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(001) [dLdOdAD12]. (100) [MFK+12]. ($1 \leq n \leq 6$) [UDVD10]. ($2 \leq n \leq 8$) [BLRdA+10]. ($3 + 2$) [WLS+19]. ($3 + 3$) [LFTL18]. ($A = N, B$) [ASW13]. ($k + l + m = 4$) [KYLC19]. ($m + n = 3$) [UKF+11]. ($m = 5, n = 2$) [MHHPR+17]. ($m = 6, n = 3$) [MHHPR+17]. ($n = 1, 2$) [Men10]. ($n = 1, 2, 3$) [EML+11]. ($n = 1--4$) [LL11]. ($n = 1--7$) [CAZ+11]. ($n = 2, 3$) [DTEMK11]. ($n = 2--10$) [WJL+11]. ($n = 2--34$) [QSLY10]. ($N = 28$) [GD11]. (r, s) [Bib13]. ($\varphi - \psi$) [MAW+18]. + [Buc12a, CdAFS+12, DMAB12, FRNM12, GKT+12, KT12b, LWWZ13, MEEA+13, MPRCEG12, MOH+12, RSN12, SÁBA+12, SD12, WZHZ13, XZL+12, YGL+11, YZ10, ZH12]. 1 [BEM12, DFK16, JW19, PSKV19]. 1/3 [KLZQ15]. 13 [LXD13]. 14 [YD17]. 16 [GAPK+19a]. 18 [YD17, GAPK+19b]. $1^3A''$ [GWZ+14a]. 2 [ABTW14, CPL15, HMA+19, HGB08, IK14, LLZaH14, LD17, NF11, PSKV19, SPD+18, SSdS17, YSW11]. $2(N + 1)^2$ [MC18a]. $2n$ [BBYZ18].

$2n + 2\pi$ [MB13]. $2n = 68, 70, 78,$ [WLZ+12a]. $2p\pi$ [VLFG12]. 3 [ABTW14, BMX+19, GWJ12, KSO19, LQZZ12, LD17, RLW+13, SM14c, VVY18]. 30 [GGD12, SLZ+12]. $3d$ [ALA15, DD17, RZC13]. $3d\sigma$ [VLFG12]. 4 [ABTW14, CD12, GAPK+19b, GB13, GWJ12, HCL13, LKN13, SM14c, WLS+19]. $4d\sigma$ [VLFG12]. $4f\pi$ [VLFG12]. $4f\sigma$ [VLFG12]. 5 [ABTW14, BGMD15, BJdlMAV12, CDSK12, HDQ+13, MPE15, SM14d, SM16]. $5g\sigma$ [VLFG12]. $5 \leq n \leq 7$ [LCZ15]. 6 [CWSZ13, HDQ+13, LdMCdA+12, MPE15, MJ14, MMV+19, Pli18, PAKA15, SS18a, VBO+15]. $6; y = 1, 2$ [BCGC12]. $6i\sigma$ [VLFG12]. $6j$ [RBD+10]. 7 [CHV14, GGJD13, SR13, WCS+13]. $7i\pi$ [KMF+11]. $7j\sigma$ [KMF+11]. 8 [YC13]. 80 [WLZ+12a]. $8jp$ [KMF+11]. $8j\sigma$ [KMF+11]. $8k\sigma$ [KMF+11]. $8 \leq n \leq 14$ [NW12]. 9 [Ali14, SBB16]. $<$ [BTH18]. $=$ [BPG+10, BL10, BDR12, ČFČ11, DIOG12, DPDR11, ESS13, FTB11, GB13, JL12a, KyH13a, LZZ+11, LMZ+11, LLG+12, MLW10, MPRB+10, dMOB12, Qu13, SZZZ11, SYQ+10, SZL+14, TFB11, WCY+10, WSL+11, XZZ+10, XWC11a, XWCY11, YK11, YIY+13, YL11, ZQJW13]. $>$ [BTH18]. $[2 + 2]$ [MBS+18]. $[2 + 4]$ [LLF17]. $[2, 7]$ [WWL+11]. $[2n, 2]$ [LSW19]. $[3 + 2]$ [ZRGE+19]. $[3 + 3]$ [ZQW+17]. $[4 + 2]$ [HZZ+19]. $[4 + 3]$ [XZG+18]. $^{+}$ [ADB10, AGRI+12, BD12, BCK19, BHV+11, Ber13a, BG11c, DWJZ11, DZ11a, DCHC11, FBM+10, GWHH17, GFB12b, GR10, HMI+15, HHCA10, HDC+11, JMPP19, KH12, KMF+11, KHH10, LCL+10a, LP10b, LGP+11, LPG+12, LLC+11, LLZZ10, LdAA+11, Ma14, MT11, MMRRA10, NKWT19, NWQX11, NZLG15, RFEGPP+16, RI19, RRCO11, SLZ+11a, SLS+11, SZZZ11, SLZH12, SSW16, SWS12, TFB11, Vik13, WLG+11, XWCY11, YLW+13, ZQJW13, ZLWL16, ZCG+17]. $^{++}$ [ZPM10]. $^{+}_{5}$ [BN12]. $^{-}$ [ADB10, BCK19, CS17, DZO11, DSZB18, FT15, KMM16, LCL+10b, LIK15, Ma14, MPM15, McC13a, MEEA+13, MMRRA10, RWW+19, RGR12, SSAM13, TFB11, XWCY11, YGLL10]. $^{-\bullet}$ [ZLWZ16]. $^{0,\pm}$ [ZPR10]. ^{1} [DSD18, Kan11, LGW11, MKD19, OD12, RR19, SBMM11, STL12, SZY17, TSL11]. ^{1,3} [DSSM18, ARG11]. ^{13} [TKSK17]. ^{14}N [BJ12]. $^{1}\Sigma^{+}$ [LJSS12, SPO+11, SLZ+11b, SLZ+11c, YLC17]. $^{1}\Sigma^{+}_{g}$ [YLC17]. ^{2} [FRNM12, LV12, LGW11, MCV11, NCMC+18, PBR18, RRCO11, She13, SLS+12, YLC17, ZCG+17]. $^{2+}$ [ASHF13, BJ17, CRB+12, CLMY12, GR11, LWL+12, MRT11, MG12, NZLG15, OPC17, RFEGPP+16, VO12, YLW+13]. $^{2-}$ [Fuk12, SBSD18]. $^{2\cdot-}$ [LGW11]. $^{2}\Pi$ [SZS+10, SLS+11]. $^{2}\Pi_{g}$ [SSAM13]. $^{2}\Pi_{u}$ [RS12a]. $^{2}\Sigma^{+}$ [SLZ+11a]. $^{2}\Sigma^{+}_{g}$ [ZCG+17]. $^{2}\Sigma^{+}_{u}$ [RS12a]. $^{2}\Sigma^{+}_{u}(2p\sigma_{u})$ [GWHH17]. ^{3} [ACMRN10, CdAFS+12, DVDBM11, DSSM19, GWZ+14a, HHL+12b, MCK17, OD12, ZCG+17, ZPB12]. $^{3+}$ [CRB+12, DSZB18, SS13]. $^{3-}$ [Bou12b, WZC+12]. $^{3}\Delta_{u}$ [SXS+12]. $^{3}\Pi_{g}$ [SXS+12]. $^{3}\Sigma^{-}$ [SSAM13, ZCG+17]. $^{3}\Sigma^{+}_{u}$ [SXS+12]. ^{4} [Kin13, RCGLV+14, SLS+12]. $^{4+}$ [NCMC+18, ZCG10]. $^{4}\Sigma$ [LDADB+15]. $^{6+}$ [DI18, ZCG10]. $^{\bullet+}$ [WSML16]. $^{\cdot}$ [CAAI12, PGG12]. ^{e} [DSSM18, DSSM19, SBMM11]. ^{II} [DS11, MC17]. ^{IV} [MLY+16, ZSHL16, ZLY+14]. $^{n-}$ [MLY+16, ZLY+14]. $^{\prime}$ [KMK+16, LZFZ13, Qu13, UJSJ13, Con10, GWM11, JWG+12, LV12, RS11b, SC12a, SKM11, YLW+13]. $^{\prime}3\Sigma^{-}_{u}$ [SXS+12]. $^{\prime}_{3}$ [GWM11]. $^{\prime\prime}$

[Dau16, LZFZ13, MCV11]. ^{q} [BLdV19]. ^{R} [Pan16]. ^{V} [ZLY^{+}14]. ^{VI}
[MLY^{+}16, ZLY^{+}14]. ^{VII} [ZLY^{+}14]. $_{0}$ [BMX^{+}19, CMCN11]. $_{0.5}$ [MGP16]. $_{1}$
[BMX^{+}19, MKD19, RDM^{+}11, SY10, VF13a, YXM^{+}18]. $_{1-x}$ [KA13]. $_{1-x/3}$
[Oni12]. $_{1.5}$ [MGP16]. $_{10}$ [LZW^{+}15]. $^{2+}_{10}$ [MCK17]. $_{11}$ [CS18, MLY^{+}16]. $_{12}$
[GAPK^{+}19b, GKGM18, HWL16, KGK13, MJ16a, MPD^{+}10, VPFD10, XCY15].
$_{120}$ [CTDOLA10]. $_{13}$ [MMBK12, SFA19, TW10, VDG13]. $_{144}$ [BDF^{+}16]. $_{15}$
[HLMO11]. $_{16}$ [CS18, TFB11]. $_{1}8$
[BDF^{+}18, yBZfC18, GKGM18, JL12a, MLY^{+}16, SCTW10]. $_{19}$ [GKGM18].
$_{1\sim2}$ [XZZ^{+}10]. $_{2}$
[AO12a, ATS15, ALA15, BDFM10, BPG^{+}10, BAP12, BDF^{+}18, BAMA12,
BL11, BGFD14, BAA^{+}18, BBYZ18, BZZ15, yBZfC18, BXZ^{+}19, BG11b, BB10,
BLKB11, BAB^{+}18, BJ17, Buc12a, BSPK11, CP10, CRSB12, CTW12, CCS13,
CS17, CC11b, Cor16, CWSZ13, CS18, DMAB12, DLCB15, DVDBM11,
DTVP^{+}12, DCDD10, Den13, DPDR11, DMG10, DZO11, DLM12, DQZF12,
ESS13, EFO11, EO11, EMSB15, Esr18, FLCHL10, FBRBR12, FTB11, Fuk12,
GP13a, GWM11, dDGNB10, GC18, GKT^{+}12, GR10, GD11, HV11, HDC^{+}11,
HSYM11, HHL12a, HHL14, HYH^{+}10, HCL13, HHL^{+}12b, JL12a, JL12b,
JLZ^{+}17, JWG^{+}12, JLG^{+}12, KWC10, Kal18, KAR12a, Kan11, KMF^{+}11,
KI12, KLK13, KK14b, KSSK16, Kim19, KSST12, KLZQ15, KDOR17, KF17,
KN15, KRG^{+}13, LZ12, Les12, LV12, LLG^{+}12, LCT14, LC16, LLL16,
LZW^{+}18, LFP^{+}19, LCZ15, LLW^{+}12, LCS^{+}11a, LXLL11, LLLB13, LEU^{+}11].
$_{2}$ [MLY^{+}16, MLW10, MFK^{+}12, MTR^{+}19, MMP^{+}18b, MMC^{+}19, MC12,
MFZ^{+}18, MBA^{+}13, MPD^{+}10, MKD19, MKM11, Mit11a, MZLM17,
MPRCEG12, MPGGS19, MPTZ13, MCV11, MKW11, MGP16, MOH^{+}12,
NW12, NTNL10, NL11, NMIP14, NH11, OCL^{+}18, Oni12, OGvSG18, PTS^{+}11,
Pan16, PWL^{+}10, PC16, PCK19, Per10b, PK13b, PRPU^{+}13, PL18b, Puz10,
QSLY10, Qu13, QCB^{+}10, RS12a, RS12b, RSL10, RFEGPP^{+}16, RWW^{+}19,
RNB^{+}10, RGR12, RRB12, RBTL19, ŞBAT16, SK14, SD16a, SCLCPB12, SR19,
SÁBA^{+}12, SVPTM^{+}10, Sat11b, SMEH15, SSAM13, SXS^{+}12, SR18, SPIL14,
SZZZ11, STL12, SLZH12, Sri18, Sri19, STU19, SYQ^{+}10, SCTW10, SW12,
SZ15, TOSN12, TSKN12, Tan13, TFSRM11, TNN16, TD11, TMC18, TSL11,
Tob19, VV18, VPFD10, VPA11, Vik11a, Vik11b, VLK^{+}11, WSCL11, WLL11,
WLG^{+}11, WZM^{+}13, WZHZ13, WZC^{+}12, WLWL14, WWGW18, WRW^{+}18].
$_{2}$ [XMZ^{+}12, XZL^{+}12, XDM^{+}10, XWCY11, XF19, YY18a, YIY^{+}13, YSK^{+}12,
YLWrL12, YGLL10, YLZ^{+}17, YC13, YLC17, YLYC18, ZZ15, ZPR10, Zha10,
ZK12, ZH12, ZQJW13, ZLWY13, ZGSM15, ZWL18, ZHL^{+}19, ZFS^{+}11,
ZLWZ16, ZLY^{+}14, ZDZL11, dHLdS12, dOR10]. $_{20}$
[yBZfC18, CWL^{+}13, GB13, WSL^{+}11]. $_{24}$
[CJMC19, HLB19, JB18, MMBK12, MC18a, MC18b, YL11]. $_{2}5$ [BDF^{+}18]. $_{28}$
[MC18a, YLH^{+}19]. $^{4-}_{28}$ [MC18a]. $^{+}_{2}$
[AC12, Ber13c, Che12, OPC17, RS12b, RAN18, SSP14, VLFG12]. $^{+\cdot}_{2}$
[FBRBR12]. $^{-}_{2}$ [SSAM13]. $^{-/2-}_{2}$ [YGLL10]. $^{2+}_{2}$ [FBRBR12]. $_{2A}$ [CSSK^{+}12].
$_{2C}$ [CSVCB12, CSSK^{+}12]. $_{2n}$ [WLZ^{+}12a, BBYZ18, EML^{+}11]. $_{2/12}$ [Kim19]. $_{3}$

[XCL+18, lAyL14, ACMRN10, AM18, BCP10, BGFD14, BAA+18, BZZ15, BXZ+19, Bou12b, CCL+13, CdAFS+12, CRSB12, CWS15, CDL+19, CS18, DS11, DS12, DPDR11, DZ11a, DQZF12, DSFT17, EMSB15, EMS16, EAV16, FRNM12, GWM11, GMT18, GZMC11, GMP+11, JCCZ12, JLG+12, KWC10, Kal18, KAR12a, KG17, KCK14, KLZQ15, Lan10, Les12, LJL+11, LZZ+11, lLBqD+19, LFP+19, LGW11, LL19, LXLL11, LdAA+11, MWH15, MFK+12, Men10, MFZ+18, MPD+10, MEEA+13, MPRCEG12, MPGGS19, Mor11, NBL12, NH11, dMOB12, Oni10, Oni12, OH12, OH13, OCGM+19, PC16, Per10b, PP14, RLTAT19, RSN12, RB11b, SMC18, SK14, SKS11, SD12, Sik18, SSP14, SZZ+12, STL12, SM17, SYQ+10, TSL11, TL15, UV18a, UV18b, VV18, VPFD10, VVY18, VLK+11, WCY+10, WLZ+12a, WLZ+12b, WZM+13, WZHZ13, WCL+17, WTP+19, WZC+12, XZL+12, XZZ+10, XWC11a, XWCY11, XCL+18]. $_{3}$ [XF19, YLWrL12, ZHL+19, ZJC+13, dHLdS12, dOR10, dOdCMUdALR11]. $_{3--5}$ [CS17]. $_{3-n}$ [SKS10]. $_{30}$ [FBO+11]. $_{36}$ [LBY+14, MS17]. $_{38}$ [MC18b, YLH+19]. $\overset{+}{}_{3}$ [MSAB19, RR11]. $\overset{-}{}_{3}$ [Sat11b]. $\overset{2-}{}_{3}$ [GPM+15, WZC+12]. $_{4}$ [BDFM10, BDF+18, BAA+18, BAB+18, CJMC19, CCL+10, DWX+16, DLM12, ESS13, FBRBR12, HLMO11, HSN+11, HHL+12b, JCCZ12, KI12, Kim13, KLK13, KSSK16, KMM16, LGHL11, LL18, LFP+19, LXD13, LW18, LKLW11, MBKH19, MPD+15, MLW10, MOE+11, MBA+13, MPRB+10, MC18a, NMIP14, OCL+18, OPP+14, PAKA15, PL18b, RPBB11, RRRV19, RFEGPP+16, RTT10, ŞBAT16, SYK+12, Sat11b, TZD+19, TGA+11, VF13a, VDG13, WWGW18, XWC11a, XWCY11, XXJ+16, XF19, YYI+13, YIY+13, YSK+12, YLWrL12, ZLY+14, dHLdS12]. $_{40}$ [LZW+15, YLH+19]. $\overset{+}{}_{4}$ [WWGW18]. $\overset{-}{}_{4}$ [Sat11a, YGLL10]. $\overset{2+}{}_{4}$ [MCK17]. $\overset{2-}{}_{4}$ [Sat11a]. $_{4/3}$ [OA12]. $_{5}$ [BDF+18, Bou12b, BDR12, CRSB12, DCDD10, Den13, DZO12b, DQZF12, GWM11, HSYM11, KMM16, LCL+10a, LFP+19, MLY+16, MBA+13, Mor11, NBL12, NTNL10, NL11, PTS+11, PP14, SYK+12, WCY+10, WCS+13, WLWL14, XZZ+10, YYI+13, YSK+12]. $_{540}$ [CCEGK12]. $_{58}$ [SCTW10]. $\overset{-}{}_{5}$ [KMM16, LFP+19]. $_{6}$ [BD14, BDF+18, BGFD14, BLdV19, BLKB11, CS18, DWPK14, ESDO16, GWM11, Kal18, KI12, KLZQ15, LCL+10a, LGHL11, Mor11, MCK17, NBL12, NH11, PP14, RLTAT19, RRRV19, Sri19, TCSD12, TZD+19, TG13, WZW17, dHLdS12]. $_{6(10-n)}$ [PAKA15]. $_{6-\delta}$ [MGP16]. $_{6-x}$ [GLF+12]. $_{60}$ [BDF+16, BCP10, DFK16, FBO+11, IMS+13, KN15, MSS11, MIN13, Nik11, PAKA15, RR11, TKSK17, XCY15, YK11, ZLWL16]. $\overset{+}{}_{6}$ [BD14]. $\overset{-}{}_{6}$ [BD14]. $\overset{2-}{}_{6}$ [KMM16]. $\overset{3-}{}_{6}$ [GGJD13]. $_{7}$ [DSFT17, LdAA+11, Sik18]. $_{72}$ [GZW16]. $_{74}$ [USL+13]. $_{76}$ [JLL+18]. $_{78}$ [ZW15]. $\overset{+}{}_{7}$ [LdAA+11]. $\overset{-}{}_{7}$ [GGJD13]. $_{8}$ [Nes11]. $_{80}$ [WLZ+12b]. $_{82}$ [SUL+11]. $_{84}$ [KK12a]. $_{86}$ [KK11b]. $_{88}$ [YLZ+17]. $\overset{+}{}_{8}$ [WWGW18]. $\overset{-}{}_{8}$ [KBF+13]. $_{8/12}$ [Kim19]. $_{9}$ [MLY+16]. $\overset{3+}{}_{9}$ [BSPK11]. $_{A}$ [TOSN12, TSKN12, BMK+14, CPL15, COCF+14, ÇT14, DQZF12, GCDNGS12, KSS12, LZ12, RZG12]. $_{\alpha}$ [FNBK17]. $_{b}$ [KSS12, LZ12, SB18, SSB19]. $_{\beta}$ [FNBK17]. $_{d}$ [YGLL10]. $_{FH}$ [CDT12]. $_{g}$ [FRNM12]. $_{H}$ [Zha14, CJMC19]. **0–14** [XF19]. $_{im}$ [WB17]. $_{\infty h}$ [YGLL10]. $_{k}$ [KYLC19]. $_{l}$ [KYLC19, PAPCMM+16]. $_{m}$ [CTW12, CD12, GWJ12, KYLC19,

LKN13, MHHPR$^+$17, PAPCMM$^+$16, UKF$^+$11]. $_N$
[DVDBM11, EHKD11, EKD12, GGD12, GD11, LJK$^+$18, MEEA$^+$13, RWW$^+$19, SM16, Ali14, BPG$^+$10, BGMD15, BEM11, BLRdA$^+$10, BJdlMAV12, CDSK12, CAZ$^+$11, CTW12, CWSZ13, CD12, DTEMK11, EML$^+$11, FTB11, GR11, GAPK$^+$19b, GGJD13, GP13b, GB13, GWJ12, HDQ$^+$13, KSSK16, Kuz19, LRKM10, LKN13, LGHL11, LWL19, LCZ15, LHL$^+$15, MCP10, Men10, MJ14, MMV$^+$19, MHHPR$^+$17, MMRRA10, NW12, PAKA15, PAPCMM$^+$16, QSLY10, RGR12, SKS10, SJZ$^+$18, SR13, SBB16, SLZ$^+$12, SM14b, SM14c, SM14d, UKF$^+$11, UDVD10, WJL$^+$11, WCS$^+$13, WJL$^+$10, XYL$^+$18, YC13, ZRR$^+$11, ZCTG18, ZCP11]. $_{n-1}$ [MCP10]. $_{n-2}$ [LCZ15]. $_n^{(n-4)-}$ [KMM16]. $_N^+$ [GGD12]. $_N^-$ [RWW$^+$19]. $_n^{-/0}$ [LL11]. $_n^{0/-/2-}$ [DHYC19]. $_n^{2+}$ [LL18]. $_n^{q-}$ [SM14c]. $_x$
[BCGC12, GLF$^+$12, HCL13, KA13, Oni12, RLW$^+$13]. $_y$ [BCGC12]. A [ASW13]. α [BWB$^+$18, HZZ$^+$19, KSAK17, MFZ$^+$18, OPAVM18, LZZ12, PEA$^+$12, QTCL10, SVRGV12]. α_2 [EPS$^+$16]. β
[AC19, GCZ$^+$14, Jeo18, JSLH14, KZZ13b, LSG$^+$14, OPAVM18, WHS$^+$13, NMHPVG12, NRP$^+$11, PEA$^+$12, SJW13, TPdMB12]. β_2 [CSVCB12]. $\cdot$ [BLWJ17, BTH18, XF19, Men10, TBHL11, XLGA12]. $\cdots$ [TG13, JLG$^+$12]. $\cdots$ [MZLM17, SPIL14, WZW17, YZZ16]. χ_1 [DSCO$^+$13]. D
[IIH16, PGMGRM15, CWW$^+$16, MVG18, MW16, OVT$^+$16]. d^{10} [DLJT14]. Δ [CC11b, Yam10]. Δ_{rxn} [DE18]. ℓ [ZHF12]. ϵ [VLM$^+$10]. η^2 [MSBF18]. η^5 [DZO12b]. f [MW16]. G [ATPRV11, DKS11, VATPR11, VAT12, SPO$^+$11]. γ [BWB$^+$18, CC11b, MFK$^+$12, PEA$^+$12]. h [PUGSFM18]. J [AAHN16]. $j = 0$ [LZFZ13]. $k(T)$ [CP11]. K_+ [GBK18]. K_+^2 [GBK18]. l [WC14]. $l + m + n = 6$ [PAPCMM$^+$16]. $l, m, n > 0$ [PAPCMM$^+$16]. λ [AM13a]. λ^5 [TM19]. $LDA + U$ [HFdGC14]. $\leftarrow$ [SB18]. M [XYL$^+$18, KC11]. $m, n = 1$ [LKN13]. $m = 1$ [CD12, GWJ12]. $m = 1{-}{-}2$ [FTB11]. m^* [Dw13]. M^{VI} [HNBS18]. μ [ESS13]. N
[CZJZ12, CPL15, DDÇY12, DPRK12, DDF$^+$12, ES17, GW18, KC11, KSAK17, MOSK10, MAN15, NJA$^+$12, Pan16, RWW$^+$19, SFW12, CMCN11, CSK12, DFK16, DHYC19, GE12b, KSSK16, KMM16, LWL19, ZYZ$^+$11]. $n + m \leq 5$ [CD12]. N, N [dAVdM17]. $n =$ [LHL$^+$15, SM14b]. $n = 0$ [GAPK$^+$19b]. $n = 0, 1, 2$ [SKS10]. $N = 1$
[SM16, CWSZ13, GGJD13, GB13, HDQ$^+$13, SR13, SM14d, WCS$^+$13, YC13, BGMD15, PAKA15, SBB16, SM14c, BJdlMAV12, CD12, GWJ12]. $n = 1, 2$ [BPG$^+$10]. $n = 1, 4{-}{-}7$ [FTB11]. $n = 2$
[Ali14, HDQ$^+$13, MJ14, MMV$^+$19, CDSK12, GGD12]. $n = 2, 3, 4$ [GP13b]. $n = 20$ [SLZ$^+$12]. N' [CZJZ12, DDÇY12, Tav11]. $n \geq 2$ [SM14c]. o [KSAK17, SR18]. p [AGJ12, AMAC12, CSK12, DLJT14, HLZ$^+$14, RRK16, SR18, SRA$^+$11, ZSASS13, ZYZ$^+$11]. π
[BWE16, CCS13, DWZZ15, HIL19, KPL$^+$17, LDKB15, LW18, LB18, MC17, MANP17, NCMC$^+$18, NIK19, NMV$^+$14, OCGM$^+$19, PC16, PNC19, SSB19, SPD$^+$18, SSS15, Szc18, TK16b, YZZ16, YD17, ZHL$^+$19, CC11b, SLS$^+$12,

TZD+19, XSLF12]. **anisol** [AMAC12]. **Anisotropic** [BMTT11, LDZG16]. **anisotropy** [Ali14, MOY13]. **annealing** [MOE+11, TCG17]. **annealing-based** [TCG17]. **annelated** [PPK+13]. **annulation** [HZZ+19, XZG+18, ZQW+17]. **anode** [UDS19b]. **anomaly** [Kar12c]. **ansatzes** [Fin17]. **Answers** [Tas14]. **anthranilic** [MC11a]. **anthropogenic** [Mor11]. **anti** [CCC19, Iku17, MPE11, ScBsR+10, Zag11]. **anti-Bragg** [Zag11]. **anti-Bredt** [Iku17]. **anti-inflammatory** [MPE11, ScBsR+10]. **antiaromatic** [RBZ15]. **antibiotics** [LSR10b]. **antibonding** [CCL+16, CFV18]. **anticancer** [CZJZ12, DSD18, MKHM11, PPK+13, XZ11]. **Antidot** [YMY+13]. **antiferromagnetism** [Fuk12]. **antiinflammatory** [YINM13]. **antimalarial** [AB16b, LTdSJ+10, RDM+11]. **antimicrobial** [ESBVJY12]. **Antioxidant** [XLZ+19, KDA+11, KK11d, ZYL+13]. **antioxidative** [TIKN11]. **antiparallel** [SJW13]. **antisense** [UJSJ13]. **antisymmetric** [TKN13]. **antitrypanocidal** [MLC+11]. **antitrypanosomal** [LWH+12]. **antitubercular** [SD13a]. **antitumors** [CCL+10]. **antiviral** [MB14]. **any** [FMPM+14, RMC19]. **AP** [NYS+10]. **AP-UBD** [NYS+10]. **AP-UCC** [NYS+10]. **apoptosis** [QZH13]. **applicability** [BJ17, FCS13a, FCS13b, WKE17, ZT13]. **Application** [ASK15, DSL15, ENV15, JH15, NMSR14, OVT+16, PBR18, RZG12, Rom10, SCBP17, TGRP19, TLC+17, TPCJ+12, AVG19b, Cha11, GfWlZ11, HW12, KLK13, LLLT12, LVP12b, MPD+15, MT10, dMOB12, SKV12, XWC10, AEM+12, DLRMFY10, HBMM11, IKS08, IKS10, KPH+12, Luz11b, LKd+16, MPRCEG12, MJ11, PCR+11, RC11, SR12, SS12]. **Applications** [CW11, HFBC19, Lar11, MSNP18, Ném14, SDP+16, AMAM18, AMMC19, CJBMMAPR19, CC12, GMM+18, HKZZ15, HIL19, Hil13, Kap12, LGL+19, LMZY15, MANP17, MPMCM+11, MML+16, MG12, MML11b, Nic11, RMC19, SSS15, TSvL+16, TSS+15, YKM+15, YFY17, ZSZ14, CW13b, ZDZO10, Mor13]. **applied** [BVRM10, CF11, CL08, FCC11, HM11, NS13, PIS18, SMV11, SXH18, SS19b, WR14a]. **Approach** [LFF+10, AV19, ATL+14, AK17, AB18, AOLB12, ART08, AT18, ALB18, BPVDB11, BLB+18, BvWG14, BVP14, BLKB11, BAB+18, CGG18, DVDBM11, DLM12, DMBL16, DLP17, Exn11, FAFR12, Fri12, FUE+12, GBK18, GFPAV19, GR10, GRD11, HR19, JLL11, KP10, KC18, Kit17, KYLC19, KSO19, LBW11, LSR10b, LSR+13, LdAA+11, Mak15, MGK+11, MNP19, MGN14, MSVMCI10, MBBT+12, Mor12, NSN17, NNSN17, NTGC19, NVPCJ+13, OT14, OPC17, OGvSG18, PT13, Pir13, PBR18, RZ17, RBGGM18, RMC19, RNC+14, RC11, RdPW+12, SCLCPB12, SÁBA+12, SB10a, SC12b, SPSA11, SSB12a, SD13b, SC10a, SSA18, Sri19, SKL10, Tou11a, TPCJ+12, UYN+13, WZ10a, WWB+14, WR14a, XNL+14, Yam11, YK13, dSdS13b]. **approaches** [AV19, AMMK11, BBA+16, Cap16, CKL16, DC14b, EML+11, IAK13, ILBS10, Jia15, LMZY15, MDC15, Men15, NYS+10, PBB15, PJP08, Sko16, TKSK17]. **appropriate** [FSB16]. **approximants** [DB13a]. **Approximate** [FKBG19, HYZS12, HYZS19, ZLJ11, AST16, HMH10b, KYH+13b, Tou11a, ZRLV10]. **approximately** [KSN+10]. **Approximating** [Fin16b]. **approximation**

MFLK11, MAPS18, MNS11, MR18b, Pea11, PSC15, Pup11a, PJ19, RZ17, RZSZ18, RAFR18a, RAFR18b, Roy15, Roy16, RRCO11, RR19, SRPD16, SK17a, SKM11, SL13, SS12, TBB+19, TW10, WWHZ13, Zak13, ZS12].
atom-bond [AD17]. **atom-centered** [KFS13, Zak13]. **atom-pairwise** [KKL+16, PSC15]. **Atomic** [AST19, Ols11b, PNC19, SV11, ABS11, ALRA10, ALRAE11, CRA+11, CF11, CB10, Fin14a, Fin15, Fuk12, Gra08, Gra11, GE12b, HST13, IFT14, Lai11, LRMAA19, MGK+12, Mam14, MC11b, May14, MS17, NDH10, Nic11, NE11, PUH+11, RLER13a, RAGM10, Rom10, SLG11, SMV11, Sch15, SD13c, STM17, TMC+13, ZY13, ZLWY13, ZZZ+18, vLRRK15]. **atomic-wire** [SD13c]. **Atomistic** [AGG+18, Mai14, BMR+13, CLKD15, MMP+18a, vL13, Zha17].
atomization [Vyb08]. **Atoms** [LSC+18, OA13, TBRIS12, AMK10, AM10, BHMN19, BAX+19, BSO11, Dil13, DSSM18, EMSB15, GBS17, GLT13, GZSMFN16, GI10, GI11b, GI11c, GI11e, GS11, Gra11, HMP+11, HMA+18, IG11, JEA13, JMX+15, Joh17, Leh19c, LKJ13, LZW+15, LHX+19, LLH15, Luz11b, MOY13, MFLK10, MJ11, NS10b, NIT16, ONBP11, OD12, PRPU+13, PWP13, PNC19, RLW+13, RD14, RBVAG18, SBMM11, SBM16, SR19, Sha18, Sto18, SKL10, TBRIS10, TBRIS11, TH12, TXK+19, TFMC19, TLC+17, UGWL18, UDS19a, WLS+19, YJ17, ZS11, ZCG+16, ZHI17, ZZZ+18, ZJS13, dSTH17, dCGAMV12, Leh19a].
Atoms-in-molecules [OA13]. **ATP** [BGJSM+18]. **attached** [HMP+11].
attachment [DSVP15, Kry12b]. **attack** [LZFZ13]. **attending** [GWME18].
attenuated [NDP10]. **attenuating** [CF14]. **Attosecond** [Vik11a, SVPTM+10]. **attraction** [MSRn+11, SYQ+10]. **attractive** [DCD11, WH18]. **Au/SAPO** [GSB10]. **Au/SAPO-11** [GSB10]. **AuCl** [SM14b]. **augment** [BDG17]. **augmented** [CLKD15, D'y16, KRC+16, SZS+10, SLZ+11c, SLZ+11a]. **AuO** [SM14c].
aureusidin [KK11d]. **aurones** [XLZ+19]. **AuSi** [BCK19]. **Autler** [HYH+10]. **autocatalysis** [Pie12]. **Autocatalytic** [dM13]. **autocorrelation** [MPV+11]. **AutoDock** [CRFR11]. **autoignition** [MOH+12].
autoionization [DE18]. **autoionizing** [Cor16]. **automated** [KMNSP19, MHO+15, NKWT19, PBB15]. **Automatic** [MML+16, CW11].
AuX [LC16]. **auxiliary** [CEFMK12, GS10, KFJ+18].
auxiliary-density-matrix [KFJ+18]. **averaged** [ABLT11, CP13, RS12b, RSN12]. **avian** [KRH13, PCML08, WZ10a, ZBK15].
axial [LGS+16]. **axiomatic** [AK17]. **axis** [Lad14, XTLA13, XTLA14]. **aza** [DC14a, VGGPdL19, WWL+11, WLWT12]. **aza-Möbius** [WWL+11].
aza-oxypentadienyl [VGGPdL19]. **azanaphthoquinone** [PPK+13].
azauracil [MPE15]. **azide** [Per10b]. **azides** [AEKGZ12]. **azidoethanamines** [SM10b]. **aziridination** [MCC13b]. **azo** [MNP19]. **azo-bridged** [MNP19].
azobenzenes [JPP+11]. **Azobis** [PP19b]. **azochromophores** [FSB16].
azocompound [NVPCJ+13]. **azodicarboxylate** [KI15]. **azoles** [SK12a].
azomethine [DI10, LFTL18, XZG+18, ZQW+17]. **azoniaallene** [WLWT12].

MSNP18, MG12, NDM+12, PCD14, PBR18, RZSZ18, RLER14, RVO+14, RLZ12, SKTI15, SXH18, SZS+10, SLZ+11c, SLZ+11a, SLS+11, TCG17, TWR15, UGWL18, UV18b, VSS11, VRO+12, WSV10, YM14, Zak13, ZF15]. **bath** [YK13]. **batteries** [Ali19a, AVG19a, KLK13, Kim18, UDS19b]. **battery** [KJ15, Oni12]. **BAu** [LL11]. **Baylis** [ZQW+17]. **BaZrO** [GMP+11]. **BB** [YGLL10]. **bc** [RDM+11, RRB12]. **BCl** [MPM15, SLZ+11b]. **Be** [BLL+13, GCD13, NW12, RFEGPP+16, WCY+10, XZZ+10, YLW+13, Kuz19, Lu15, Met11, Nes11, Sza13, AM18, DTEMK11, DZO12b, GPM+15, Mit11a, RSN12, dOR10]. **beam** [AGG+18]. **Bean** [BMB12]. **bearing** [CMR13, CJMC19, MCK17]. **BEC** [GdLT12]. **beginnings** [QBRA18]. **Behavior** [GST11, DSC+11, DLM+11, LG12, MC18a, PNC19, RF10, RGS+13, SHE10, SM14c, SMGZ13, YLH+19]. **behaviors** [HKLW13, VSL+15]. **BeN** [UDS19a]. **Benchmark** [AV19, JZZH17, OH19, PB10, HM12, LP10b, OKR12, RS12a, RS12b, RSN12, Vie17, WZW17, YWH12a, YWH12b]. **benchmark-quality** [OKR12]. **Benchmarking** [CKB18, KDOR17, MXC18, Man16, MBSAG16a, PRFR17, MBSAG16b, Rus14, VBJK18]. **benchmarks** [Lat13, LJ13]. **bending** [GFB12a, IMS+13, ZZ15]. **bent** [HV11]. **Benveniste** [WSV10]. **benzal** [YWJ+11]. **benzal-5-pyrazolone** [YWJ+11]. **benzaldehyde** [ZSHL14]. **benzamide** [DPRK12]. **Benzene** [CGM12, CL11, CCS13, DKZ+10, DJ18, FZH+18, HAX+18, HhGqZZ17, JW19, KBMM10, SPSA11, Sch12a, SGL19, TG13, VC13, WDSL14, Yu13, ZS12]. **benzenes** [JW19]. **benzenoid** [ACT19, HIL19]. **benzenoids** [BR08, BR12a, RB08, RB11a, RVNP12]. **benzimidazole** [WLL+13]. **benzimidazoles** [LZB10, XFW+14]. **benzimidazolyl** [SHW+13]. **benzo** [ÖEDB11, ZLS+18]. **benzoazacrown** [FBU+11]. **benzoazacrown-containing** [FBU+11]. **benzocatafusenes** [MA12]. **benzochalcogenadiazole** [BSSS19]. **benzodiazepin** [HMA+19]. **benzofuran** [ASMP15]. **benzoic** [PMEP19, SN12, SHL+13]. **benzoin** [ZSHL14]. **benzonitrile** [ZRGE+19]. **Benzothiadiazoles** [Net12]. **benzoxazole** [YLW+13]. **benzoyl** [LD17]. **benzyl** [EHKD11, EKD12, SJZL12]. **benzylidene** [DDÇY12]. **BeO** [Ali14]. **BEPOX** [KZZ13b]. **Berry** [DMAB12]. **Beryllium** [NW12, AM18, DZO12b, Nic11]. **BeS** [DAR+11]. **Best** [Ish14, CB10]. **beta** [MBTVR12, PTD+12]. **better** [BLL+13]. **between** [ASHF13, AD17, ALMY18, BLR12, BHA19, BL11, BLWJ17, BWB+18, BTH18, BWE16, BB16, CZJZ12, CCL+13, CCC19, Cha10, CCS13, CDL+19, CF17, DNCKCS+12, EKN10, EHKD11, EKD12, EEMSS14, EAV16, Fin16a, Fin17, GXZ+14, Gra08, Gra11, GE12a, HCH+18, Han19, HMH+13, HIL19, JEA13, JLS13, Kan11, KdPNNS16, KMMS17, Kim16, LKOS17, LdMCdA+12, LMZ+11, LLG+12, LFTL18, LFP+19, LBdV16, LWC+10, LZD+11, LCS+11a, LCH+11, LCS+11b, LXLL11, MYZ+10, MFK+12, MSY+12, NBL12, NZ13, NAK+17, NBI+10, NL11, NRGS11, OKK10, PDNC14, PM12, RYM12, RFN+12, RMJ11, RNB+10, RS13, SSI+10, SD16b, SKHN13, Sch15, SM17,

SBD+16, SCZH16, SC18, Tav12, TDOD17, TYL10, TXL10, TL15, UV18b, WWC17, WLL11, WLWT12, WWD+15, WHM14, WWX+11, XZYS10, XCL+18, YM12, Yak11, YWY+12, ZLWZ16, ZMB+17, dCSDdMC13, dSdSPG11, dCDC+11, dLRR11]. **Beyond** [Chu12, DCD11, Dob14, EAA17, ZWE12, CTVA12, MA10, RB18, SK17a, Var14, VVN+16]. **BGlu1** [WHS+13]. **BH** [Kim13, XZZ+10, SLZ+11a]. **bi** [MMR+10, MHHPR+17]. **bi-cations** [MMR+10]. **biaryl** [TPdMB12]. **Bias** [BVRM10, CCC19]. **Bias-exchange** [BVRM10]. **BiBO** [MLK17]. **bicyclam** [SK11]. **bicyclic** [DZ11b, JA12, MMM19]. **bicyclo** [Sat11b, WLS+19]. **bidipyrrins** [JWG+12]. **biexciton** [LEU+11]. **BiFeO** [lLBqD+19]. **bifunctional** [XZ11]. **bifurcate** [dOdCMUdALR11]. **bifurcation** [MHO+15, YW11b]. **Big** [CF11, MSAB19]. **Biginelli** [LCZL11]. **bilayer** [KMT+12, SMK+12, SIT+12, YINM13]. **bilayers** [MP12, MCKD11]. **bilinear** [MPMCM+11]. **bimetallic** [GB18, MHHPR+17]. **Bimolecular** [LQ13, DAA16, WLWL14]. **binary** [AD17, CLL+11, GE12a, Kan18, LMC19, MS14b, RKCK19]. **Binding** [ESLM19, GB18, RWW+19, ZFW+13, ATS+11, BLB+18, BBM17, BJ17, CSSK+12, DPK18, DTF+11, DMG10, EKN10, FYhC11, GM11, GGD12, KKM+12, KB19, LCT14, LNI12, MS14a, MZB+13, MPTR12, MS14c, OT14, PSK+16, PP14, SH19, SAHA12, Shi13, ŚKB18, SW12, SJW13, VBJK18, WTH+11, WDJ+17, XZ11, dCSDdMC13]. **Binuclear** [RALK18, SS19a, WLS+19, ZLY+14]. **bio** [Swa13]. **bioactivation** [MMÅ13]. **bioactive** [MKHM11, dSSdSGA12]. **bioactivity** [MKHM11]. **Biochemistry** [AM13a, KRH13, KyH13a, KGK13, LSR+13, OM13b, PSK+13, PPK+13, SKHN13, Shi13, TYN13, XTLA13, YYI+13, YIY+13]. **biodiesel** [MCRS16]. **bioenergetics** [Blo15]. **biogenic** [MBTVR12]. **bioinformatics** [RNP13]. **bioinorganic** [BBA+16]. **biological** [Brä11a, CWL+13, CAPGAIG18, Chu12, LB14a, MG12, MMP11, XHZXXZ10]. **biologically** [ASHF13, KM12b, KSD10, VO11]. **bioluminescence** [CYLL11]. **biomimetic** [ADR+18, WRW+18, ZSHL16]. **biomolecular** [Mit11b, SKV12]. **biomolecules** [BMTT11, Dum12, IKS08, IKS10]. **biophysical** [WSV10]. **Biophysics** [AM13a, KRH13, KyH13a, KGK13, LSR+13, OM13b, PSK+13, PPK+13, SKHN13, Shi13, TYN13, XTLA13, YYI+13, YIY+13]. **biorelated** [LGZC15]. **biorthogonal** [BVP14]. **bipartition** [Du12]. **Biphenyl** [JMX+15, BMF13, RS11b]. **bipolar** [RS11b, Sil14]. **bipolaron** [PFdM13]. **bipyramid** [SALK19]. **bipyridine** [LKZ+16]. **bipyridine-ligated** [LKZ+16]. **biradical** [KMK+16, KMM+18, KSN+10, KYH+13b, ZZW11]. **bird** [WLZ18]. **birefringences** [RC11]. **Bis** [BSM+15, Jac12, LYW11, LWJL10, LZZ+17, MCC13b, Pli18, RNdA+10, SDR+13, SAHAA16, ZQCJ10, ZQXP17, dARAV12, JWG+12]. **bis-actinyl** [ZQXP17]. **bis-azopyrroles** [Jac12]. **bis-dithiolene** [SDR+13]. **bis-furylfulgimide** [LZZ+17]. **bis-heterocyclic** [LWJL10]. **Bis-imino** [BSM+15]. **bis-tert-alcohol-functionalized** [Pli18]. **bisadduct** [LYS+19]. **biscycloheptatrienyl** [ZFC+17]. **bisdiselenolene** [BB16]. **bisdisphenoid** [SALK19]. **bisdithiolene** [BB16]. **Bishop** [Ano11c, Ano11b, RC11, Sau11].

TKS11, XCL+18, YSS+10, YYI+13, YGLL10, YWH+12c, ZZL+11, ZHL+19, ZLWZ16, ZYL+14, ZJS13, dAVdM17, dLRR11, dOR10]. **Book** [Ban12, Brä12, Kry11a, Li11, Lin12, Mas11, Mor13, Mue12, SGJ10, Sch10a, Tay12]. **boosters** [HEVMSA+19]. **borane** [LCZ15, MFOH18, MC12]. **boranes** [GWM11]. **borazine** [Kal18, RLTAT19, STM18, ZHL+19]. **border** [AGOP18, CN12, GMT16]. **borides** [ČFČ11]. **Born** [BPL13, GVPCK10, RSM12, RAN18, SK17a, Sut12, VVN+16]. **borofullerenes** [YLH+19]. **boron** [ALHC18, BCGC12, Buc10, DWGX12, ES17, Esr18, FZX18, For12, GWZ+14b, GAMM10, HIL19, HNBG15, KC19a, LQ13, LC12, Mar11, MJSC18, OVT+16, PPDF11, RRCO11, TNT18, TCSD12, UDS19b, WG18, XYL+18, ZDF13, ZCG+16, YGLL10]. **boron-** [HNBG15]. **boron-arsenide** [UDS19b]. **boron-nitrogen** [KC19a]. **boron-rich** [TCSD12, WG18]. **boroxine** [Kal18]. **boroxol** [LFP+19]. **Bose** [DCD11]. **Bound** [Agb12, AY15, PGMGRM15, TD19, DSSM19, Fin16b, FDA16, FRGC10, GWHH17, KH10, LDADB+15, ONK+13, Ril10, WC14]. **Bound-states** [Agb12]. **boundaries** [WLH+19]. **Boundary** [LZ12, CW13b, MFLK11, UYN+13]. **bounded** [LLP17]. **Bounds** [MC11b, PR10a]. **Box** [GZSMFN16, NCMC+18, GZF14, Lun13a, Lun13b, Roy15, Tou13]. **boxed** [RAFR18a, RAFR18b]. **bpy** [DS11]. **Br** [DVDBM11, EMSB15, EMS16, HNBG15, JLG+12, Kuz19, LCL+10a, LMZ+11, LLG+12, RLTAT19, SB18, SZL+14, TL15, WZW17, XZL+12, JLZ+17, LWL19, OK16, TSL11]. **bracteatin** [KK11d]. **Bragg** [Zag11]. **branched** [SPD+18]. **branching** [MOY13, RSL10, TSL11]. **Brändas** [Ban12]. **Bravyi** [TSS+15]. **Brazilian** [DC10, DC12]. **Br —** [LLG+12]. **BrBr** [LGW11]. **BrCl** [JLZ+17]. **BrCN** [BMBD10]. **breaking** [AGB19, DLCB15, SSK+12, SC18, Tob19, WLZ18, YIY+13]. **Bredt** [Iku17]. **BrF** [JLZ+17, Wu11]. **BrF-HX** [Wu11]. **BrHBr** [GRLA18]. **bridge** [CLMY12, HSS18, KyH13a, Nal12, Nal13, SSK11]. **bridge-acceptor** [SSK11]. **bridged** [MNP19, ZZR+12, ZLS+18]. **bridges** [ATS+11]. **bridging** [MG10]. **Brief** [Ano11a, BC15, BC16, Mai14, YZ13]. **Brillouin** [BG11a]. **broad** [FCS13a, FCS13b, TZ11]. **Broder** [PR11a]. **Broken** [FDNR10, SC10a, CR18, GFRdG11, Tob19]. **broken-symmetry** [CR18, GFRdG11]. **brominated** [MFB11]. **bromine** [FGD+19]. **bromo** [OA13]. **Brønsted** [GI14, RDB19]. **brookite** [GP13a]. **BS** [YGLL10]. **BSE** [RAMB18]. **B —** [MGB18]. **bt** [Qu13]. **Bu** [GWM11]. **buckyballs** [GKGM18]. **buckybowl** [LZW+15]. **Buckycatcher** [DI15]. **build** [GBK18]. **building** [JHL+18, KS19, LLZ+14, MDC15, MSOV13, Sza13, XWP+18, CNBPR+11]. **bulk** [TFB11]. **bundle** [GWME18, JE10]. **bupivacaine** [MP12]. **butadiene** [SKTI15]. **butadiynol** [ŞBAT16]. **butadiynyl** [KI12]. **butanetriol** [LL17]. **butatrienone** [ŞBAT16]. **butene** [IK14, TFA10, ZPB12]. **butyl** [AMAC12, MFK+12, WZZL10, dOLdlV13]. **bzq** [ZQJW13].

[RZG12, RLER14, RAMB18, RCGLV+14, RVO+14, Rud12, RRCO11, RTT10, RMY+13, SH19, SMEH15, SAHG11, SAHA12, SJZ+18, SL13, Sko16, STL12, SRA+11, SN11, SW12, SJW13, SCBP17, Tan13, TNN16, TSH17, TWR15, UTTn13, UGWL18, USL+13, VVVB10, Wag14, WWC17, WYM15, WZW17, YYI+12, YIY+13, YSK+12, YKM+15, YHL+13, Zak13, ZST+10, ZQCJ10, ZCC11, ZF15, ZZC12, ZZZ+18, dSM19a]. **calix** [Pli18]. **CAM** [JdOS16]. **CaMn** [SYK+12, YYI+13, YIY+13, YSK+12]. **Can** [ADR+18, Kuz19, Lu15, Met11, Nes11, Sza13, TFA10, Blo15, Luz11a, PWP+18, WLZ18, ZLWL16]. **cancer** [LB14a]. **candidate** [AB16b, XWP+18]. **candidates** [Ali19a, KMRG13]. **Canonical** [GW13, CCL+16, JH15, Jør15, Jør18]. **Canuto** [Ano11a, RdA11]. **CaO** [SAHA12]. **capabilities** [AG19, OCGM+19]. **capability** [CJSNLM11]. **capacities** [GVPCK10, UDS19b]. **capacity** [KDA+11]. **capped** [SALK19]. **capsules** [KKH+13]. **capture** [GSaY11, Mai14, PRPU+13, Sri19]. **carbazol** [MUNZVR12]. **carbazol-oxadiazole** [MUNZVR12]. **carbazole** [ZBBB17]. **Carbene** [CDL+19, HZZ+19, LWC+10, LCS+11a, LCH+11, LCS+11b, LXLL11, RMP+14, ZFS+11]. **carbenes** [ABTW14, ALB18, CDL+19, MAN15, Pan16, SZL+14]. **carbide** [NEEV15, RK14]. **carbides** [GM11]. **carbocyanine** [Mas10]. **carbodiimides** [WLWT12]. **carbodithioic** [SJZL12]. **carbohydrazide** [HZZW11]. **Carbon** [DSFT17, MPL+11, AKC10, AEM+12, ACT19, Bas11, BEPZ10a, Buc10, Buc11b, BSO11, CS13, CTDOLA10, DI10, DM16, EBR11, ETGLMJ+19, FC19, GAMM10, GT13, GZBH18, GGP13, HCH+18, HNBG15, HNBS18, Hog13, JW19, JR19, KKC14, KKT13, KKT14, KG08, LV19, LMC19, Mai14, MAT19, MSOV13, OPS10, OCGM+19, OD12, PP14, PNC19, RRK16, SA18, SD13a, SC10a, SQ10, TZD+19, TDOD17, TC10, Wan11, WW11, WHY+14, WJY15, WDJ+17, Yam10, ZCX+16, ZMB+17]. **carbon-carbon** [FC19]. **carbon-hydrogen** [GZBH18]. **carbonate** [DLO16, YM12]. **Carbonates** [RBLZ15, ZQW+17]. **carbonic** [dM13]. **carbonmonoxy** [CHSO13]. **carbonyl** [BLdV19, BH10a, DWJZ11, GGJD13, MTS15, MG10, RCM+19, WLS+19, YYS15, dCSDdMC13]. **carbonyl-coordination** [GGJD13]. **carbonyls** [LLW+12, RALK18]. **carborane** [FSQ+11, LCZ15]. **carborazine** [Kal18]. **carboryne** [HhGqZZ17]. **carboxaldehyde** [TBA13]. **carboxylase** [WLD+10]. **Carboxylate** [SCB+14, KSAK17, LYL+12]. **carboxylic** [KC11, LGM+18, MK10b, SAG13, TPT+13, VF13a, WJ11]. **carcinogenic** [DKZ+10]. **Carlo** [ÁFV12, ABG12, ANC+15, ASK15, Cal10, CKB+19, CCC19, CP16, HCH+18, Hog13, HB14, HM12, JCCZ12, PDR+14, PIS18, RCGLV+14, SGC13, SCBP17, Wag14, WCM14, ZLR15, ZCC11]. **Carlos** [HS15]. **carrier** [GNM+12]. **carriers** [NMV+14]. **Cartesian** [GMR18]. **cascade** [Fra17]. **case** [AGRI+12, BDF+16, Bas11, BBM17, BLdV19, CCL+16, DMAB12, DVDBM11, DAA16, DCDD10, DFF+13, GS11, GB18, GWME18, KLE+19, Kuz19, Mar12, MVG18, MSC10, MURR13, Oni10, Ped16, PK13b, SS10, TC12, TWR15, YLZ+17, CTVA12, DB12]. **cases**

[Zak13]. **CASPT2** [BDFM10, BDR12, ČFČ11, GLOGM+11, KZZ13a, LCL+11, LGP+12, MR11, Pul11, RS12b, SKTI15, SZZ+12]. **CASPT2//CASSCF** [GLOGM+11]. **CASSCF** [BDFM10, DAR+11, GLOGM+11, Lar11, Ols11a, PE11, RS12b, RSN12, SZZ+12, SBL11]. **CASSCF/CASPT2** [SZZ+12, BDFM10]. **CASSCF/MRCI** [DAR+11]. **Catacondensed** [RB08, RB11a]. **catalysed** [SMRK18, ZYSW17]. **catalysis** [BvWG14, KJ14, MMM+12, MCRS16, PIS18, Sic16, SLS+15, XDM+10]. **catalyst** [ENV15, Esr18, EM19, GB18, Hog13, JXX+15, LCM+11, TM19, Var14, ZQW+17, ZBG+19]. **catalyst-free** [ZBG+19]. **catalysts** [BAB+18, TFZ+15, WR14a]. **Catalytic** [BD14, PM17, SS18b, AGOP18, BGFD14, CLY12, DMBJ15, ED16, GGZZ16, GSB10, HSN+11, HSYM11, LPOP12, MLW+14, MMP+18b, NEEV15, TK16a, TTD13]. **catalyze** [XGH18a]. **catalyzed** [AKC10, AZD+11, CAPGAIG18, CWZ+10, Che12, GCZ+14, HZZ+19, JL12b, JSLH14, KUTS10, LGM+18, LZZ12, LQ13, LYR+17, LLF17, LD17, LTL18, LFTL18, LMCZ11, LCZL11, LW13, LW15, LKZ+16, MPGGS19, MCC13b, PRFR17, SH18b, SHL+13, SR11a, SLS+15, TTD13, TFA10, WML10, WWLZ17, WZZL10, WRW+18, XZG+18, YS18, ZCZ+12, ZSHL14, ZZC15, ZQW+17, ZSS+13, ZLY+14, ZPW16]. **catechin** [MKHM11]. **catecholamines** [MBTVR12]. **cathode** [KLK13, Kim18]. **Cation** [ZLWZ16, ATS+11, Ber13a, BMX+19, DWJZ11, DAE+12, HV11, LCL+10a, LLC+11, MMMM12, MS14c, ONBP11, Oni10, OCGM+19, PDR+14, PvS10, SPSA11, SZZ+12, XZL+12, YM12, ZFC12]. **cation-** [OCGM+19]. **cation-exchange** [PDR+14]. **cation-exchanged** [PvS10]. **cationic** [BCGC12, FTB11, ZQJW13]. **cations** [BMF13, ESLM19, GK12, HFA+19, IGMK11, LGP+11, LPG+12, MMR+10, MKM11, NKWT19, PDR+14, SHE10, WLWT12, YLW+13, ZLWZ16]. **caused** [HYH+10]. **causes** [ABP13, MFM18]. **causing** [MFR10]. **cavernous** [CJMC19]. **cavities** [MGK19, Pup11a]. **Cavity** [PCR+11, OPC17, RAFR18b, RAFR18a]. **CBr** [WZHZ13]. **CBS** [CFOC+10, VF13a]. **CBS-Q** [VF13a]. **CBS-QB3** [CFOC+10]. **cc** [SLS+11]. **cc-pV5Z** [SLS+11]. **CCH** [EMS16, LZZ+11]. **CCl** [SKS11, LGW11]. **CCSD** [CK13, VV13, BL12, CPF+11, DVP18, JdOS16, SLS+11, TD19, VV12]. **CD** [SZY17, ASHF13, XZZ+10, XWC11a, LKLW11, XWC11a]. **CDO** [ADR+18, SAHG11]. **CdS** [XWC11b]. **Ce** [WLG+11, WSL+11]. **cefotaxime** [LBM11]. **Cell** [KMT+12, CWB+13, JK12, LGS+16, MANP17, QJ13, SSS15, TGRP19, WLL+13, WWB+14]. **Cell-penetrating** [KMT+12]. **cells** [AGJ12, BDG17, FFPD16, FM16, cLqFtW+14, LYS+19, MY17, PMAP12, SG19, TZ11, ZSAP11, Zha17]. **cellular** [Kuv10]. **cellulose** [FNBK17]. **center** [Buc10, Buc11a, CRSB12, CN12, Hog10, HZS14, Koc13a, MSNP18, Tal11, Yam10, YD17]. **centered** [GAPK+19a, KFS13, Zak13]. **centers** [ASD14, YGLL10]. **centrifugal** [CLXD15, IIH16, ZLJ11]. **centrosymmetric** [KPL+17]. **century** [Pup11b]. **CeO** [QCB+10]. **ceria** [KJ14]. **ceric** [BSPK11]. **cerrado** [CCA+12]. **cesium** [MMR+10]. **CF** [lAyL14, Mor11, Mor11]. **CFCl** [dOdCMUdALR11]. **CFP** [KyH13a]. **CGR**

ASMP15, AD17, AMMB+18, BF11, Bal16, BL10, BL11, BG11b, Brä13, BVRM10, CJBMMAPR19, CKL16, CLXD15, CFGC11, CPAT11, DKZ+10, DPK18, DSL15, DPRK12, DFK16, DMS+10, DLM+11, DMBL16, DSFT17, EAK+10b, EML+11, EMED+12, EMEPD15, FBO+11, FBD+13, Gag11, GP13a, GRCGRRHT19, GFPAV19, GA19, GI11a, GbZA10, Gru17, HMA+19, Hop15, HAX+18, JN13, KWC10, Kal18, KBGC12, KMK+16, KM12c, KUTS10, KK11d, LZZ12, LYR+17, LL17, MC11a, MPE15, MTR+19, MC14, MG12, MQA17, MKM11, MBBT+12, MML11b, MGP16, NC11, Nal12, NZ13, Ném14, NVPCJ+13, NRP+11, NJA+12, OS10b, OWD18, OSJ+12, ÖEDB11, PWY+18, PO15, Qu13, RLW+13, RGTS11, RNE10]. **chemical** [RMP+14, RR19, RBTL19, SSI+10, SSK+12, SAG13, SBEH11, SKHN13, SC12a, SW10, SN15, SM19, SC10a, She14, Shi13, SIS+08, SKM11, SR13, Sko16, SFY12, SBKJ18, SRA+11, SK10, SSB+12b, TFBG14, TYN13, Tap15, TMC18, TKSK17, UTTn13, UJSJ13, VOK+18, VO11, VO12, WYM15, WLD+10, WLWL14, YNLD18, YSS+10, YYI+13, YB11, ZBK15, ZZC12, dHLdS12, vL13, vLRRK15]. **chemiexcitation** [dSM19a]. **Chemiluminescence** [dSdS13b]. **Chemisorption** [OD16]. **chemistries** [Vie17]. **Chemistry** [AH19, ÁIGVZW12, Brä13, Hog13, IFT13, KYS13, KYH+13b, TBRIS12, ZJS13, Ban12, Bar16, BMRM19, BZBZ13, Blo15, BHH+13, BT15, Buc12b, Cav13, CAA19, CM16, CSG14, DC12, Gag11, GGZZ16, HR13, HEVMSA+19, IK14, Jia15, Kap12, Kar09, Kar10, KC19b, KN15, LSR+10a, LSR+11, LJ16, LFS+11, LCZL15, LSKM19, Luz11a, MMŁ+16, MEF+15, MMCNV19, MQG13, MPGGS19, Mor13, NBZG16, NTCK13, Nic11, Nic14, NMSR14, OM13b, PTH11, Pup11b, Puz17, Rei15, RNB+10, SDP+16, She13, SG14, SPM+15, Tch16, TBB+19, TBRIS10, TBRIS11, Tri14, TB15, VVN+16, VMR11, VBJK18, WYWL13, WWX+11, WR14b, YZ13, ZLWY13, ZWSF16, DC10, SG14, BT17, Tch13]. **Chemists** [RA10b]. **chemogenomics** [IAK13]. **chemometric** [LSR+10a, LSR+11]. **chemosensor** [LWZ+14]. **CHF** [STL12]. **Chiral** [YWR+18, BdTG11, CPL15, KGVG11, LPM+11, LMCZ11, LW13, QCW+12, SFW12, WTZ+11, YWY+12, ZSS+13]. **chirality** [Luz11b, SD13a]. **chiroptical** [Cap16]. **chirp** [GRLA18]. **CHITEL** [RA10b]. **chloramine** [SZL+15]. **chloride** [EHKD11, EKD12, MMM+12, SKS11, dOLdlV13]. **chlorides** [BLM+12, HSN+11]. **chlorinated** [FBO+11, KZA+17]. **chlorine** [DWGX12, cLqFtW+14, MOY13, XXbX+13]. **chlorins** [CJSNLM11]. **chloro** [DDÇY12, DPRK12, PSKV19]. **chloroalkenes** [MLB+12]. **chloroaniline** [HLZ+14]. **chlorobenzaldehyde** [SRA+11]. **chlorobenzene** [SGL19, SC18]. **chlorobenzofuran** [ASMP15]. **chloroethyl** [CZJZ12]. **chloroethylnitrosoureas** [ZMZ13]. **chlorophenol** [ASW13]. **chlorophenyl** [ÖEDB11]. **chloroquine** [KdPNNS16]. **chlorotrifluoroethylene** [OCB+10]. **CHN** [RB11b]. **CHNC** [DW12]. **CHO** [DZ11a, Sch10b]. **choice** [AGPDZ13, FSB16]. **Cholesky** [BVA+14, CPF+11]. **Choosing** [KBJ17]. **Chou** [QZH13]. **chromites** [Zen11]. **chromium** [HM12]. **chromogens** [JA12]. **chromophore** [BF11, BSM+15, GLOGM+11, LORR+12, TCM+12].

VOK+18, FMCA11, FC19, RCM+19, SCZH16, ZZL+11]. **Comparisons** [CA17, PGG12]. **compass** [ZBK15]. **compatibility** [Fin17]. **compensating** [FUE+12]. **compensatory** [Chu12]. **Competition** [GE12a, SM17, TL15, GHS12, LFP+19, NRGS11, YZZ16]. **Competitive** [LLG+12, AMMB+18, SBKJ18]. **compilation** [TB15]. **complementary** [Yak11]. **complemented** [WJY15]. **complete** [CHH+19, CC19, GS10, LV12, SGB11, SXH18]. **Complex** [GLT13, IA13, JH13, KBF+13, ONK+13, BSS16, Bou12b, Cho16, DSD18, DI15, DZO12b, FDNR10, GRLA18, GR10, IKC18, JLG+12, JR19, KRG+13, LZ12, LV16, LLG+12, LSR+13, LBdV16, LDADB+15, LKZ+16, MNC12, MIN13, MMT+13, MSBF18, NS10a, NTGC19, NBI+10, NMIP14, OAA19, PEA+12, PWY+18, Puz17, Qu13, RW11, SS19a, SY10, Sat11b, Sic16, SLS+15, VDG13, VPOG19, WRW+18, XZ11, XCD18, XCL+18, YSS+10, YYI+13, YSK+12, YS13, YW16, ZSASS13, ZSHL16, dCSDdMC13, dOdCMUdALR11]. **Complex-scaling** [JH13]. **complex-valued** [YW16]. **complexant** [XWCY11]. **Complexation** [ESLM19, SHE10, ZKKR11, ZAE10]. **Complexes** [ALMY18, GHGF12, AC19, ADR+18, AM18, BHMN19, BPG+10, BAP12, BHA19, BZBZ13, BLdV19, BPK19, BCS+12, BB16, BSV12, CRB+12, CPF12, CTW12, Con10, CLMY12, CADSG18, DSD18, Den19, DPDR11, DG19, DCdG10, DdG+11, ED16, ESS13, EMSB15, EMS16, FBRBR12, For12, FBD+13, HS11b, HL19, HYD11, HZZW11, JW19, KRK+17, KV11, Kry12c, KBMM10, LJL+11, LYW11, LXW+14, LYR+17, LYL+12, LXD13, Lu10, MZB+13, MCE11, MNV+17, MC17, MGK19, MC12, Men10, MG12, MKM11, MS14c, MPRCEG12, ND11, NFD+10, OAC17, OPP+14, OVT+16, Owe17, PCMG12, PRG+10, PAKA15, RFEGPP+16, RB11b, SS10, SVRGV12, SG19, SGKG12, SRASZ16, SAHA12, SLS+14, SK11, SSP+17b, SPIL14, SHW+13, SM17, SK12b, SS13, TTD13, TMM+14, TL15, UDVD10, VO12, WLS+19, WXB+11, WZW17, WHM14, Wu11]. **complexes** [YZL+10, YZL+11, YZW+15a, YWH+12c, YZZ16, ZPR10, ZQCJ10, ZLLS10, ZQJW13, ZLZ+14, ZZC15, ZHL+19, ZSQ+10, ZFS+11, ZLWZ16, ZSZ14, ZQXP17, ZBBB17]. **Complexity** [GN19, EMED+12, LRMAA19, SMOD11]. **compliance** [NH18]. **component** [AB18, CW16, FZC14, KKT13, KKT14, MHT+08, MM19, SN15]. **components** [LVP12a, NIK19, Nal12, RLZ12]. **composed** [TK16a]. **Composite** [KO10, ZJS13, CC19, Mor12]. **Composite-system** [KO10]. **composites** [KT12b]. **composition** [GLF+12, GbZA10, IBA+11, Lad14, LKN13, QZH13, XTLA13, XTLA14]. **composition-dependent** [LKN13]. **Compound** [ZST+10, KWC10, LLLB13, MQA17, PGG12, RCM+19, SKS10, SSW16, TYL10, TXL10, WR14b, vL13]. **compounds** [AMK10, ASD18, BG13, BH10a, Buc11b, CCA+12, CHV14, FC19, GZMC11, HZG12, KM12b, LOHB13, LV19, LTdSJ+10, LTL18, LWJL10, MLC+11, MPMCM+11, MW16, Mor12, MSRn+11, OPAVM18, OG19, Pan19, PP19a, PI13, PH12, Pie11, PP19b, RDM+11, RRK16, RR19, SMC18, SLC+18, Shi13, TSvL+16, TWR15,

[EAK+10b, EAK+10a, EI11, THSR13]. **corrosion-inhibition** [THSR13]. **cosine** [GH11, GE12b, LLH15]. **Coulomb** [SS12, CF14, ARG11, BPL13, BBL12, Fin16b, FRGC10, Fuk12, GH11, IOO18, JH13, KH12, KWWH18, KK13, LLH15, Luz12, Nag16b, NDP10, PGGRMP10, Rit12b, Roy13, Roy16, SMOD11, Sil14, TC12, WWGW18, ZX12]. **Coulomb-attenuated** [NDP10]. **coulomb-attenuating** [CF14]. **Coulomb-like** [PGGRMP10]. **Coulombic** [Roy15, YW11b]. **Coulombic-like** [YW11b]. **coumarin** [MNP19, MDNDO+16]. **coumarins** [GTSC+19]. **Counter** [XLGA12, ZLWL16, MMSC19, Oni10]. **Counter-ion** [XLGA12]. **counterpart** [KC16]. **counterpoise** [KPH+12]. **counting** [JL12a]. **Coupled** [BJ12, Cam10, Cam12, Car19, PCV19, Sto18, VVVB10, WWC17, BVP13, BVP14, BSM+15, CSVCB12, DMAB12, DLM12, LRP+11, LP10b, Luz08, MPT11, PB10, RS12b, RSN12, SZS+10, Sza13, Tob19, Var11, XDM+10, YK13, ZE18]. **Coupled-cluster** [Cam10, Cam12, PCV19, LP10b, PB10, SZS+10, Sza13]. **coupling** [ATL+14, Ash18, BJ12, BSV12, CCP18, CFGC11, CSP+10, CDT12, IROW10, Kry10, Lar10, LKOS17, LW15, MKD19, MC18b, PM12, RCP14, SSI+10, Shi18, SHS+13, WTP+19, Wit18, YSS+10, YH14b, ZLS+18]. **couplings** [HKLW13, Kaw15, LB19]. **course** [HSYM11]. **covalency** [MML11b]. **covalent** [ABS13, AB16a, MURR13, NE11, YLH+19, KK13]. **covariant** [Luz08]. **Cover** [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano13k, Ano13q, Ano13r, Ano13s, Ano13t, Ano13u, Ano13v, Ano13w, Ano13a, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g, Ano13h, Ano13i, Ano13j, Ano13l, Ano13m, Ano13n, Ano13o, Ano13p, Ano13x, Ano13-35, Ano13-41, Ano13-42, Ano13-43, Ano13-44, Ano13-45, Ano13-46, Ano13-47, Ano13y, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13-32, Ano13-33, Ano13-34, Ano13-36, Ano13-37, Ano13-38, Ano13-39, Ano13-40, Ano13-48, Ano14a, Ano14b, Ano14n, Ano14t, Ano14u, Ano14v, Ano14w, Ano14x, Ano14y, Ano14z, Ano14c, Ano14d, Ano14e, Ano14f, Ano14g, Ano14h, Ano14i, Ano14j, Ano14k, Ano14l, Ano14m, Ano14o]. **Cover** [Ano14p, Ano14q, Ano14r, Ano14s, Ano14-27, Ano14-37, Ano14-43, Ano14-44, Ano14-45, Ano14-46, Ano14-47, Ano14-48, Ano14-28, Ano14-29, Ano14-30, Ano14-31, Ano14-32, Ano14-33, Ano14-34, Ano14-35, Ano14-36, Ano14-38, Ano14-39, Ano14-40, Ano14-41, Ano14-42, Ano15a, Ano15b, Ano15c, Ano15d, Ano15e, Ano15t, Ano15x, Ano15y, Ano15z, Ano15-27, Ano15-28, Ano15-29, Ano15-30, Ano15-31, Ano15-32, Ano15-33, Ano15-34, Ano15f, Ano15g, Ano15h, Ano15i, Ano15j, Ano15k, Ano15l, Ano15m, Ano15n, Ano15o, Ano15p, Ano15q, Ano15r, Ano15s, Ano15u, Ano15v, Ano15w, Ano16a, Ano16s, Ano16t, Ano16n, Ano16u, Ano16v, Ano16w, Ano16x, Ano16y, Ano16z, Ano16-27, Ano16-28, Ano16b, Ano16c, Ano16d, Ano16e, Ano16f, Ano16g, Ano16h, Ano16i, Ano16j, Ano16k, Ano16l, Ano16m]. **Cover** [Ano16o, Ano16p, Ano16q, Ano16r, Ano17a, Ano17b, Ano17m, Ano17n, Ano17t, Ano17u, Ano17v, Ano17w, Ano17x, Ano17y, Ano17z, Ano17c, Ano17d,

[OK16]. **Dative** [AM18]. **David** [Ano11c, Ano11b, RC11, Sau11]. **Davydov** [BEPZ10a, BEPZ10b, Lak10]. **DBUH** [RI19]. **dC** [XLGA12]. **DDQ** [YYS15]. **deacetylase** [dSMPRSF18]. **deactivation** [MR11]. **deal** [PBB15]. **Dealing** [AAHN16]. **deamination** [AASU+17]. **dear** [Sau11]. **Debye** [KWLS15, LKJ13, MGK+11, SMV11, Win10]. **decades** [Nes10]. **decahedral** [VS19]. **decanethiol** [FFF10]. **decapeptide** [DGA+13]. **decarboxylation** [EAH13]. **Decay** [AC11, ASD14, Cao17, CCM08]. **Decisive** [SC18]. **decoherence** [Brä11b]. **decomposition** [ÁFV12, CPF+11, CWS15, DWPK14, ENV15, HSN+11, LPOP12, LdAA+11, MCC12, MOSK10, MML+11a, MJ11, NB19, NEEV15, PWL+10, PMEP19, RLW+13, SKS11, SZ11, SLS+19, WLWL14, Yu13, ZL10, ZDZL11, dM13]. **decompositions** [BVA+14]. **Deep** [MVC13]. **defect** [BXR+13]. **defective** [ATS15, BAP13, Esr18]. **defects** [ES17, KC19a]. **deficiency** [MFR10]. **defined** [Fin16a, Gru17]. **Definition** [LVP12a, Kon11, MBTVR12]. **definitions** [Tch16]. **Deflation** [MQG13]. **deflection** [AOLB12]. **deformation** [GMP+11, KK12a]. **deformations** [KMT+12]. **deformed** [Agb12, MJ11]. **deg** [FDG18]. **degeneracies** [Lev10, RMG+19]. **Degeneracy** [MSC10]. **degenerate** [BDPT12]. **deglycosylation** [WHS+13]. **degradation** [HYZ13, SZL+15, dlLIAI+12]. **Degree** [YIY+13, CAAI12, GV19, LSW19, LWY19, PR11b, PL18a]. **degree-Kirchhoff** [LSW19, LWY19, PR11b, PL18a]. **dehalogenase** [ZCZ+12]. **dehalogenation** [PSKV19, ZCZ+12]. **Dehydration** [MMM+12]. **dehydrofulvene** [LVP12b]. **dehydrogenase** [SSB+12b, dCDC+11]. **dehydrogenation** [HSYM11, NTNL10, WZM+13]. **Delayed** [SGG+10, GMM+18]. **Deletion** [Cin11a]. **delivery** [RdPW+12]. **Delocalization** [DZO11, LNI12, ARH+13, AT18, LDKB15, MJ16b, NE11, NRGS11, RBVAG18, WDSL14, WWD+15]. **delocalized** [ALK18, DG19, Joh17]. **delta** [DAC11]. **demon** [CD15]. **denaturation** [BMB12]. **Deng** [Roy14]. **denoising** [SRMB15]. **denominators** [CPF+11]. **dense** [BN12, DW12, Ng12]. **densities** [ALRA10, ALRAE11, BPL13, Fin15, LS17, MAT19, MT11, MNZPT19, SS19b, WGLX10, ZL12]. **Density** [Ano13-49, BHA19, BGBV12, BJdlMAV12, CCL+13, CM12, CD12, DCBB11, DSZB18, DQZF12, EM16, ED16, FZX18, GMR18, GGD12, HLZ+14, HKLW13, HYD11, ISN13, IKN13, JS17, Kar13, KCC13, KK14b, KSAK17, Kit14, Kit17, Lae14, LWL+12, LWX+14, LBY+14, MLC+11, MW16, MUNZVR12, MIN13, MLB+12, MM13, MCRS16, MOH+12, NTNL10, NZAVR10, PS10b, PS14, PMH+16, RGPZD13, SA18, SVRGV12, SKY+13, SS13, TOSN12, Tan12, TIN13, TDOD17, TFZ+15, UMS13, VUC13, WJL+11, Wit18, YKM+15, YL11, ZCX+16, ZRR+11, dCSDdMC13, AC19, ABLT11, AK17, AM13b, AB18, ATM17, AGPDZ13, AST16, BMK+14, BD14, BCGC12, BVCAP12, BL19, BDF+16, BDF+18, BLdV19, BLKB11, CDSK12, CEFMK12, CM15, CNSK11, CH17, CZLD17, CLH14, CC19, CK17, CF14, CC11b, CSTA16, DWJZ11, DKS11, DPRK12, DW12]. **density** [Dil13, DZ11a, DGR+16, DG19, FO10, FDNR10, Fin16a, Fin17, FA17,

FSB16, GFPAV19, GCK+17, GM11, GJ18, GHCMCMQ17, GWME18, GD11, GCZ+14, HMA+19, HR19, HHCA10, HZZ+19, HMH10a, HMH10b, HKIH13, HZZW11, IN15, JR12, JPP+11, Jan13, JW18, Jeo18, JW19, Jou13, KK13, KME+18, KPCV18, KJ16a, KJ16b, KKL+16, Kit15, KYLC19, KDOR17, KJ14, Kri13, KFS13, KG08, KMU+13, KFJ+18, Kuz19, Lat13, LPO+12, LSR10b, Leh19a, Leh19b, LW11, LC16, LSP+16, LLW+11, LCK+16, LDZG16, LNI12, MYZ+10, MLW+14, MJ16a, MFK+12, Mas10, MKSG13, MLK17, MJ11, MBBT+12, MBSMJC18, MNS11, MKW11, MJM19, Nag15, Nag17, NAK+17, NDP10, NL11, NMIP14, NMSR14, NIT16, OD16, POLV12, PI13, PK13a, PABSK16, PP16, PTH11, PL11, PCV19, PR10b, PSMD16, PRFR17, PFdM13, Per18, PBR18, PJP10]. **density** [PMAP12, PI16, PC13, QHS11, RLER13a, RCM+19, RPVM10, RGTS11, RAMB18, RBVAG18, Rud12, RSCS10, RLZ12, RS13, RKCK19, SS10, SLG11, SB18, SFC16, SLC+18, SN12, SAHG11, SHL+13, SJZ+18, SIS+08, SDM12, SSP+17b, Sri19, SRA+11, SK12b, SX15, Tan13, TÁ10, TCA10, TGRP19, TLC+17, TRZ+19, UV18a, VPGC12, Vik13, VBO+15, VSL+15, WKE17, WW11, WJY15, WDJ+17, WTZ+11, WR15, XNL+14, XSLF12, fXxBhD19, XGH+18b, YLH+19, YWH12a, YWH12b, YRN+11, Yu13, YF16, ZT13, ZKKR11, ZQCJ10, ZLWY13, ZBG+19, ZMZ13, ZCG+16, ZSZ14, ZKW17, ZZ18, Zho18, dCGAMV12, CTDOLA10, LLZ+12, Ven12]. **density-based** [ZKW17]. **density-dependent** [IN15]. **Density-functional** [FZX18, BDF+16, BDF+18, BLKB11, CF14, DW12, JR12, LNI12, MYZ+10, WR15]. **Density-functional-theory** [SVRGV12]. **Density-matrix** [EM16, Kit14, Kit15]. **deoxygenated** [TYN13]. **deoxyguanosine** [SKM11]. **deoxyribonucleoside** [MB14]. **Dependence** [AG10a, BLWJ17, Buc12a, BN11, BSV12, CAAI12, GLF+12, KP11, KSG+12, KKH+13, LZFZ13, Mar11, MIN13, MKSG13, PMMGL+11, Rud12, WR15]. **dependent** [ASD18, Bae16, Bae14, BDF+16, BDF+18, CP10, CEFMK12, CW11, CW13b, DCZ17, DM16, FMMD+10, GFPAV19, GSR12, HS11a, HHCA10, HKZZ15, IN15, ILBS10, IG11, JPP+11, LKN13, LV19, lLBqD+19, LMZY15, Luz13, MJM19, NMS+10, NSN17, NNSN17, NDP10, Oht13, PVS11, PVS12, PSC15, PJP10, PMAP12, PI16, SFC16, SLC+18, SSAM13, SL13, Sko16, SHW+13, Vik11a, Vik11b, WKE17, WYWL13, YLYC18, ZQCJ10, ZCG+17, ZLE17, ZSZ14, ZZ18, Zho18]. **dephasing** [Gan14]. **Depicting** [LBdV16]. **depolarization** [AEM+12]. **deposited** [SAHG11, SAHA12]. **deposition** [TFBG14]. **deprotonation** [CFOC+10, Kry12b, PUGSFM18, Shi18, WXB+11]. **depth** [LYS+19]. **Depurated** [Cin20, MMM16, MMM20]. **derivation** [BR10, BR16, Bra10]. **Derivative** [HSN18, BSSS19, DWPK14, KGVG11, LWZ+14, TPT19, WLZ+12b]. **derivatives** [ALMY18, BSS15, CWL+13, CCL+16, CFV18, CWB+13, CSG14, DKZ+10, DWZZ15, DNCKCS+12, EI11, FSQ+11, GTR11, GB13, HNH+12, HMA+19, HS11b, HLB19, ILBS10, JLZ+17, JB11, JFDD10, KZA+17, KKM+12, KSN+10, KKG12, LGM+18, LWL+12, LYS+19, LWY19,

LCCH10, LWH+12, LCH+11, LCS+11b, LW15, MLY+16, MNV+17, MLPT10, MDNDO+16, MBBT+12, NRHJ11, OAA19, PPK+13, QHS11, RYM12, RBZ15, RMP+14, SF13, SSTÖ11, SRMB15, TZ11, TKSK17, Val17, VV18, VMC11, VHTEG15, VBO+15, WGLX10, WLL+13, WJ11, YWR+18, ZSAP11, ZZX10, ZZR+12, ZYL+13, ZMB+17, ZFC12]. **derived** [CADSG18, MAN15, NH18, PAKA15]. **describe** [CB10, MMG15, PABSK16, Sza13]. **describing** [Gar08, JCC10, dGR14]. **description** [AB18, DVDBM11, DCFD10, DMBL16, Fer19, FGD+19, GC19, HFdGC14, KO14, LORR+12, MPMCM+11, MBA+19, Nas19, NGS11, SIM14, SFL+10, TCA10, TRZ+19, ZZ18]. **descriptions** [PC16, PCK19]. **descriptor** [AKR12, FDG18, PUGSFM18]. **descriptors** [GI10, GI11b, GI11c, GI11e, JS18, LV19, LNV+18, Nag16b, Nal15, OPAVM18, PH12, Pog12, TFA10]. **Design** [FZH+18, HSS18, IIS+17, cLqFtW+14, Val17, BJ17, CAA19, DC14b, GbZA10, HM10b, LLZ+14, LZZ+17, MY17, MSM16, Ném14, Oni12, OWD18, SRASZ16, SAHAA16, Sik18, SLA12, SSS15, STM18, THL+15, TK16b, VVY18, WWB+14, WR14a, WR14b, XFW+14, YZZH15, YHLC15, ZFW+13, ZWZK19]. **designed** [NTGC19, OAA19]. **designing** [SSB12a, ST15]. **desorption** [ÁFV12, FTB11, GD11]. **Dess** [TM19]. **destructuring** [KRG+13]. **desulfurization** [VPGC12]. **detachment** [DZO12c, DZO12a]. **Detailed** [Sch13, Fin14a]. **Details** [Lar10]. **detector** [BMB10]. **determinant** [RLZ12]. **determinants** [CSSK+12]. **Determination** [ATL+14, GI11b, GI11c, IKN13, SN12, Ali14, AGPDZ13, AST16, MLW10, PT13, Ser11b, GBK18]. **determine** [SFW12, Tob19]. **determined** [Mor12]. **Determining** [MGM11, AGB19, Bon17, IKN13]. **detonation** [LZZ+13, RGTS11, WGLX10, ZZX10, ZL12]. **Detours** [DB13a]. **deuterium** [NHB12]. **deuterons** [HITU16]. **developed** [AY15]. **Developing** [AV19]. **Development** [KSN+10, Lin14, NSN17, NNSN17, SR11b, SKV12, SZ15, GEL18, Kap12, KKL+16]. **developments** [AMMC19, HJK14, Jør18, Mur12]. **device** [yBZfC18]. **devices** [Jan10]. **dfppy** [ZQJW13]. **DFT** [YSK+12, AEKGZ12, AFC+10, ACF+11, BVCAP12, BPVDB11, BP13, Bas11, BZBZ13, BLRdA+10, BAA+18, BS14, BDR12, BAB+18, BJ12, BO11, BW13a, BW13b, BSV12, BSPK11, CRB+12, CR18, CPF12, ÇAS13, CRSB12, CW16, CCL+10, CKYR18, CKB18, CFGC11, DSCO+13, DSD18, DCDD10, DCFD10, Dw13, DAE+12, DPDR11, DP16, DdG+11, DB15, DFF+13, EG10, ESDO16, ESS13, EFO11, EO11, ES17, EM19, ESBVJY12, FSQ+11, FV11, FRNM12, FPRGMHGB12, GAPK+19b, GC18, GJ18, HS11b, HFdGC14, HNBS18, HhGqZZ17, JPPA10, Jan10, JL12b, JB11, JLL11, KMS+11, KP10, KP11, Kar12b, KBF+13, KAG08, KMM+18, KG17, KI15, KKG12, KBMM10, LJ13, LGM+18, Les12, Lev16, LYW11, LLP+13, LLF17, LZW+18, LTL18, LYW+19, LGW11, DVMC19, LKZ+16, LGS+16, MXC18, MCP10, Mar12, MCC12, MGK19, Mas10, MMP+18b]. **DFT** [MMC+19, MFZ+18, MCL11, MS17, MML+11a, MMM+12, MAN15, Nag16a, NEEV15, OKK10, OGvSG18, OCB+10, OCGM+19, OPP+14, OVT+16, PS10a, PTS+11, PK13a, PWL+10,

PAD+10, QCW+12, RK14, RRVJ10, RGST12, RFEGPP+16, RDB19, RYW+15, RNdA+10, RFMC19, RS11b, Rua10, SSP+17a, SSB19, SMGZF19, Sat11b, Sch12a, SMEH15, Ser11a, Ser11b, SAHA12, SHE10, SM13, SS18b, SB10b, SBB16, SHW+13, SMGZ13, SWS+14, Tas14, Tav12, TGRP19, TG13, Tug13, TKSK17, UV18b, VF13a, VV18, VLG12, VSN+11, Vie17, WLWT12, XX12, XZ11, XZG+18, YNLD18, YYS15, YY18a, YY18b, YYI+12, YIY+13, YZL+11, YWY+12, YZW+15a, YZZ16, ZSAP11, ZLWL16, ZL10, ZQXP17, ZLY+14, ZPW16, ZCP11, ZDZL11, dSdS13a, dSdS13b, dSM19a].
DFT-based [BP13, Dw13, MCP10]. **DFT-D** [BAB+18]. **DFT-D3** [SSB19]. **DFT-treatment** [AEKGZ12]. **DFT/M08** [Vie17]. **DFT/M08-HX** [Vie17]. **DFT/TB** [ZCP11]. **DFT/TD** [LGS+16]. **DFT/TD-DFT** [LGS+16]. **DFT/TDDFT** [BAA+18, YZW+15a, ZSAP11]. **DFT/UFF** [JLL11]. **DFTB3** [PSC15]. **dG** [XLGA12]. **di-anionic** [DHYC19]. **di-enol** [Val17]. **di-lanthanide** [OAC17]. **Diabatic** [CHM+17, ART08, DMAB12, DM12, KUY16, MHOG18, MKD19, SHS+13]. **diacetyl** [TM13]. **diagonalization** [GBK18, Man16, MBSAG16a, MBSAG16b]. **diagonalizations** [CKYR18]. **diagrams** [FMKJ14, Jen13]. **dialkaline** [BHMN19]. **dialuric** [KB13]. **diamagnetic** [Pit12, RP11a]. **diamantane** [BBKO16]. **diamines** [LKOS17]. **diamino** [LLW+11]. **diaminoanthraquinone** [DKS11]. **diamond** [GZ14, ZWWY10]. **diamond-like** [GZ14]. **dianions** [TIN13]. **diarylethenes** [MPJ12, YXM+18]. **diarylethylenes** [Bud12]. **diastereocontrol** [SFW12]. **diastereoselectivities** [TFZ+15]. **diasteroisomers** [BCF+11]. **Diatom** [CNBPR+11]. **diatomic** [Agb12, BKM15, BB10, CP13, CJOOW11, GM11, GS11, HRT12, HVR18, Ish14, JZP17, KBGC12, KBG17, Leh19c, LLP17, MPM15, NDH10, RC11, Roy14, SYY16, Tou11a, VOAH18, Leh19b]. **diatomics** [GI11b, GI11c, IM15]. **diaza** [ZLS+18]. **diaza-benzo** [ZLS+18]. **diazaadamantane** [KMK+16, KMM+18]. **diazadiborinine** [GC18]. **diazine** [BHA19, CW16]. **diazo** [LTL18, LDW+11]. **diazonium** [Bon17]. **diazotization** [LLW+11]. **dibenzothiophene** [VPGC12]. **dibenzothiophene-like** [VPGC12]. **diborane** [ZYL+14]. **diborane···** [SSB19]. **dicarbon** [FC19]. **dications** [Buc12b, GNM+12]. **dichalcogen** [KM19]. **dichloro** [LCS+11a]. **dichloro-germylene** [LCS+11a]. **dichloroketene** [CHH+19]. **dichloromethylbenzimidazole** [PMC11]. **dichloropropene** [ASMP15]. **dichlorosilylene** [LLLB13]. **dichotomy** [GMT18]. **dichroism** [PCR+11, SB10a]. **diclofenac** [KK19]. **dicopper** [BH10b, RNdA+10]. **dicyclobutadieno** [LWY19]. **dielectric** [CN12, KP10, KT12b, Ng12, NDM+12, OA13, RTG+19, Ser11a, Ser11b]. **dielectron** [LB19]. **Diels** [CM12, Iku17, LW11, MIKH19, ZLWL16, ZXY13]. **Diels-Alder** [MIKH19]. **dien** [WLS+19]. **diene** [EI11]. **dienes** [LW11, LKZ+16]. **dieniminium** [BMX+19]. **dienone** [KAOB11]. **diethyl** [KI15]. **diethyldichalcogens** [Dum12]. **difference** [AD17, Fin16a, Kim16, LCZ15, WH18]. **differences** [ALK19, BWB+18, BB16, MK10a]. **Different** [MAT19, ABP13, ABA11,

BS16, CW16, CP11, FM16, GI11e, GGP13, HGB08, JdOS16, KP10, LZZ+17, MNP19, MIKH19, TW10, TFZ+15, YŞÖ12, ZCW16, Zil14]. **differential** [Ali14, yBZfC18, CRA+11, HVR18, Nag10]. **differentiation** [CW11]. **difficult** [KLE+19, Mar12]. **difficulties** [Sut12]. **diffraction** [ÖEDB11]. **diffuse** [SZS+10, SLZ+11c, SLZ+11a]. **Diffusion** [JCCZ12, PP10, ABG12, BR12b, HKZZ15, LWX+14, MFOH18, RJLPGH+13, SR19, UDS19a, WLH+19]. **difluorohydroxyborane** [MMCN+11]. **dihydro** [SC12b, TAY11]. **dihydrobenzimidazole** [KKG12]. **dihydrobenzoxazoles** [ZBG+19]. **Dihydrogen** [dOR10, AKHS13, GD11, GT13, MS14c]. **dihydrolipoic** [PM17]. **dihydrolutidine** [TM13]. **dihydrolysergol** [RGS+13]. **dihydropyridines** [ZYSW17]. **dihydropyrrolones** [VGGPdL19]. **dihydrothiophene** [HL19]. **dihydroxyacetone** [BGJSM+18]. **dihydroxybenzene** [YY18a]. **diimide** [HSS18]. **diiso** [LKOS17]. **diketonato** [AC19]. **diketone** [SKS10]. **diketopyrrolopyrrole** [MSG16, PWP+18, WWB+14]. **diketopyrrolopyrrole-analogue** [PWP+18]. **diketopyrrolopyrrole-thiophene** [MSG16]. **dilauroyl** [MKSG13, TTM16]. **Dimensional** [DTF+11, ART08, Beh15, BEPZ10b, Cho15, CYK17, Dau16, DLRMFY10, DBTA19, Dw13, DMS+10, Mam13, MPD+15, MDC15, MSC10, MLDP10, PGMGRM15, RZSZ18, RNC+14, SPD+18, SD13b, SSAM13, VBC+12a, VBC+12b]. **dimensionally** [Yam11]. **dimensions** [IIH16, RPVM10, RAK10]. **dimer** [AM13a, BF11, CHL+19, GIO12, HM12, KS18, MPT11, NTGC19, NVI10, NHB12, PMMGL+11, SH19, SXH18, SKY+13, SS13, TNN16, TBB+19, Zak13]. **dimeric** [Rua10]. **Dimerization** [LSR10b, LS19, Rua10, SKTI15, TFA10]. **Dimers** [TBRIS12, BCF+11, Cas15, CZCW19, FSB16, GORW19, KM12a, KK11a, KSS+19, KDOR17, MT10, PP10, PMEP19, RPBB11, RNE10, SZZ+19, TBRIS10, TBRIS11, TPT+13, VSS11, WJ11, dSCC12]. **dimetal** [ZFC+17]. **dimetallocene** [LYD+18]. **dimethoxyphenol** [Tan12]. **dimethyl** [JSLH14, JAB12, LdBF+12, LXLL11, NMHPVG12, Owe17, SJZL12, SSP14, SCZH16, TAY11, TXL10, WXZ+11]. **dimethyl-germylidene** [TXL10]. **dimethyl-silylene** [LXLL11]. **dimethylallene** [CPL15]. **dimethylamine** [LLZZ10]. **dimethylaminophenyl** [FO10]. **dimethylaminopropanol** [WZX11]. **dimethylcyclobutene** [MB13]. **dimethylmethylene** [LWC+10]. **dimethylnitrosamine** [LVdSdM14, dAVdM17]. **Dimethylphenyl** [Tan12]. **dinitrogen** [VPOG19]. **dinitrophenol** [LDW+11]. **dinitrophenyl** [RNdA+10]. **dinitrosamine** [JN13]. **dinuclear** [FDNR10, PEA+12]. **dinucleoside** [PAD+10]. **dinucleotide** [Cys11]. **dinucleotides** [HW12]. **dioctahedral** [PDR+14]. **diodes** [MUNZVR12, NZAVR10]. **diols** [LKOS17, SBEH11]. **dione** [OPP+14, QJ13, IK14, KDÇ12]. **dioxabicyclo** [VOK+18]. **dioxane** [Cha10, CNSK11]. **dioxetanone** [dSdS13b]. **dioxetanones** [dSM19a]. **dioxide** [JLS13, KKT13, KKT14, MPL+11, PP14, TDOD17]. **dioxin** [MSY+12]. **dioxolene** [DG19]. **dioxy** [KMK+16, KMM+18]. **Dioxygen** [MMÅ13]. **dioxygenase** [ASD18]. **Dioxygenation** [ADR+18, ASD18].

BGL+16, Bra10, BEPZ10b, CNBPR+11, CCC19, CYLL11, COP16, DKS11, DK13, GWZ+14b, GZMC11, HV11, HR19, HSN+11, IGMK11, JN13, JLG+12, Lad14, LSR10b, LZ12, LPOP12, LWL+12, LLC+11, LWJL10, LB19, MNP19, MG12, MS10, MSK+12, MPT11, MW15, NTCG18, ND10, OKK10, OA13, PCMG12, RY12, RMTG11, RRK16, RR19, SD13a, SIM14, SM19, SAHAA16, SPIL14, SK10, STU19, TYN13, TMC18, TJS17, WWL+11, XTLA13, XTLA14, XWCY11, XZJ+16, YRN+11, YKN13, YD17, ZGSM15, ZKWZ17, dSSF16b, dSSF16a, dAVdM17, Jan10, JWG+12, ZAE10].
Effective [AST19, CEM14, Liu15b, May14, TSvL+16, Vik11b, YHL+13, BCGC12, CCBR+12, Dw13, GbZA10, KUY16, MPTZ13, MZST16, PGGRMP10, TG16, ZE18, Liu16]. **effectively** [ABM+19]. **Effects** [ABA11, BS16, Bla15, CAO18, KSAK17, LLZ+12, MSRn+11, PETB18, AGOP18, ACF+11, Ali14, AEM+12, ALMY18, BHMN19, BH10a, BSO16, Chr10, CFGC11, DCD11, DPDR11, DWZZ15, DLLA10, EHKD11, EKD12, EEMSS14, EAV16, Fer11, GR11, GBS17, GWM11, GZF13, GR10, GRCATG19, HZW18, Ire12, IROW10, IK14, JA12, JHSG18, KI15, KRG+13, LDKB15, LGHL11, LDW+11, MNZPT19, MZLM17, MKHM11, MURR13, MPE11, NG11, NMHPVG12, Oni10, OGvSG18, OK19, PCR+11, PWP13, QHS11, RLTAT19, RP11b, RFN+12, RS12a, RSN12, RSM12, RdA11, Ril10, SH18a, SKTI15, SP19, TK16a, TV13, TFSRM11, TH12, Tob19, VFCSC17, VSMK13, WDR+11, WLC+17, XX12, XLGA12, XDM+10, YZW+15a, YMY+13, YT14, YFY17, ZH12, ZLS+18, ZBG+19, ZYL+13, ZBBB17, ZFC12, dCDC+11, dSMT+18, dSNBG08, SMK+12]. **Efficiency** [Cal10, AGOP18, ATPRV11, BDG17, Mai14, THSR13, VRO+12]. **Efficient** [BŁ16, KI15, SHW+13, SCBP17, YM14, ZWSF16, ZRLV10, CKB+19, FZH+18, FM16, IIS+17, LCK+16, OAA19, SKLC19, SGH10, SAHAA16, WTP+19, WZX15b, ZCX+16, ZKW17, dSM19a]. **EGEE** [LG10]. **Ehrenfest** [KUY16]. **eigenfunctions** [PMGMGR12, PBR18]. **eigenstates** [KB12]. **eigenvalue** [Mit11c]. **eigenvalues** [Mit11c]. **eigenvector** [LHX+19]. **eight** [SALK19]. **eight-vertex** [SALK19]. **Einstein** [DCD11]. **elastic** [Per10b, UV18b]. **Electric** [CB19, MJM19, SS12, BŁ16, CHL+19, CKB18, DB15, EBR11, GMR18, GV11, KA11, KT12b, LB19, MM19, PCD14, SMEH15, SMEH16, SM19, VRO+12, YŞÖ12, Zha17]. **electrical** [GKS10]. **electride** [OCL+18]. **electrides** [HWL16]. **electrocatalysis** [MLW16]. **electrocatalytic** [FFPD16]. **electrochemical** [AVG19b, NBZG16]. **electrochemistry** [FFPD16]. **electrode** [KJ15, Tug13]. **electrodes** [Che13]. **electrodynamics** [FNIT16, IFT14, Lin14, Liu15b, Liu16]. **electrolyte** [DLO16]. **electrolytes** [AVG19a, MNE+13, Pha19]. **electromagnetic** [Bae14, NTGC19]. **Electron** [Bas11, DZO12c, DJ18, DSVP15, LC16, LRMAA19, LZ10, MT11, PUH+11, PI16, RVNP12, RBVAG18, SLG11, VBC+12a, AA11, AOT+18, Ali14, AEM+12, AGG+18, ALRAE11, AM18, ARH+13, AST16, AT18, BLL+13, BHMN19, Ber13a, BL10, BL11, BSSS19, BKM15, Buc10, Buc11a, CMR13, ČW13a, CM15, CG12, CH17, CSMZ10, CSTA16, DLCB15, DAA16, DLJT14, DTEMK11, Dil13, DZO12a, DLLA10,

Dum12, DSSM18, ETGLMJ+19, FYhC11, Fin15, FA17, FMMD+10, GAPK+19b, GSaY11, GTR11, GS10, HSN18, JdL08, Jan10, Joh17, KWLS15, Kar12c, Kha16, KPL+17, Kit15, Kri13, KM19, Kuz19, Lar10, LCH14, LZZ+11, LWY13, LYL+12, LG12, Lu10, MGK+11, MR12, MW16, MJ16b, MPD+10, MPZWD10, MGB18, MJ11, MNS11, NA14, NCMC+18, NIK19, NBZG16, NAK+17, Nes11, Ng12, NDM+12, NE11, NRGS11, NMV+14].
electron [OAT+13, POLV12, PL11, Pir13, PNC19, RBGGM18, RNV+12, RCM10, RAGM10, RS13, RKCK19, SDS19, SDS20, SS10, SBMM11, SBM16, SYK+12, SPD+18, SSAM13, SHS+13, SM12, Sit15, SL13, ScBsR+10, SBKJ18, Sri18, SP19, Tob19, TC12, VF13a, VBC+12b, WLS+19, WWD+15, WH12, XZYS10, YNLD18, YM14, YRN+11, YHLC15, YD17, ZDZO10, ZFS+11, ZZZ+18, ZSZ14, ZJS13, dA12, dCDC+11]. **Electron-density** [RBVAG18]. **electron-group** [WH12]. **electron-muon** [RAGM10]. **electron-N** [SSAM13]. **Electron-pair** [LRMAA19, MT11, WH12]. **electron-proton** [DLCB15]. **electron-rich** [YNLD18]. **electron-withdrawing** [BSSS19]. **electronegativity** [CG12, GI11b, GI11c, GI11e, GI11f, Kan18, TSBSM12]. **Electronic** [AB16b, AC19, AGB19, AVG19b, BZBZ13, Ber13b, BVP14, BBYZ18, BBAL12, BG11b, BG11c, CZLD17, CJGTL12, DZO12b, DLLA10, FBO+11, FMCA11, GZF13, HHCA10, IA13, KK11b, KLZQ15, KP13, LVdSdM14, MLY+16, MFZ+18, MS14b, MKM11, NBL+14, NDM+12, Pup11a, RKM12, RZC13, SGC13, SBB16, TNT18, TSKN12, TSH17, VSN+11, VBO+15, XTLA13, XTLA14, YW11a, YH14a, AEKGZ12, AO12a, Ale13, ART08, AST16, BVCAP12, BPVDB11, BPL13, BS11, BL10, BW15, BBB16, BSV12, CWL+13, Cas15, CMCN11, CWW+16, CHSO13, COP16, DIOG12, DAR+11, DDÇY12, DD17, DWX+16, DG19, DCHC11, DHYC19, DHZS11, DSH+13, DB13b, Dun15, D'y16, ETGLMJ+19, Fin14b, FSK+11, GBS17, GAPK+19b, GSZ10, GWM11, GFB12b, GP13b, GMT16, GEL18, GJ18, GB13, GMM+18, GC19, HMI+15, HTM10, HIL19, HJ13, HWWW18, HhGqZZ17, IGMK11, IK18].
electronic [JL12a, KG17, KRK+17, KMF+11, KCK14, KJ15, KJ16a, KJ16b, KSD10, Kle11, KYLC19, KSY+11, KFY+12, KZZ13a, KHH10, KAOB11, KMM16, Kri13, KO12, KUY16, Lai11, Leh19c, LL11, lLBqD+19, LMZY15, LL19, LLZ+14, LBdV16, DVMC19, LHL+15, LZ10, Lya14, MSG16, MLC+11, MC11b, May14, MMWA11, MUNZVR12, MBA+13, MPZWD10, MGB18, Mil12, MS17, MKD19, MA11a, MA11b, MMRRA10, MJ11, MB13, MPT11, MPTZ13, MM13, MW15, MSRn+11, MCRS16, MC18b, NS19, NA12, NIT16, NZAVR10, OGvSG18, PE11, PCR+11, PAKA15, PMAP12, QJ13, QCB+10, RMLPGGGH16, RS12a, RMJ11, RRRV19, RNC+14, RMTG11, Rus14, RMY+13, SRPD16, SR12, SD13a, SB10a, SLC+18, SYL+18, SLS+14, SXS+12, SLS+12, SLSZ13, SIS+08, SRS+17, SSTÖ11, SR11b, SZZ+12, ScBsR+10, SSW16, SK12b, TYN13, TZ11, TV13, TD11, TBB+19, TFB11].
electronic [TRZ+19, TG13, UTTn13, Var14, VPA11, VLFG12, WWC17, WFS13, WDS19, WJL+10, YZL+10, YZL+11, YZW15b, YH14b, ZQCJ10, Zha10, ZLLS10, ZZR+12, ZCG+16, ZQXP17, Zho18, ZCP11, dSSF16b,

dSSF16a, Bou12b, Lad14]. **electrons** [BEM12, BMB10, BB10, BMB16, Dw13, Fer19, Ign11, Ign12, ISRK12, KK13, KK14a, KV19, Kry12c, Nas19, Nes10, QCB+10, RP11a, RPVM10, RS13, SALK19, She12, SS19b]. **electrons-Nd** [BB10]. **Electronuclear** [SL13]. **electrophilic** [Buc11b, YSA+11]. **Electrophilicity** [PC13, IG11]. **Electrostatic** [HL19, NMHPVG12, TH12, TCS10, AC19, CDSK12, DPRK12, IG11, KKS+11, KRG+13, PK13a, TYN13, ZCZ+12]. **electrostatics** [BWE16]. **element** [OVT+16, SHS+13]. **elementary** [EMED+12, EMEPD15, SOF+10, Zil14]. **elements** [AÖ12b, ČW13a, GI10, LXD13, NZ13, RRK16, SW10, TMC+13]. **eleven** [DCFD10]. **ELF** [Fin14a]. **eliciting** [TPT19]. **elimination** [BLM+12, FZC14, MM19, MLB+12, Zha10]. **elliptical** [MFLK11]. **elongated** [ALHC18]. **Elongation** [KdSM+10, XLGA12]. **else** [Kry10]. **Elso** [COP16, HS15]. **elucidating** [Kaw15]. **elucidation** [MMP+18b, SBKJ18]. **elusive** [SSP14]. **elymoclavine** [RGS+13]. **embedded** [BA13, Lan10, LC19, SMV11, SRN+19, JLL11]. **Embedding** [ABS11, DB13a, QB15, AB16a, GCK+17, HJK14, SRN+19, TGRP19]. **embeddings** [AF19b]. **emeraldine** [RMTG11]. **Emergence** [LFP+19]. **emergent** [SMMT13]. **Emerging** [AH19, GP13a]. **emission** [BS11, BSO11, CFP+10, LXW+14, ORJ18, PSK+13, dSdS13a]. **emissive** [ZKWZ17]. **emitter** [OAA19]. **emitting** [MUNZVR12, NZAVR10, SHW+13]. **empirical** [Hat13]. **Employing** [Tob19]. **enable** [LSKM19]. **enal** [HZZ+19]. **enantiomeric** [LW13]. **enantiomers** [MP12]. **enantioselective** [LCZL11, QCW+12, WTZ+11]. **enantioselectivity** [LCM+11]. **encapsulated** [CWL+13, JL12a, KG08, TPT+13, WW11, ZLWL16]. **Encapsulation** [RR11]. **endic** [ZPW16]. **Endo** [Jal10]. **Endohedral** [JW19, ACL12, BBYZ18, GAPK+19a, HLB19, JLL+18, LYW+19, MS17, SCTW10, WLZ+12a, WSL+11, YL11]. **endohedrally** [NW12]. **endohedrals** [YK11]. **ene** [IK14, Sat11b]. **Energetic** [GB13, GAMM10, HLB19, HM11, HZZW11, Kar15, LCCH10, LL17, MTS15, SRA+11, TCSD12]. **Energetics** [MNC12, ACMRN10, CdAFS+12, CdLdSC18, DCBB11, GCD13, KUTS10, PMMGL+11, Puz10, QTCL10, TBA13]. **Energies** [BBKO16, LBW11, SCZG12, ASHF13, AC12, Ali19a, ABA11, BVCAP12, Bla15, CFOC+10, CHH+19, DZO12c, DZO12a, EKN10, FLvLA15, FYhC11, FC19, GMA+19, GM11, GFRdG11, HNH+12, HIL19, HM10b, IKN13, Kin13, KKS+11, KB19, LDKB15, LORR+12, MMM19, Mas10, MS14c, NA14, Nal13, NVI10, OKR12, OK16, Pea11, PBB15, SH19, SR19, SOM10, SZL+14, Tsu15, VF13a, VLFG12, WWC17, WZW17, WR15, XX12, YÇÖ11, YWH+12c, ZZX10, ZCC11, ZZC12]. **Energy** [CC11b, FDA16, AV19, AG10b, AK17, AB18, AOLB12, AEM+12, ART08, AZD+11, AST16, ALK19, BXR+13, BPVDB11, BP13, BAP12, BSS16, BBL12, Ber13c, BVA+14, Bou12b, Bud12, CPF+11, CWW12, CNBPR+11, CDS+18, CCL+16, CFV18, CLH14, CSG14, COP16, DK13, DB11, DHZS11, EMK14, Fin16a, FMMD+10, GST11, Gra08, Gra11, HR19, Han19, HJRO13,

HFD11, HMH10b, HFdGC14, HM10b, HM11, HBMM11, ISN13, IK18, Jeo18, JZP17, KKH18, KyH13a, Kim16, KSN+10, KMNSP19, KMM16, KPH+12, Kri13, Kuz19, LFF+10, LSR10b, LV12, LWWZ13, LDZG16, LG12, LDADB+15, LVP12a, LSC+18, MZB+13, MGK+11, MDC15, MCP10, MHT+08, MA12, McC13a, MOE+11, MOLF11, MIN13, MAF19, MJSC18, MGD11, MPRCEG12, MLB+10, NA12, Ném14, Ng12, NDP10, NIT16, OPAVM18, OH19, PML+11, Per18, PMEP19, Pha19, PP14]. **energy** [RBGGM18, RPVM10, RGTS11, RCP14, RLER10, SAS+12, SIM14, SFC16, SGL+16, SCLCPB12, SA11a, SB16, SXH18, SLZ+11b, SRS+17, SK11, SGC13, SS19b, SSW16, STU19, SZ15, SZY17, SC18, TNN16, TSL11, Tou11b, VPA11, Vik11b, Vyb08, Wag14, WKE17, WWL17, WH18, fXxBhD19, XZZ+10, YH14b, YLC17, YLYC18, ZWL18, ZS12, ZRLV10, dHLdS12, dSSF16b, dSSF16a, Yu13]. **energy-based** [SK11]. **energy-dependent** [FMMD+10]. **energy-loss** [AEM+12]. **energy-relevant** [Wag14]. **Energy-surfaces** [FDA16]. **engineering** [RI19, WCL+17]. **enhance** [ZLWL16]. **Enhanced** [BGL+16, TZD+19, DSD18, LLZ+14, Mas14, MS14c, MPE11, SKV12, Sri19, TFSRM11, TSBSM12]. **Enhancement** [GV19, KKT13, KKT14, SJW13]. **enhancements** [ATPRV11]. **enhancing** [MZLM17, WLC+17]. **enol** [AZD+11, Coo12, GW18, MPGGS19, VF13b, Val17]. **enol-imine** [Coo12]. **enols** [MPGGS19]. **enones** [LMCZ11]. **enough** [MSS11]. **ensemble** [AM13a, Jou13, PP16]. **Entangled** [Xu16, EMEPD15, SK17b, Xu19]. **Entanglement** [Kar15, Tap15, BT15, BT17, SPM+15, XZJ+16, ZZ15, ZBK15]. **Enthalpies** [Mor12, dSNBG08, HZG12]. **Entropic** [DTPC17, LSS19, SMOD11, LRMAA19, MR18b]. **entropies** [HN12, OH19]. **Entropy** [AZD+11, DBTA19, Gra08, Gra11, JZZH17, NTCG18, PD11, PKK+16, PSGK17, Sit15, SDL+15, WSV10]. **envelope** [MMA10]. **envelopes** [BW15]. **environment** [AG10a, GC19, JCC10, TYN13, MPL+11]. **Environmental** [OK19, RdPW+12]. **environments** [AM10, Mar13, MVA19]. **Enzymatic** [SCB+14, BMB12]. **enzyme** [DPRK12, ZST+10, dSSdSGA12]. **enzymes** [AHC+18, WYWL13]. **EOM** [DVP18, TD19]. **EOM-CCSD** [TD19]. **EOMCC** [DSVP15]. **E'Ph** [WSML16, WSML16]. **epoxidation** [LMCZ11, ZLY+14]. **epoxide** [KMS+11, KUTS10]. **eQE** [GCK+17]. **equalization** [GI11a, GI11f]. **Equation** [FKBG19, UV18a, Agb12, ATPRV11, Bay19, BKM15, BR10, BR16, Cam10, CW11, CW13b, Cho16, GMGRMP12, HYZS12, HYZS19, KC16, Kha16, Kri13, MNZPT19, Nag16b, NF11, PGGRMP10, PVS11, PVS12, PGMGRM15, RZ17, RW12, RA10a, VATPR11, VAT12, WC14, Zak16, ZLJ11]. **equations** [CRA+11, DSCO+13, Per10b, ZLE17]. **equilateral** [RSN12]. **equilibration** [Nes11]. **equilibria** [Kim19]. **equilibrium** [KS18, LDW+11, Nal15, NB17, SXH18, TSH17, Zak16]. **equivalences** [ZWE12]. **Equivalent** [GSZ10]. **era** [IAK13]. **Ergodicity** [NE11]. **Erratum** [BR12a, BC16, BT17, BW13a, DJ12, FCS13a, Ign12, IKS10, Kar10, LSR+11,

CNSK11, CH17, CM12, CZLD17, CC19, CK17, CF14, CTDOLA10, CSTA16, CD12, DWJZ11, DCBB11, DKS11, DW12, DZ11a, DGR+16, DG19, DSZB18, DQZF12, ED16, FCS13a, FCS13b, FZX18, FO10, FDNR10, Fin17, FA17, FSB16, GFPAV19, GCK+17, GMR18, GM11, GGD12, GHCMCMQ17, GD11, GCZ+14, HMA+19, HR19, HHCA10, HLZ+14, HZZ+19, HMH10a, HMH10b, HKIH13, HYD11, HZZW11, IN15, JR12, JPP+11, JA12, JS17, JW18, KME+18, Kar13, KPCV18, KK14b, KKL+16, KSAK17, KYLC19, KSG+12, KJ14, Kri13, Kry12c, KG08, KMU+13, Lat13, LPO+12, LSR10b, Leh19a, Leh19b, LW11, LWL+12, LWX+14, LBY+14, LLW+11, LCK+16]. **functional** [LDZG16, LLZ+12, LSC+18, LNI12, MYZ+10, MLW+14, MJ16a, MLC+11, MFK+12, MA10, MW16, MUNZVR12, MG12, MKSG13, MLK17, MLB+12, MBBT+12, MM13, MKW11, MJM19, MCRS16, MOH+12, Nag15, Nag17, NH18, NDP10, NTNL10, NL11, NMIP14, NMSR14, NDM+12, NZAVR10, OD16, POLV12, PS10b, PS14, PI13, PMH+16, PABSK16, PP16, PTH11, PR10b, Pir13, PU14, PJP10, PMAP12, PI16, PC13, QHS11, RGPZD13, RS12b, RCM+19, RPVM10, RAMB18, Rud12, RSCS10, SB18, SA18, SGL+16, SVRGV12, SLC+18, SN12, SAHG11, SHL+13, SJZ+18, SIS+08, SDM12, SRMB15, Sri19, SK12b, SS13, TOSN12, Tan12, TIN13, Tan13, TDOD17, TFZ+15, TLC+17, UV18a, UMS13, VPGC12, Ven12, VUC13, Vik13, VBO+15, WKE17, WJL+11, WW11, WJY15, WDJ+17, WTZ+11, WR15, Wit18, XNL+14, XSLF12, XGH+18b, YLH+19, YWH12a, YWH12b]. **functional** [Yu13, YL11, ZT13, ZKKR11, ZQCJ10, ZLWY13, ZCX+16, ZBG+19, ZRR+11, ZMZ13, ZCG+16, ZSZ14, ZZ18, Zho18, dCSDdMC13]. **functionality** [ATS+11]. **Functionalization** [ZWWY10, JNY17, YLH+19]. **functionalized** [LRKM10, MSOV13, MLW16, OD16, Pli18, SPPT15, TDOD17, WLZ+12b, ZK12, ZBG+19]. **functionals** [AF16, Ali19b, AK11, DCDD10, DCFD10, Fin16a, HFdGC14, Jan13, Jou13, KDOR17, Lae14, LCT14, LSP+16, LORR+12, Lu15, MXC18, PSMD16, PRFR17, SFC16, SMOD11, SOF+10, SSP+17b, SGC13, SX15, TÁ10, TCA10, UV18b, VSL+15, YF16, YFY17, dSdS13a]. **Functions** [GLT13, IA13, KBF+13, ONK+13, CSMZ10, CML+16, FRGC10, GBK18, GBS17, GTR11, GN19, GS10, HITU16, HGB08, Hog13, Hor13, KH10, Kar13, MPV+11, MSNP18, MJ11, NS13, NDLC19, Oht13, OH19, PABSK16, RZSZ18, SPO+11, SZS+10, SLZ+11c, SLZ+11a, SKL10, VSL+15, WH12, YM14, vLRRK15]. **Fundamental** [Brä13, Hor13, IFT13, MSH13, Mar13, YK13, ZJS13, Blo15, CK13, GI11b, GI11c, GI11e, VVVB10, VV12, VV13]. **fungal** [VGS10]. **furoic** [GIO12]. **Further** [Jør18, ZLWL16]. **furylfulgide** [LZZ+17]. **furylfulgimide** [LZZ+17]. **fused** [RGTS11, WDS19, Yam11]. **future** [BJ17, MGN14, Sic16]. **fuzziness** [Tch16].

G [KK12b, CSVCB12, DE18, ZR13]. **G1** [PWP13]. **G3** [DCR10]. **G3B3** [LVP12a]. **G4MP2** [VF13a]. **Ga** [CWS15, JLL11, LXD13, MLW10, BXR+13, CCM08, GWJ12]. **Ga-like** [CCM08]. **GABA** [Ser11a]. **gain** [Luz11a]. **Gaining** [RNdA+10, vL13].

FNBK17, KPL+17, KSAK17, LPO+12, NHG+12, Ril10, ScBsR+10, Tri14]. **growing** [CD12]. **growth** [LVP12b]. **Grx3** [Dum12]. **Grx3-like** [Dum12]. **GTP** [MMT+13]. **guanidine** [LW13]. **guanidine-catalyzed** [LW13]. **Guanine** [SL10, BSV12, KMMS17, POLV12, YM12, ZRY+13]. **guess** [LCK+16]. **Guest** [DC14a, XXbX+13]. **guests** [NCMC+18]. **guide** [SLS+19]. **guided** [SRS+17]. **Guseinov** [Mam14]. **Gutzwiller** [YWH12a, YWH12b]. **GW** [RAMB18].

H [BDF+18, BGFD14, BJ17, BTH18, Buc12a, BSPK11, CRSB12, CS17, DMAB12, DPDR11, DZO11, DZO12b, DQZF12, EML+11, EMS16, FBRBR12, GWM11, GB13, GR10, GKGM18, HJRO13, JCCZ12, JLG+12, KWC10, Kal18, Kan11, KI12, KSSK16, KSST12, KRG+13, LZ12, LCL+10a, LJL+11, LZZ+11, LMZ+11, LBY+14, LZW+15, LCZ15, LXD13, LdAA+11, LEU+11, MLY+16, MC12, MMBK12, MPRB+10, MC18a, NBL12, NL11, NMIP14, NH11, OCL+18, PTS+11, Pan16, QSLY10, RLTAT19, RFEGPP+16, RGR12, ŞBAT16, Sat11b, SZZZ11, SCTW10, SZL+14, SZ15, SZY17, TBRIS12, TG13, VLK+11, WCY+10, WZW17, WLWL14, WWGW18, XLLZ10, XCL+18, XF19, YIY+13, YSK+12, YLYC18, ZGSM15, ZCG+17, ZWL18, ZHL+19, AC12, AST19, BN12, BDFM10, BPVDB11, BP13, BPG+10, BAP12, BEM11, BHV+11, Buc12a, CLXZ12, CP10, CC11b, Cor16, DLCB15, DSD18, Den13, DMS+10, DLM12]. **H** [DMBL16, FBM+10, GWM11, GZSMFN16, GMT16, GKT+12, GJ18, GD11, HV11, HSYM11, IKS08, IKS10, IROW10, JL12b, KWC10, KH12, KdPNNS16, KMF+11, KI12, KDA+11, KF17, LZ12, LZZ+11, LZFZ13, LWWZ13, LGW11, LKLW11, LCM+11, MMC+19, MKW11, MSAB19, NW12, NWQX11, OPC17, PWL+10, PL18b, RLW+13, RR11, RNB+10, Roy15, Roy16, RR19, SB18, SSB19, SD16a, SR19, SH18b, SVPTM+10, SMEH15, SMEH16, SSP14, SL13, SS11, SK10, STU19, SCTW10, Tan13, TBRIS10, TBRIS11, VVAO12, VPA11, Vik11a, Vik11b, VLFG12, WZC+12, XDM+10, XCL+18, YY18a, YS18, YZ10, YLC17, ZWL18, ZJC+13, GLT13]. **H-abstraction** [LGW11]. **H-atom** [KDA+11]. **h-BN** [GLT13]. **H-Bond** [LCM+11, SMEH16]. **H-bonded** [DLM12, DMBL16, IKS08, IKS10]. **H-bonding** [CLXZ12, DMS+10, KdPNNS16]. **H-bonds** [IROW10, SS11]. **H-passivated** [GMT16]. **H/D** [SK10]. **H2** [ZCG+17]. **H5N1** [KRH13, WZ10a]. **HAl** [Sat11a]. **HALA** [RRK16]. **Half** [KMS+11, AAAM12, AAA12, DZO12b, SMOD11, Pup11b]. **Half-a-century** [Pup11b]. **half-line** [SMOD11]. **half-metallicity** [AAAM12, AAA12]. **half-sandwich** [DZO12b]. **halide** [DZO12c, HNBG15, LGM+18, XZL+12]. **halide-exchange** [XZL+12]. **halides** [BMBD10, For12, LC16, MML+11a, RYM12, RKCK19]. **Hall** [Bra10]. **halo** [EMK14, LGP+11]. **halo-** [EMK14]. **haloalkane** [ZCZ+12]. **haloammonium** [XZL+12]. **Halogen** [DLP17, SC18, VVY18, BLL+13, Buc11b, CLXZ12, DPK18, DWZZ15, EMSB15, FGD+19, GLXL18, JLZ+17, KKC14, Kuz19, LJL+11, LLG+12, LDZG16, LZD+11, LLZ+12, MS14c, Sch13,

SMP10, SPIL14, SYY16, SCZH16, TL15, VVJ15, WTW+15, XZYS10, YZZ16, ZZL+11, ZLWZ16, ZYL+14, dOdCMUdALR11]. **halogen-bonded** [LJL+11]. **halogen-bonds** [JLZ+17]. **halogen-hydride** [BLL+13]. **halogen-oxygen** [dOdCMUdALR11]. **halogen-substituted** [CLXZ12]. **halogenabenzene** [WLZ18]. **halogenated** [GHS12, LLW+12, TL15]. **halogen**$\cdots$ [LDZG16]. **halomethanes** [HLJZ11]. **halonitrenes** [SYL+18]. **halopyridinium** [ZLWZ16]. **HAlS** [LPG+12]. **Hamiltonian** [Bra10, FYhC11, IM15, Kry12c, Mos14, SPSA11, SA11a, SKG11, TD11, TSvL+16, YYI+12]. **Hamiltonians** [Liu16, Cal10, CCBR+12, Liu14, Liu15b, MQA17, SR12, ZE18]. **Hammett** [DNCKCS+12]. **happens** [Tou11b]. **hardness** [Bar11, GI10, GI11a, GI11b, GI11c, GI11d, GI11e, GI11f, VO11]. **HArF** [GWZ+14b]. **harmful** [dSMT+18]. **harmful-gas-sensing** [dSMT+18]. **harmonic** [CB19, CML+16, DTPC17, DBTA19, MR18a, PVS12, PABSK16, YK13]. **harmonicity** [CTVA12]. **harmonics** [BAP12, Kit15, MFLK10, Nik11, RLER13b]. **Hartree** [AHT12, CC12, FA17, GST11, HZS14, Leh19a, Leh19b, Luz13, MdAdCS12, Mys12, NSN17, NNSN17, PI13, RBVAG18, SL13, SZ11, TTT13]. **HAu** [CS18]. **HAuF** [CS18]. **having** [BB10, KP10, RNV+12, SALK19, SN11]. **HB** [XZZ+10]. **HBeN** [LCL+10b]. **HBN** [LCL+11]. **HBNH** [BL12]. **HBr** [LGW11, SLS+11, WZHZ13]. **HC** [EAA17]. **HCCH** [BL11]. **HCF** [dOR10]. **HCl** [LGW11, SPIL14, YGL+11, EI11, MPRCEG12, SZS+10]. **HCN** [JLG+12, Tap15]. **HCN/CNH** [Tap15]. **HCNO** [MKW11]. **HCNS** [KZZ13a]. **HCO** [WB17, WZC+12, YL10]. **HCOOH** [XDM+10]. **HCu** [ALMY18]. **HD** [ZGSM15, GWZ+14a, GWHH17, Kan11, SZ15]. **HDCH** [SZY17]. **H**$\cdots$ [DB15, MNV+17]. **healing** [ES17]. **Heat** [MMP11, FUE+12, GVPCK10]. **Heats** [PP19b, ZZX10]. **heavier** [ALB18, YD17]. **heavy** [BMRM19, ND10, RRK16, RR19]. **HeH** [NWQX11, OPC17, Vik13]. **HeI** [DTVP+12]. **Heisenberg** [ATL+14]. **Heitler** [CC12]. **helical** [MCE11, NRI15]. **Helium** [Var11, AC11, CS13, HMP+11, Ign11, Ign12, KH10, KWWH18, KT12a, LLH15, OH19, Pop19, SXH18, YÇÖ11]. **Helium-fullerene** [Var11]. **helium-like** [KWWH18, YÇÖ11]. **helix** [PAD+10]. **Helmholz** [Koc13b]. **hemagglutinin** [KRH13]. **heme** [LVdSdM14, LdMCdA+12, SBSD18]. **hemerythrin** [TYN13]. **hemispherands** [SHE10]. **heptagon** [SCTW10]. **heptagon-containing** [SCTW10]. **herbicides** [CRB+12]. **Hermitean** [Brä12]. **heroin** [RCM10]. **Hess** [SN15]. **hetaryl** [MMW19]. **hetarylazo** [ÇAS13]. **heteroaromatic** [WWQG17]. **heteroatom** [GAPK+19a]. **heteroatom-centered** [GAPK+19a]. **heterocycles** [VOK+18]. **heterocycles-6** [VOK+18]. **heterocyclic** [ABTW14, CYL+19, CDL+19, GZ14, HZZ+19, LWJL10, LZD+11, LLLB13, MAN15, Pan16, WLL19]. **heterogeneous** [Lya19, MCRS16, PCV19, PIS18]. **heterojunction** [OKK10, WCL+17]. **heterojunctions** [IMS+13]. **heteroleptic** [SK12b]. **heterolytic** [GWM11]. **heteronuclear** [GI11b, GI11c, LYD+18].

[PTD+12, SLS+10, CSVCB12]. **homolytic** [KZA+17, OKR12, OK16]. **Homonuclear** [EMS16, KBGC12, NZ13, SZZ+19, SM14a]. **HONPAS** [QSX+15]. **HOO** [YL10, ZZW11]. **Hooke** [BPL13]. **Hookean** [LEU+11]. **hopping** [MMG15]. **horseradish** [ZST+10]. **HOSO** [STU19]. **host** [DC14a, MSS11, OCGM+19, XXbX+13, YBMK12]. **hot** [BW15]. **HOX** [LLG+12]. **Hras** [MMT+13]. **Hras-GDP** [MMT+13]. **Hras-GTP** [MMT+13]. **HRh** [DPDR11]. **HS** [dDGNB10, LZFZ13]. **HSAB** [ZXY13]. **HSAl** [LPG+12]. **HSH** [SKS10]. **Hsp90** [KTI+12]. **HT** [CSVCB12, CSSK+12]. **Hua** [FKBG19, HYZS19, KBG17, AAHN16, HRT12, HYZS12]. **hubbard** [LNI12, HFdGC14, WDJ+17]. **Hubbard-corrected** [HFdGC14]. **hubbard-like** [LNI12]. **Hückel** [Koc13b]. **Huge** [FBD+13]. **Hulburt** [Haj18]. **Hulthén** [Roy15]. **Human** [CSVCB12, WTH+11]. **humans** [KRH13]. **Hund** [KT12a, MHT+08]. **HX** [SPIL14, HNBG15, SPIL14, Vie17, Wu11]. **hybrid** [AV19, AF16, Ali19a, AK11, CF14, FCS13a, FCS13b, HZZW11, Kry12c, KSO19, LPO+12, MCK17, NMSR14, SB10b, SX15, TFSRM11, XCY15, YYI+12, YIY+13, Yu13, YF16, ZPR10, MPE15, SIS+08, YSK+12]. **Hybrid-density** [SIS+08]. **hybridization** [ABS11]. **hybrids** [MJM19]. **hydantoin** [ND11]. **hydratase** [MLW+14]. **hydratase-lyase** [MLW+14]. **hydrate** [XXbX+13]. **hydrated** [BMF+14, EPS+16, MNC12, SMEH16, SCS15]. **hydrates** [LB19]. **Hydration** [Ma14, Pat15, PBM10, RGR12, RBTL19, SL10]. **hydrazide** [DDÇY12]. **hydrazine** [SC12a]. **hydrazono** [KDÇ12, SC12b]. **hydride** [BLL+13, Ber13a, HMI+15, JL12b, Mar11, MHOG18, OA12, YYS15]. **hydrides** [AO12a, BDR12, CP13, EAA17, SH18a, SSA18]. **hydroacylation** [WML10]. **hydroaminations** [ZSS+13]. **hydroboration** [SLS+15]. **hydrocarbon** [MSY+12, WLS+19]. **hydrocarbons** [BRS10, Bla15, CA17, DI18, FC19, GMT18, GHS12, HIL19, LVP12b, RNV+12, SFM13, VRO+12]. **hydrochloric** [dLdOdAD12]. **hydrofluoropolyethers** [Vie17]. **Hydrogen** [AO12a, BLR12, BAP13, Cha10, CTDOLA10, GZ14, HS15, JLG+12, KK11a, MSVMCI10, MURR13, ND11, NBL12, OA12, PCMG12, SGKG12, SJZ+18, SKM11, WWGW18, YL10, dFR15a, dLRR11, AV19, AKHS13, BCGC12, BN12, Bay19, BL11, BWB+18, CdLdSC18, CDS+18, CNSK11, CCP18, CC11a, Coo12, COP16, DAC11, DAC12, Den13, DLG12, DLM12, DLP17, DB15, EKN10, EPS+16, FAFR12, FRNM12, FMCA11, FKC12, GI14, GIO12, GH11, GORW19, GZBH18, GZMC11, HNH+12, HL19, HNBG15, HYD11, IAA15, IK18, JN13, JCCZ12, JZZH17, Kar12c, KKG12, KS18, Kry10, LLF+12, LJW+11, LLG+12, LWX+14, MS14a, MdAdCS12, MK11, MK12, MNV+17, MCARL11, MTL+12, MT10, MFOH18, MFLK11, MMBK12, MS14c, MMM+12, MAPS18, MNS11, MR18b, NW12, NG11, NMIP14, NH11, NHB12, NRGS11, NRP+11, NRHJ11, NEEV15, OH12]. **hydrogen** [OH13, OHDA13, OA13, PM17, Pup11a, RZ17, RZSZ18, RJY+10, RJA+10, RYM12, RI19, Ril10, Riv11, RAFR18a, RAFR18b, RNE10, RB11b, SRPD16,

SS10, SMRK18, Sch10b, Sch13, SK17a, SM19, SMP10, Sic16, SSP14, SPIL14, SYS14, SS12, SCL19, SW12, SCZH16, SCBP17, TL15, UDVD10, Var14, VSMK13, WLS+19, WCGD12, WWHZ13, WZHZ13, WWLZ17, WJ11, WH18, XDM+10, YW11a, YWH12a, YWH12b, YRN+11, YWH+12c, ZAE10, ZZL+11, ZLZ+14, ZL10, dSCC12, dSSF16b, dSSF16a, dFR15b, dAVdM17, dOR10].
hydrogen-bond [OHDA13, SCL19]. **Hydrogen-bonded** [SGKG12, CdLdSC18, CCP18, KS18, LJW+11, MT10, OA13, RNE10, ZLZ+14, dSCC12]. **hydrogen-bonding** [DB15]. **hydrogen-like** [SS12]. **hydrogenase** [BGFD14, BAA+18, MG10, DMG10]. **hydrogenated** [IIW+11]. **hydrogenation** [TGA+11, VPGC12, XSLF12, ZZC15]. **hydrogenic** [DLRMFY10, DBTA19]. **hydrolysis** [CCL+10, DSZB18, KFS13, PRFR17, PMC11, RNdA+10, YTY19]. **Hydronium** [DE18]. **hydrophobic** [NHG+12, SMK+12]. **hydroquinone** [NP18]. **hydrosulfide** [HLJZ11]. **hydroxamates** [TPdMB12]. **hydroxamic** [KK11a]. **hydroxide** [DE18, RGR12, WZZL10]. **hydroxides** [DCDD10]. **hydroxy** [TAY11, YLW+13]. **hydroxyacetone** [SSdS17]. **hydroxyanthraquinone** [JB11]. **hydroxybenzaldehydes** [EKN10]. **hydroxybenzenes** [ATM17, KM12a]. **hydroxybenzylamine** [AFC+10]. **hydroxycarbene** [Buc12b]. **hydroxycarbonyls** [SSdS17]. **hydroxycinnamoyl** [MLW+14]. **hydroxycinnamoyl-CoA** [MLW+14]. **hydroxyfullerene** [KK11c]. **Hydroxyl** [TWHZ14, CGIAI12, FNBK17, KAR12a, LLP+13, LCM+11, Ril10, XNL+14, YM13, YY18a, ZZC12]. **hydroxyl-thiourea** [LCM+11]. **hydroxylapatite** [UV18a, UV18b]. **hydroxylated** [MDNDO+16]. **hydroxylations** [SSI+10]. **hydroxylbutyloxy** [RS11b]. **hydroxylbutyryl** [MFR10]. **hydroxymatairesinol** [SBEH11]. **hydroxymethyl** [KAOB11]. **hydroxyphenalenone** [OA13]. **hydroxypropanal** [SSdS17]. **hydroxyquinoline** [CHV14]. **Hylleraas** [OH19, PSGK17]. **Hyper** [LXW+12, DW12, FKL+12, KP11, Kha16, Mar12, XWCY11]. **hyper-netted-chain** [DW12]. **hyper-radial** [Kha16]. **hyperbolic** [AY15, GE12b, SDL+15, dAB17]. **hyperbolic-type** [AY15]. **hyperbolical** [WC14]. **hyperconjugative** [CSP+10]. **hyperfine** [Bou11, Bou12a, Kin13, Wit18]. **hypergeometric** [PMGMGR12]. **hyperpolarizabilities** [AK11, CEFMK12, NKF+13, OCL+18, YMY+13, dWLC14]. **hyperpolarizability** [BHMN19, FSB16, GXZ+14, Kar12b, Mar11, RVO+14, WWL+11]. **hyperspherical** [BAP12, PML+11, RPBB11]. **hypersurfaces** [PBM10]. **hypervirial** [ATPRV11, VATPR11, VAT12]. **hypochlorous** [TV13]. **hypoelectronic** [SALK19].

I-converting [dSSdSGA12]. **i-motifs** [KUS19]. **I.** [KK12b]. **IB** [DWX+16]. **ibuprofen** [XNL+14]. **ice** [Mil12, Wan13]. **ices** [LRP+11]. **ICN** [BMBD10, McC13a]. **iconicity** [Tch16]. **icosahedral**

SAHAA16, STL12, SM14c, Sri18, SN11, SJW13, SPM+15, TK16a, TNN16, TSL11, THVP14, UGWL18, UV18b, VPFD10, Var11, WZX11, Wit18]. **initio** [Wu11, WLWL14, YKM+15, YZL+11, Yu13, ZDZO10, ZZL+11, ZLZ+14, ZF15, ZXY13, ZZZ+18, ZRLV10, DAE+12, GWJ12, MPM15, SW12, Wag14]. **initio-based** [LV12]. **injection** [ZQJW13]. **inner** [BB10]. **inner-transition** [BB10]. **innovator** [SL11]. **inorganic** [BMRM19, BMF+14, BGJSM+18, KSO19, MCCGM+19, Swa13, YSA+11]. **inserted** [KRH13, LWL19]. **insertion** [DPDR11, RRVJ10, SMC18]. **Insight** [DMWY11, HFL+17, She12, She13, TFZ+15, WLL+13, BGMD15, DGR+16, EM17, KCDC15, MNV+17, MC17, MMSC19, RNdA+10, SAG13, SACA18, SC11, VHTEG15, YWJ+11, AF16, Tan13]. **Insights** [CP13, CADSG18, GJ18, HNBS18, MS14a, MC18b, SLA12, TFBG14, VBO+15, Bal16, BHA19, DJB10, LXW+14, LKZ+16, MNE+13, NP18, Pan16, SMGZF19, SR11a, ŚKB18, XZYS10, XLZ+19, YHLC15, dSM19a, dARAV12, KMS+11, QTCL10]. **instability** [Pat15]. **instanton** [Buc12a]. **insulator** [BEM11, Lar12, SAHG11]. **insulators** [YZZH15]. **Int** [BR16, COP16, HS15, Man16, dFR15a]. **integral** [HSN18, HFBC19, KSST12, LWY13, Mak15, RCGLV+14, SGC13, YK13, ZLR15]. **integrals** [AEÖ12, AA15, GTR11, GS10, Hog10, YM14, YŞÖ12]. **Integrated** [Cap16, HCH+18]. **integration** [BG11a]. **integrations** [Koc13a]. **intelligence** [Ezz10, SRS+17]. **intense** [DLCB15, SRPD16]. **intensities** [VVVB10]. **inter** [Tav11]. **inter-** [Tav11]. **interact** [NCMC+18]. **interacting** [Cap16, DM12, Dil13, KWWH18, Nes10, RP11a, RS13, SGL+16]. **Interaction** [ASHF13, DWPK14, EG10, JLS13, MYZ+10, MRT11, RNB+10, SPD+18, SK11, TBRIS10, ZT13, Ali19b, Bae14, BLL+13, Bas11, BEM11, Ber13b, CAZ+11, CCL+13, CGM12, CGG18, CRSB12, Cha10, CC11a, CYL+18, CP16, DC14a, DVDBM11, DTVP+12, DLG12, DWZZ15, ELC08, Eng16, EBH11, EAV16, FZX18, GWZ+14b, GD11, HFD11, HM10b, JFT13, JH15, JLG+12, KMM+18, KV19, KPH+12, LLG+12, LBdV16, Luz08, MMR+10, Mar12, MMC+19, NL11, NVI10, NFQ+11, OA12, PSK+16, PBR18, RYM12, RFN+12, RFMC19, RS11b, RRCO11, SSB19, SA18, SD13a, SD16b, SKHN13, SYL+18, Sha11b, SLZ+11c, SS11, SM14d, SWS12, SZL+14, SYY16, SCZH16, TK16b, TG16, VHTEG15, VVVB10, WLL11, WZW17, WWQG17, WG18, Win10, XXbX+13, ZST+10, ZCZ+12, ZS12, ZMB+17, TBRIS11, TBRIS12, YL10]. **Interactions** [KMMS17, MFK+12, dCDC+11, AGRI+12, BMR+13, BAP12, BMRM19, BLWJ17, BDG17, BLdV19, BWE16, Buc12b, CNBPR+11, CdLdSC18, CNSK11, CCS13, CKL16, Chu12, CSP+10, Cys11, DJB10, Dob14, DLP17, EAA17, EA12, EMS16, FNBK17, FRGC10, FKC12, HCH+18, HMA+19, HYD11, Jal10, JEA13, JLZ+17, KdPNNS16, KMK+16, KP12, KKG12, Kry12a, Kuv10, Kuz19, LMZ+11, LC16, LYW+19, LZZ+13, LDZG16, LB18, MZB+13, MHZ18, MS12, MIKH19, MSNP18, MPD+10, MPZWD10, MS10, MSY+12, MZLM17, MAW+18, MURR13, MMSC19, NH18, Nal13, NRI15, OA13, PML+11, PABSK16, PP16, Pie12, PETB18,

RK14, Ril10, Riv11, RGR12, SB18, Sch15, SSAM13, SM14b, SM14c, SS13, TH12, TDOD17, TCS10, Var11, VBC+12b, VSMK15, Yak11, YJ17, Yu13, YF16, YFY17, Zak13, ZRY+13, ZFS+11, ZLWZ16, dCSDdMC13].
interactions [dOdCMUdALR11]. **intercalated** [CWF11]. **intercalation** [KKS+11, MS10]. **intercalators** [Net12]. **interchain** [FNBK17]. **interconversion** [AZD+11, SAS+12, SSdS17]. **interdigitation** [MCKD11]. **interelectronic** [ALRA10, PWP13]. **interest** [Sko16]. **Interesting** [KBGC12]. **interface** [DLZ11, LLM13, RTG+19, SFNC+18, MRS15]. **interfaces** [NBZG16, OK19, SFL+10, TTM16, WML11]. **Interfacial** [IMS+13, LYS+19]. **interference** [YS13]. **interhalogens** [LWL19]. **interleukin** [WLL+13]. **interleukin-2** [WLL+13]. **Intermediate** [RMP+14, JL12b, MPRCEG12, Tal11]. **intermediates** [GGZZ16, KZZ13b, SMRK18, SBSD18, VGGPdL19]. **intermetallic** [AO12a]. **Intermolecular** [EAA17, LZZ+13, MZB+13, Pie12, Yu13, ZRY+13, BPG+10, Buc12b, EML+11, EA12, KP12, KMNSP19, MB15, OA13, OD12, PML+11, SPIL14, TNN16, Tav12]. **Internal** [MPC10, DDF+12, NH18, Sch15]. **International** [Ano13-49, NYA+13, Brä14, SG14]. **internuclear** [GI11b, GST11]. **Interplay** [MK11, Sch15, dCDC+11]. **interpolated** [ZRLV10]. **Interpolating** [MQA17]. **Interpolation** [RP16, DTVP+12]. **Interpretation** [CFP+10, Kar12c, Mor13, DHZS11, DSH+13, MHT+08, MAW+18, ZPM10]. **interpreted** [Nes11]. **Interpreting** [LB18, ZP16]. **intersection** [MSH13]. **intersections** [BMX+19, GSaY11, HV11]. **Interstellar** [TBRIS12, BN12, BRS10, CM17, LRP+11, RR11, TBRIS10, TBRIS11, XDM+10]. **Interstitial** [LLF+12]. **interstrand** [ZMZ13]. **intersubband** [BN11]. **intersystem** [LKd+16, MMG15, RMJ11]. **intra** [EML+11]. **Intramolecular** [BMR+13, RJY+10, RJA+10, AV19, Buc12b, CNBPR+11, COdF+11, CKL16, EKN10, FSBA12, HNH+12, JN13, JS17, KMM+18, KSAK17, KAOB11, Kry10, LXW+12, MK11, MK12, MB15, MSBF18, NRGS11, NRP+11, NRHJ11, Tav11, Tav12, UTTn13, YRN+11, ZZ18, dSM19a]. **Intriguing** [LB19, WSML16, ZLS+18, YHLC15]. **Intrinsic** [Lai11, MHO+15, NH18, GJ18]. **Introduction** [CCC11, KKL+12, LP10a, ÖS10a, ÖS12a, PBL12, Sch12b, SE11, Tch11, BC15, BC16, KCK14, KSAK17]. **Intuitive** [OS10b]. **Invariance** [Laz14, Kon10]. **invariants** [LZ10]. **Inverse** [CCA+12, Kar09, LXD13, WR14b, BMB12, BN11, CYK17, JW18, KM12c, PT13, WR14a, Kar10]. **Inversion** [MMM20, Cin20, DI18, MMM16, NKWT19, PM12, SH18a]. **inverted** [AAHN16, BW18, KMT+12]. **investigated** [CP16]. **Investigating** [BS14, MB15, CHSO13]. **Investigation** [EAV16, Gan14, HLB19, HWWW18, KG17, KLK13, KCK14, SM12, VO12, ASMP15, ATM17, AAA12, AZD+11, BXR+13, BAA+18, BWE16, Buc11a, CZJZ12, CHM+17, CNSK11, CC11a, DDÇY12, DMG10, DOE+14, DSVP15, Exn11, GWJ12, HDQ+13, HWHZ11, HCL13, JFT13, KB13, KSSK16, Kim19, LB14a, LOHB13, LRP+11, LPO+12, LL11, LDW+11, LXD13, LZZ+17, LMCZ11, LCZL11, LW15, MWH15,

Man16, MBSAG16b, PS13b, Tou13, VV13, VUC13, XTLA14, dSSF16a]. **level** [AOT+18, AST19, BLdV19, KK13, KdSM+10, LCL+10a, MAN15, NBI+10, PAD+10, PWH+12, RNE10, Shi13, SZL+14, WWHZ13]. **levels** [CDS+18, DK13, Kin13, MA12, SA11a, Tou11b]. **levodopa** [EAH13]. **Levy** [SGC13]. **Lewis** [EMSB15, GCZ+14, PP14, dSTH17]. **Li** [BCGC12, BL10, ČFČ11, HHL12a, HHL14, HWL16, MLW10, MPRB+10, OCL+18, RFEGPP+16, Sat11b, SM17, Sri19, XWCY11, YK11, YC13, BGL+16, CDSK12, DLZ11, GGD12, HMP+11, HYH+10, JMPP19, JCCZ12, KH12, LKJ13, LdAA+11, MT11, MJ14, SM16, TL15, UDS19a, VVAO12, WCY+10, XWCY11, YZ10, YLC17, ZLWL16, ZCG10, dOR10]. **Li-B-H** [VVAO12]. **Li-like** [ZCG10]. **LiBH** [WZM+13]. **library** [DSM+19b]. **Lieb** [SGC13]. **LiF** [YZ10]. **life** [BHH+13]. **lifetimes** [Ber13a, SCZG12]. **ligand** [BZBZ13, BLdV19, BPK19, CPF12, CSSK+12, DS11, DPDR11, DCdG10, GZMC11, Joh17, KKG12, MCE11, SLS+14, WLS+19, WTH+11, XWC11b, YZW+15a, ZLLS10, CSVCB12]. **ligands** [AC19, ASHF13, Con10, CADSG18, DPK18, DG19, DdG+11, LYW11, LXW+14, LGS+16, SHW+13, SM14b, YZL+11, ZKKR11, dCSDdMC13]. **ligated** [LKZ+16]. **light** [ALB18, BSS15, CSS16, DS11, MUNZVR12, MGB18, NZAVR10, WCL+17, dSCC12, dSdS13a]. **light-emitting** [NZAVR10]. **light-induced** [CSS16, DS11]. **lignan** [SBEH11]. **LiH** [YLC17, FBM+10, LWWZ13, RAN18, SPO+11, SCTW10]. **like** [BRBRS11, CEM14, CCM08, DTPC17, Dum12, GZ14, JL12a, JHL+18, KWWH18, KP11, LORR+12, LSKM19, LC12, LNI12, PGGRMP10, She13, SLS+19, SS12, SCZG12, VPGC12, VBC+12b, WCY+10, YÇÖ11, YW11b, ZCG10]. **limit** [CHH+19, KYS13, LV12, RPBB11]. **limits** [Coo12, Kry11b, RBD+10, RBTL19]. **LiMn** [KLK13]. **LiN** [Per10b]. **line** [Bib13, BR12b, IROW10, SMOD11, TY17]. **Linear** [D'y16, UYN+13, ABA11, BEM11, Boe12, Buc10, CKB18, EBH11, GRLA18, KJ16a, KJ16b, LWY19, LZZ19, MMWA11, MM19, MMF+13, NIK19, NMV+14, OPAVM18, PVS11, PL18a, PCD14, PBB15, QSX+15, RSN12, RCP14, WZ10b, Yam11, ZY13, ZLE17, dOdCMUdALR11]. **linear-response** [Yam11]. **linear/cyclic** [MMF+13]. **Linearity** [IKN13]. **linearized** [Liu15a]. **linearly** [YF16]. **lineshape** [LC19, SB10a]. **LiNH** [WLL11]. **LiNi** [Kim19]. **linkage** [MMSC19]. **linked** [Dum12, LYW11, NKF+13]. **linking** [PWH+12]. **Lipid** [Kuv10, KMT+12, MCKD11, SMK+12, SIT+12, YINM13]. **lipids** [FMP+17]. **Lippmann** [DJ12, DJ95]. **liquid** [AMMK11, CSTA16, KME+18, MMP+18a, MFK+12, MPV+11, OHDA13, Pha19, Riv11, SSKS12, TGRP19, WZZL10, ZSASS13, dSdSPG11, dOLdlV13]. **liquids** [AVG19b, AVG19a, HFL+17, RI19, RdA11]. **LiRb** [GFB12b]. **List** [Ano10a, Ano10b, Ano10c, Ano10d, Ano11d, Ano11e, Ano12p, Ano12q, Ano12r]. **lists** [TY17]. **lithium** [Ali19a, AVG19a, BCGC12, DLO16, EEMSS14, HFBC19, KLK13, Kim18, Kin13, MJ14, Per10b, SD16a, SKY+13, WWL+11, WLH+19, YC13, ZLZ+14]. **lithium-iodide** [MJ14]. **lithium-ion** [Ali19a, Kim18]. **lithium-orientation**

KJ16a, KJ16b, Kit14, Kit15, Kit17, KFS13, KFJ+18, Lan10, Lat13, SHS+13, YKM+15]. **Matrix-covariant** [Luz08]. **matter** [AF19b, DW12, Ng12, Tap15]. **Matthews** [BSS16]. **Matthews=** [MSBF18]. **Matthews=-Olson** [MSBF18]. **Mattsson** [MA10]. **MAu** [FTB11]. **Maximum** [EMEPD15, GGJD13]. **Maxwell** [CD15]. **May** [LW18]. **mazzite** [RDB19]. **MCCH** [DD17]. **MCI** [TIKN11]. **MCI-186** [TIKN11]. **MCSCF** [OD12]. **MD** [AHC+18, Eil14, MFB11, SLA12, YWY+12]. **MD/QC** [Eil14]. **MD/QC-simulated** [Eil14]. **MD/QM** [MFB11]. **Me** [ČFČ11, GWM11, HHL14, RBTL19, HHL12a]. **mean** [DCD11]. **mean-field** [DCD11]. **Meaning** [Gao11]. **means** [AGNS14, BL10, Ném14, OK16, RNdA+10, TH12, ZXY13]. **measurement** [Ezz10]. **measurements** [Bra19, KDA+11, ZPM10]. **measures** [Ale13, DTPC17, IOO18, Kan18, LS17, LSS19, Lat13, LRMAA19, Luz13, MR18b, SLG11, YOS15, ZYL+14]. **MeB** [ČFČ11]. **mechanical** [CPAT11, DKR10, DC14b, LV19, MMP+18b, MPD+10, MPL+11, Pan19, PP19a, RDM+11, SSA18, VPFD10, XS18, YZ12]. **mechanics** [BBB+12b, EAH13, IAK13, Ma14, MPE15, MSC10, Rup15a, Rup15b, SK17b, SIB+13, UV18b, Brä12]. **mechanics/molecular** [Ma14]. **Mechanism** [KBF+13, MCC13b, Pli18, SH18b, WML10, ZQW+17, ZL10, AG10a, Bal16, BCP10, BL11, BLWJ17, yBZfC18, CCL+10, CWS15, DS12, DP12, DZ11a, DSZB18, EAH13, EM17, FZX18, FDMR11, HWHZ11, HhGqZZ17, JSLH14, LGM+18, LJK+18, LLL16, LZW+18, lLBqD+19, LS19, LWJL10, LWC+10, LCM+11, LCS+11a, LCH+11, LCS+11b, LXLL11, LLLB13, MLW+14, MOSK10, MR11, MML+11a, MKW11, NE11, OH12, OH13, PL18b, PO15, RY12, RFMC19, SAS+12, SSI+10, SAG13, SKS10, SKS11, SDR+13, SDM12, SR18, SLS+15, SZL+15, SSdS17, TM13, TYL10, TXL10, VPGC12, VLK+11, VOK+18, WGLX10, WXZ+11, WHS+13, WWLZ17, WWX+11, WLD+10, XDM+10, XZCH11, YM12, YNLD18, YWJ+11, YZZH15, ZRGE+19, Zha10, ZZW11, ZCZ+12, ZBK15, ZBG+19, ZSS+13, ZCTG18, ZTC11, ZLY+14, ZPW16]. **Mechanisms** [CGIAI12, LLF17, LFTL18, PWL+10, XZG+18, AGNS14, CWZ+10, FTB11, HLJZ11, HZZ+19, HNBS18, HYZ13, JLS13, LNGW14, LD17, MXC18, MMP+18b, MLB+12, NKWT19, NZLG15, OD12, PTS+11, PRG+10, RFEGPP+16, SYK+12, SSK+12, SS18a, VHTEG15, WLWT12, YSS+10, ZPB12, ZMZ13, ZSHL16]. **Mechanistic** [Buc12b, GMT18, LTL18, LKZ+16, NP18, SGL19, WRW+18, dSM19a, AASU+17, AEAS+19, RNdA+10, VPOG19, dlLIAI+12]. **mechanochemical** [TJS17]. **mechanochemistry** [QBRA18]. **media** [CPL15, Ser11a]. **mediated** [Dau16, FDMR11, SGL19, WTP+19, ZL10]. **mediating** [Var14, ZYL+14]. **Medium** [TBRIS12, BRS10, BBB16, EAK+10b, EAK+10a, MPMCM+11, PBB15, Puz16, Ser11b, TV13, TBRIS10, TBRIS11, XDM+10]. **medium-sized** [Puz16]. **medium-to-large** [BBB16, PBB15]. **MEDT** [ZRGE+19]. **meeting** [Tch13]. **Meetings** [ÁIGVZW12]. **meets** [Puz17]. **melamine** [AASU+17]. **member** [RNV+12]. **membered** [ABTW14, BBKO16, MSK11, WvRSW+11, Zha14]. **membrane**

[Agb12, Ale13, Ali19a, ACL12, AT18, BMK+14, BdTG11, BCHN16, BRS10, BAX+19, BDG17, BBB16, BB10, Cam12, CM17, CPL15, CRSB12, CKB18, CB19, CK17, CF17, DIOG12, DK13, DSRGD12, Dil13, DCR10, EML+11, EMS16, GFB12a, GMR18, Gin10, GS11, GHP11, HRT12, HMH+13, HST13, HNBG15, HYH+10, HMA+18, Jen13, JMX+15, Jeo18, JZP17, JCCZ12, KBGC12, KBG17, KKL+16, Kim16, KKH+13, KKS+11, KKT13, KKT14, LKDC11, Leh19b, Leh19c, LHX+19, LSKM19, LPM+11, LLP17, Luz12, MSG16, MCE11, MK10a, Mar12, May14, MFLK10, MCL11, MGB18, MSM16, Mit11a, MB15, MJ11, MCK17, MPE11, Nal15, NS10b, OKK10, OA13, OD16, PL11, PWY+18, PKK14, PWP13, PB10, Puz16, Puz17, RBGGM18, RGTS11, RWW+19, RC11, Roy14, RAK10, SGB11, SD16b, SSKS12, SA11a, SKG11].
molecules [SMEH15, Sha18, SB16, SMR14, SRN+19, Sto18, SYY16, Sut12, SCZH16, SV11, THL+15, TK16b, TH12, TXK+19, TFMC19, Tou11a, UGWL18, VO11, XHZXXZ10, YZZ16, YD17, ZS11, ZDF13, ZP16, ZCC11, ZZZ+18, ZS12, ZI19, dSCC12, dSTH17]. **Møller**
[RS11a, BVA+14, NMIP14, RS09, TH13]. **molten** [BM10, DLZ11]. **moment**
[AM12, Ber13c, BVP14, HK11, KSG+12, Kri13, MdAdCS12, YŞÖ12].
moments
[AM10, Ber13a, DPRK12, GFB12b, GI11a, GI11c, LMC19, MD11, TW10].
Momentum
[SH19, ALRA10, Ash18, AKR12, HSN18, MOY13, TCG17, TÁ10, YOS15].
Moniliophthora [PTD+12]. **mono**
[Buc12b, DHYC19, Jac12, MMR+10, PS13a, ZQXP17, BL10]. **mono-**
[Buc12b, DHYC19, Jac12, MMR+10, PS13a]. **monoacetylides** [DD17].
monoamines [MBTVR12]. **monoanions** [CYL+19]. **monoatomic** [Bar11].
monoboronyl [MLK17]. **monobromide** [HTM10]. **Monochloride**
[MOY13]. **monoclinic** [DWX+16]. **monocyclic** [Du12]. **monodentate**
[ZKKR11]. **monofluorides** [KWC11]. **Monofunctional** [XZ11].
monofurazan [ZZX10]. **monohalogenated** [MNV+17]. **monoiodide**
[HTM10]. **Monolayer** [UDS19b]. **monolayers**
[KC19a, MDP12, RZC13, TTM16]. **monolithiated** [WWL+11]. **Monomer**
[Cas15, BHA19, JWG+12, MM13, BMR+13]. **monomeric** [Rua10].
monomers [MBA+13, UJSJ13]. **Monometallic** [ZW15, GZW16, ZCTG18].
monomolecular [MOSK10]. **mononitride** [DSH+13, HFD11, KLE+19].
monooxygenase [SSI+10]. **monophosphates** [PAD+10]. **monosulfur**
[WJ11]. **monovinyl** [dlLIAI+12]. **monoxide** [AKC10, Hog13]. **monoxides**
[TG13]. **Monte** [ÁFV12, ABG12, ANC+15, ASK15, Cal10, CKB+19, CCC19, CP16, HCH+18, Hog13, HB14, HM12, JCCZ12, PDR+14, PIS18, RCGLV+14, SGC13, SCBP17, Wag14, WCM14, ZLR15, ZCC11]. **montmorillonite**
[BJdlMAV12]. **MoO** [MFZ+18]. **moracin** [MGK+12]. **mordenite** [NL11].
Morita [ZQW+17]. **morphine** [RCM10]. **Morse**
[Agb12, PSGK17, Sta10, Tou11a, ZLJ11]. **MoS** [LZW+18]. **most** [GI10].
Mostar [ACT19]. **motif** [SLZ+12, YD17]. **motifs** [CJMC19, KUS19, Kry10].
motion

[GHGF12]. **oligomer** [KFS13, MM13]. **oligomeric** [TDOD17]. **oligomers** [CZLD17, SMA11]. **oligonucleotides** [ACF+11]. **oligopeptide** [MM10]. **oligopyrroles** [DCBB11]. **oligosilane** [ZYZ+11]. **oligothiophene** [TZ11]. **Olof** [Pyy11]. **Olson** [BSS16, MSBF18]. **OMC** [WCY+10]. **On-site** [DLJT14]. **on-the-fly** [UTTn13]. **One** [Ber13a, CG12, Dum12, LCH14, Bud12, CAZ+11, CM15, CLY12, CYK17, FCS13a, FCS13b, GTR11, GI11e, GAMM10, GS10, HZS14, Kri13, LW15, Luz11a, MSC10, MBBT+12, PVS12, RZSZ18, SC12b, SZZ+19, SWS+14, TAY11, VBC+12a, VBC+12b, WWC17, WLZ+12b, YF16, ZZZ+18, TC12]. **One-** [CG12, WLZ+12b]. **one-center** [HZS14]. **one-dimensional** [CYK17, MSC10, RZSZ18, VBC+12a, VBC+12b]. **One-electron** [Ber13a, Dum12, LCH14, CM15, GTR11, GS10, Kri13]. **one-mode** [PVS12]. **one-parameter** [FCS13a, FCS13b, YF16]. **one-photon** [Bud12]. **one-pot** [LW15]. **one-to-one** [WWC17]. **One-two** [TC12]. **ones** [HMA+19, LW13]. **Onicescu** [OH19]. **ONIOM** [EFO11, EO11, KYH+13b, MTL+12, ŚKB18]. **ONO** [XX12]. **onset** [LB14a]. **onto** [CA17, CAO18, SFW12, SRS+17, Sta10]. **OO** [SBSD18, SSK+12]. **OOH** [NP18, PGG12]. **OPAL** [CwCW+11]. **Open** [CP16, DSM+19b, Gan14, GCK+17, GHP11, HNH+12, JEA13, JE10, MAT19, NSN17, NNSN17, QSX+15, RAMB18, Sha18, YMY+13, dGR14, GXZ+14]. **open-close** [HNH+12]. **Open-shell** [CP16, JEA13, NSN17, NNSN17, YMY+13, dGR14, GXZ+14]. **open-source** [DSM+19b, GCK+17, QSX+15, RAMB18]. **Opening** [TFBG14, AMMB+18, BAX+19, KMS+11, MBSMJC18, QB15, TXK+19]. **openings** [KUTS10]. **OpenMP** [WMK+19]. **Operator** [DJ95, CD18, DJ12, IM15, Mys12, Yos20]. **OPh** [DPDR11]. **Oppenheimer** [BPL13, GVPCK10, RSM12, RAN18, SK17a, Sut12, VVN+16]. **opportunities** [FAK19]. **OPPS** [ZPM10]. **opsin** [TU10]. **optic** [Zen11]. **Optical** [LRKM10, YBMK12, AMK10, ABA11, BF11, BSM+15, BSO16, CPL15, CZLD17, DWX+16, FSQ+11, FZX18, FBU+11, GAPK+19b, GDM+10, GKGM18, GRCATG19, Hat13, HWL16, HWWW18, HSS18, IGMK11, JdOS16, JFDD10, KC11, KPL+17, KL11, KMU+13, LYW11, LZW+15, LYL+12, MPC10, MNP19, Mas14, MPJ12, MFZ+18, MA11a, MMF+13, NKF+13, NMHPVG12, OGvSG18, RKM12, RRRV19, ŞBAT16, SSKS12, SLS+14, SM17, SYQ+10, WLZ+12a, YK11, YLWrL12, YHLC15, ZSQ+10]. **optics** [DSRGD12, LKDC11]. **Optimal** [FT15, GSPR19, NVI10, NB19, TCG17, YWR+18]. **optimally** [NTGC19, ZZ18]. **Optimization** [CL08, FCC11, HJ13, KYH+13b, Kub12, Lu15, MHT+08, SGH10, SPM+15, WWL17]. **optimizations** [YIY+13]. **optimized** [ANC+15, KPH+12, SXH18]. **Optoelectronic** [AFA13, JR19, BHAH+18, KA13, MANP17, OAA19]. **orbit** [Ash18, Ber13b, BDR12, CYL+18, KV19, LWL+12, MLK17, MC18b, RS12a]. **Orbital** [BT15, Kon10, MMM20, AOT+18, AK17, Ash18, ABA11, Bar11, CPF+11, Cin20, DVDBM11, Fin17, FA17, FMPM+14, FC19, GR10, Hog10,

AFM$^+$10, AMK10, AMAM18, ABA11, BŁ16, BHAH$^+$18, BSM$^+$15, BGKK16, Bon17, Bou12b, BH10b, Cap16, COdF$^+$11, CGM12, CdLdSC18, CWB$^+$13, CWW$^+$16, CZLD17, CKB18, CB19, CSMZ10, Cor16, CADSG18, CHV14, DKS11, DCFD10, DAE$^+$12, DWX$^+$16, DHYC19, DWGX12, FZX18, FZC14, FPRGMHGB12, FBU$^+$11, GAPK$^+$19b, GLF$^+$12, GWZ$^+$14a, GMT16, GMR18, GB13, GKGM18, GRCATG19, GMM$^+$18, HWL16, HWWW18, IGMK11, JA12, Jac12, JL12a, JWG$^+$12, JR19, Jou13, JFDD10, KBGC12, KA13, KV19, KRK$^+$17, KMF$^+$11, KCK14, KJ15, KSSK16, KPL$^+$17, KL11, KYLC19, KSY$^+$11, KP12, KLZQ15, KMU$^+$13, KK11d, KM19, Kuz19, LRKM10, Laz14, LZ12, LVdSdM14, LCH14, LZB10, LJW$^+$11, LXW$^+$14, LZW$^+$15, LC16, LL19, LZZ$^+$13, LLZ$^+$14, LZZ$^+$17, DVMC19, LHL$^+$15].

properties
[MLY$^+$16, MMP$^+$18a, MCCGM$^+$19, MBKH19, MSG16, MZB$^+$13, MLC$^+$11, MANP17, MNP19, MPTR12, MPMCM$^+$11, MFZ$^+$18, MG12, Mil12, MS17, MHHPR$^+$17, MA11a, MA11b, MLDP10, MBA$^+$19, MMF$^+$13, MW15, MSRn$^+$11, MC18b, NBL$^+$14, NBI$^+$10, NMHPVG12, NB19, NDM$^+$12, OAA19, OGvSG18, OCB$^+$10, OK19, OMĐ13a, Pan19, PP19a, PK13a, PCD14, PFdM13, Pit12, Pog12, PAKA15, PMAP12, PSK$^+$13, QHS11, QJ13, QCB$^+$10, RMLPGGGH16, RRRV19, RGTS11, RZC13, RC11, RSCS10, RBLZ15, SD13a, SMOD11, SSKS12, SLS$^+$14, SB16, SXS$^+$12, SLS$^+$12, SLSZ13, SR13, SSTÖ11, SBB16, SM14b, SM14d, SM17, SRN$^+$19, SYQ$^+$10, TIKN11, TZ11, Tas14, TD11, TBRIS10, TBRIS11, TFMC19, THVP14, TFB11, TRZ$^+$19, TCG13, TPdMB12, UTTn13, VOAH18, VMC11, VRO$^+$12, VBO$^+$15, WGLX10, WXB$^+$11, WLZ$^+$12a, WLZ$^+$12b, Wan13, WDS19, Wu11, XLZ$^+$19].

properties
[YK11, Yam11, YZL$^+$10, YZL$^+$11, YLWrL12, YZW$^+$15a, YBMK12, YZW15b, ZZX10, ZLLS10, ZZR$^+$12, ZQJW13, ZKWZ17, ZSQ$^+$10, ZL12, ZCG$^+$16, ZS12, ZCP11, dSdSPG11, dSMT$^+$18, dOLdlV13, vL13, vLRRK15].

properties/activities [MPMCM$^+$11]. **property**
[BXR$^+$13, CWL$^+$13, CJSNLM11, FSQ$^+$11, GI11e, GMP$^+$11, MY17, MCL11, MMP11, Nic11, Pea11, RGST12, ZYZ$^+$11]. **property-specific** [Nic11]. **proportions** [Lu15]. **proposed** [TCA10]. **propyl** [CMCN11]. **propylene** [LS19, WML10]. **protease** [VHTEG15, dAGNJT12]. **proteases** [SKS10]. **protected** [MC18b]. **Protection** [CAPGAIG18, BSS15, GAI19]. **Protein** [PT13, AGRI$^+$12, CR18, CHSO13, CSVCB12, DFF$^+$13, GSR12, HXDY16, KFY$^+$12, KKG12, LLZaH14, MYZ$^+$10, MRT11, MRS15, MSK$^+$12, Pop15, TYN13, TCM$^+$12, TBHL11, YSW11, ZPM10, ZWLC12, ZTC11, dA12, TBST10]. **protein-coupled** [CSVCB12]. **Protein-nucleic** [TBST10].

proteins
[LDKB15, LKd$^+$16, NTCK13, QZH13, RP16, RAK10, Sch10b, TCS10, YSG10].

protic [HFL$^+$17]. **ProtNA** [TBST10]. **ProtNA-ASA** [TBST10]. **protochlorophylide** [SR11a]. **protocol** [BDF$^+$18, CwCW$^+$11, SCBP17]. **protocols** [COCF$^+$14]. **Proton** [SCS15, DLCB15, DLM12, DSZB18, FDMR11, IKS08, IKS10, KAOB11, Kry11b, Kry12b, LZZ12, LYL$^+$12,

[AHC+18, AMMK11, DMG10, Exn11, GFRdG11, MOLF11, MG10, SD16a, SD16b, ST15, SLA12, TIKN11, UYN+13, VHTEG15, ZKW17, dAGNJT12]. **QM/MM-ER** [TIKN11]. **QM/MM/MD** [AHC+18]. **QM/polarizable** [Cap16]. **QM/QTAIM** [BTH18]. **QMMM** [HCH+18]. **QR** [BB10, Bou12b]. **QR-SCMEH-MO** [BB10]. **QSAR** [KKM+12, MPMCM+11, PH12, XFW+14, ZFW+13]. **QSPR** [CD18, MPMCM+11, SN12, TFA10]. **QSPR/QSAR** [MPMCM+11]. **QSTR** [PI13]. **QTAIM** [BTH18, DP16, MAW+18, NH18, Sha11a, VHTEG15, XXJ+16, XWP+18, YXM+18, ZLZ+14]. **quadratic** [FYhC11, OPAVM18, RSN12]. **quadratically** [ISRK12]. **quadratric** [ZST+10]. **quadricyclane** [TTD13]. **quadrilateral** [LZZ19]. **quadruple** [MPT11, NZ13]. **Quadrupole** [MdAdCS12, AC11, BJ12]. **quality** [OKR12]. **Quantal** [SIB+13, SHKS15]. **Quantification** [SP19, Gru17, ORJ18, Rus14]. **Quantifying** [Mar12, MML11b]. **Quantitative** [CJSNLM11, HSN+11, Zha17, MY17, MBTVR12]. **quantities** [FSST16]. **quantization** [HKLW13, Kle11, SD13b]. **quantized** [Tou11b]. **Quantum** [Bal16, BSS16, BL10, BR16, Bra19, Brä13, CJBMMAPR19, Cav13, CKL16, Cho16, Cho19, COP16, DKZ+10, DLCB15, DFK16, DLM+11, DC14b, EAK+10b, EML+11, EMEPD15, Ezz10, FMKJ14, For17b, GbZA10, GGZZ16, HGB08, HS15, Hog13, HB14, Hop15, IFT13, IAK13, IOO18, IK14, Jen13, JXX+15, KWC10, KYS13, KMK+16, KYH+13b, KUTS10, LB14a, LZZ12, Luz11b, Mak15, Man16, MMP+18b, MNE+13, MBTVR12, NTCK13, Nic14, OWD18, ÖEDB11, PH12, PWY+18, PETB18, PKK+16, PSGK17, Puz17, Qu13, RGTS11, Rit11, RMP+14, SAG13, Shi13, SR13, SG14, ŚKB18, SBKJ18, SZY17, SSB+12b, Tap15, TFSRM11, UJSJ13, VVN+16, VBJK18, Wag14, WDSL14, WYWL13, WZX+15a, WWX+11, WCM14, WLD+10, XS18, XZJ+16, Xu16, YM12, YW11b, YZ12, YB11, ZCC11, ZJS13, dFR15a, dFR15b, dSMT+18, ASMP15, ABG12]. **quantum** [ANC+15, ASK15, BF11, Ban12, BAX+19, Blo15, BGL+16, BHH+13, BT15, BT17, BM16, BBB+12b, Bra10, Brä12, Buc12a, BN11, CD18, CKB+19, CM16, CSK12, CSG14, CW13b, Cho15, CYK17, Coo12, CPAT11, CN12, Dau16, DPK18, DSL15, DPRK12, Dil13, DMBL16, DSFT17, EAH13, FLCHL10, FBO+11, FNIT16, FSST16, Gag11, Gan14, GWZ+14a, GRCGRRHT19, GB10, GS11, GR10, HR13, HS11a, HITU16, HS11c, HEVMSA+19, HM12, Hor13, HMA+18, IFT14, Ish14, JN13, JHSG18, JMX+15, Kap12, KB12, KCDC15, KC18, Kar09, Kar10, Kha16, KCC13, Kit14, Kit15, Kle11, KN15, KK11d, LS17, LSS19, LV19, LSR+13, LCZL15, LHX+19, Lin14, Liu15b, Liu16, LSKM19, LEU+11, Luz11a, Ma14, MC11a, MR12, Mam14, MDC15, MPE15, Mar13, MSC10, MMŁ+16, MPD+10, MQG13, MPL+11, MBBT+12]. **quantum** [Mor13, MLDP10, MB12, MGP16, NC11, NKKN15, NS10b, NGS11, NBZG16, Ném14, Nic11, NVPCJ+13, NMSR14, NRP+11, NJA+12, Nym14, OPS10, OK19, OM13b, OSJ+12, PABSK16, PTH11, PMGMGR12, PMHM19, Pup11b, RP11a, RP11b, RL12, Rei15, RDM+11, RNE10, RNB+10, Rup15a, Rup15b,

SDS19, SDS20, SOF+10, SBEH11, SKHN13, SC12a, SPSA11, SN15, SK17b, SKLC19, SD13b, Sha18, She13, SIB+13, SHKS15, SKM11, SSA18, SGC13, Sjö15, SS19b, SFY12, SRA+11, STU19, SZ15, SCBP17, SPM+15, Tch13, TBB+19, TK16b, TH12, TXK+19, TFA10, Tri14, TB15, UTTn13, UV18b, VPFD10, VMR11, VVVB10, Vik11a, VOK+18, VO12, WYM15, WR14b, YNLD18, YÇÖ11, YZ13, YW11a, YS13, YH14a, YW16, YLC17, YLYC18, ZS11, ZX12, ZGSM15, ZH15, ZWSF16, ZZC12, ZWE12, ZRLV10, dHLdS12].
quantum
[dSTH17, vLRRK15, AGNS14, BMRM19, DMS+10, GP13a, SP19, ZBK15].
Quantum-chemical [DLM+11, ÖEDB11, Qu13, BF11, DMBL16, DSFT17, MGP16, Ném14, NVPCJ+13, SN15, VOK+18, YNLD18, DMS+10].
Quantum-chemical-aided [GbZA10]. **Quantum-classical**
[Cho16, Cho19, Mak15, SPSA11]. **Quantum-matter** [Tap15].
quantum-mechanical [LV19, VPFD10]. **quantum/classical** [CP11].
Quantumness [CD15]. **quartet** [HK11, SCZG12, ZCG10]. **Quartic**
[VBC+12b, FT15, dAB17]. **quartz** [LLM13]. **Quasi**
[XLLZ10, YZ10, BDPT12, Hog13, KUY16, MPM15]. **Quasi-classical**
[XLLZ10, YZ10]. **quasi-degenerate** [BDPT12]. **quasi-diabatic** [KUY16].
quasi-exact [Hog13]. **quasi-stable** [MPM15]. **quasiparticle** [MS12]. **qubit**
[MR12]. **quenching** [SAHG11, SAHA12]. **quest** [GI11d, GI11e, GI11f, LL18].
questions [Ng12, VATPR11]. **quinacridone** [Gao12]. **quinoline**
[MLPT10, MAN15]. **quinoline-derived** [MAN15]. **quinolinecarbonitriles**
[ZFW+13]. **Quinone** [XWP+18, KSAK17]. **Quinone-based** [XWP+18].
quintuple [SZS+10, SLZ+11c]. **quotient** [Tra19].

R [DPDR11, DQZF12, GWM11, NBL12, Pan16, CPL15, ESS13, GWM11, LL17, PCR+11, ZSHL14]. **R-** [PCR+11]. **racemase** [LZZ12]. **radial**
[IG11, Kha16, RZ17, SPO+11, vLRRK15]. **radiation** [TK16a]. **radiative**
[Ber13a, CCM08, SCZG12]. **radical**
[BLL+13, BAMA12, BRS10, BCS+12, CWZ+10, GAI19, GK12, HWHZ11, IUMVB10, JB11, JAB12, KAR12a, KZA+17, KI12, KZZ13b, LCG12, Les12, LLP+13, LSG+14, LVP12b, MMMM12, OKR12, dMOB12, PM17, RCM+19, SSI+10, SK14, SS18a, SPSA11, Sch12a, SB16, SLZ+11b, SLZ+11c, SLS+12, SKM11, SWS+14, WLWL14, XNL+14, YM12, YY18a, YSS+10, Zha14, Zha15, ZBK15, ZLWZ16, ZJC+13]. **Radicals**
[TWHZ14, lAyL14, Buc12b, CGIAI12, DI11, DFK16, HXX15, KK14a, KDA+11, LCL+11, LVP12b, MXC18, NP18, RLW+13, RMG+19, SZL+15, TIN13, TCA10, Wit18, YM13, YL10]. **radii** [GI10, SV11, TMC+13]. **radius**
[Bar11]. **Radu** [Tou13]. **rain** [PL18b]. **Ramachandran** [MAW+18]. **Raman**
[CK13, VV13, ÇAS13, KV11, LMZY15, PM12, TFSRM11, TSBSM12, VPFD10, VVS+18, VV12, YJ17]. **Ramos** [COP16]. **Randić** [AD17, DZ11b].
random [HFBC19, PR10a, Per18, Pog12, SSB12a]. **randomly** [GB10].
Range [BPG+10, AM10, Dun15, GW13, Haj18, IKN13, KAR12a, MJ16b, MIN13, MC18a, RR19, SSK11, SKY+13, ZZ18]. **range-determining**

MFB11, Rit12a, Rit12b, SCB+14, SK10, TKSK17, XGH18a]. **shifted** [AAHN16, Kry10, Roy14]. **shifting** [dOR10]. **shifts** [CRSB12, CFGC11, FBD+13, RR19, Tap15]. **SHN** [NRP+11, SS11]. **short** [Dum12, GST11, NWQX11, RMC19, SB16, WWL+11, XCD18]. **short-living** [SB16]. **short-loop** [Dum12]. **shortcomings** [MGN14]. **should** [She13]. **showing** [DSD18]. **shuttle** [Ali19a, FDMR11]. **SHX** [EMSB15]. **Si** [GLF+12, JL12a, MGD11, TW10, TFB11, UKF+11, VPFD10, XCL+18, ZHL+19, CN12, ENV15, Esr18, GKGM18, LKN13, LBY+14, LW18, LLLB13, MCP10, MBA+13, MSVMCI10, OD16, PWL+10, WLWL14, ZCX+16]. **Si-** [ZCX+16]. **Si-doped** [ENV15]. **SiC** [LXLL11, TCCI10]. **SiCH** [FT15]. **SiCNT** [SD16a]. **side** [DSCO+13, MPE11, NHG+12]. **side-chain** [DSCO+13]. **sieve** [SACA18]. **SiF** [KMM16, KMM16, SLS+12]. **SiGe** [LLLB13]. **Sigma** [DAC11, FC19]. **sigma/pi** [FC19]. **signal** [GSPR19, QZH13]. **signature** [GDM+10]. **signatures** [BR08, BR12a, RB08, RB11a, SCL19, ZR13]. **signed** [SK17b, SKLC19]. **Significance** [Chu12, ELC08, Kut10]. **SiH** [HCL13, RLW+13]. **sila** [FC19]. **silapolycyclic** [TYL10]. **silica** [CRSB12, SFNC+18]. **silicate** [Ped16]. **silicene** [WLH+19]. **silico** [DAA16, ST15]. **Silicon** [Cza18, GKGM18, AMK10, CSK12, DHYC19, JLS13, KAG08, KMM16, LRKM10, LHL+15, MSK11, NEEV15, RK14, RKM12, XCL+18, dSMT+18]. **silsesquioxanes** [TDOD17]. **Silva** [COP16, HS15]. **silver** [AMK10, Boe12, BPK19, RFMC19, SS18b, YJ17]. **silver-ligand** [BPK19]. **silylene** [LCH+11, LXLL11]. **SIMD** [WMK+19]. **similar** [Pup11a]. **similarities** [BB16, MK10a]. **similarity** [ART08, Luz11b, MBTVR12, MBBT+12, Sat11b]. **Simple** [QBRA18, BM16, DCR10, Fin15, FB17, KV11, Lev10, LPM+11, MA12, MT10, SAS+12, SGL+16, SGKG12, STM18, SLS+19, Szc18, TLC+17, TC12, VSL+15, YZZ16, ZT13, ZDF13]. **Simplification** [CFOC+10]. **Simplified** [GZF14, GZSMFN16]. **simulant** [HYZ13]. **simulate** [SKLC19, SKV12]. **Simulated** [TCG17, VVS+18, AM13a, Eil14, JPP+11, MOE+11, VVN+16]. **Simulating** [DMBJ15, GMA+19, MRS15]. **Simulation** [LPM+11, CwCW+11, CSK12, CS17, CTDOLA10, DKZ+10, DGR+16, DLZ11, FFF10, Fra17, FNIT16, GW18, Hog13, IFT13, IFT14, Kim19, KSST12, LCT14, LL17, Mas14, MPD+10, MPZWD10, MG12, NKKN15, Net12, NDM+12, PP10, PMH+16, SLS+10, Tan13, UTTn13, YAF+15, YT14, YINM13, ZWSF16]. **Simulations** [Hor13, MSH13, Mar13, OHDA13, SIB+13, SHS+13, UYN+13, UTTn13, YK13, ÁFV12, AF19b, ATS15, BMF+14, BM10, CLKD15, CKYR18, GVPCK10, GSR12, GSPR19, HFBC19, IKC18, Kit15, KKH+13, KFS13, LFS+11, MGN14, MM10, MMT+13, MBS+18, PDR+14, Pha19, PIS18, PPK+13, QSX+15, RP16, RNC+14, SHKS15, SBL11, TGRP19, TSH17, TPdMB12, UV18a, ZWLC12, Zha17]. **sinc** [KRC+16]. **sine** [dAB17]. **Single** [Esr18, Sri18, Bar11, Bas11, DI10, DCZ17, ETGLMJ+19, EM19, Fra17, HNBG15, KG08, LZZ+11, DVMC19, MR12, MSOV13, RLZ12, SD13a, SD16a, SVPTM+10, SWS+14, TKS11, TC10, XGH18a, YW16]. **Single-**

ZWLC12, ZLE17, ZSZ14, ZQXP17, ZI19, dARAV12]. **Spectral** [LLH15, Mys12, CdLdSC18, FBU+11, KP12, KM19, LYR+17, SMGZ13, XLZ+19]. **spectral-luminescent** [KP12]. **Spectral/structural** [LLH15]. **spectrometry** [ABKJ18]. **Spectroscopic** [BH10b, Jac12, Mag14, NC11, NVPCJ+13, SZS+10, SLZ+11c, SLZ+11a, SLS+11, SXS+12, SLS+12, WFS13, BD12, CHM+14, CWB+13, CJOOW11, DAE+12, GFB12a, KSSK16, LJSS12, LZZ+17, MG12, MPTZ13, QHS11, RNdA+10, Sch10b, SYL+18, SLSZ13, SWS12, Tas14, VLG12, VLFG12, VBO+15, WXB+11, YZL+10, YZL+11, ZLLS10, ZR13, dSdSPG11]. **Spectroscopical** [MSBF18]. **Spectroscopies** [KKT13, MOY13, McC13a, OA13]. **spectroscopy** [Ber13a, BDR12, BWB+18, For17b, GFB12b, LdBF+12, Mas10, MML11b, ORJ18, Ped16, Puz17, SA11b, UTTn13, YJ17, ZPZ15, RdA11]. **spectrum** [AA11, BS16, BDF+18, BBB+12b, Bou12b, CWF11, CRSB12, DSD18, DHZS11, DWGX12, HHCA10, HRT12, HMH+13, HYH+10, JCC10, KBG17, NDM+12, QD10, RS12a, SBKJ18, WWC17, Zha17]. **Speculation** [KRH13]. **spent** [HB14]. **spermine** [SGB11]. **Spherical** [Kit15, PML+11, Roy15, CH17, CB19, CN12, GAPK+19b, Nik11, OHDA13, RLER13b, RAFR18a, RAFR18b, Roy16]. **Spherical-harmonics** [Kit15]. **spherically** [JZZH17, Nag16b]. **spheroconal** [MFLK10]. **spheroidal** [OPC17]. **Spin** [BDR12, DCdG10, JR12, Kle11, Luz11a, MLK17, NKWT19, SAHG11, SAHA12, Swa13, YYI+12, ATL+14, Ash18, Ber13b, Bla15, Bra10, CR18, CCP18, CYL+18, CFGC11, CSP+10, CDT12, DS11, DM16, FSST16, GXZ+14, GLXL18, GFRdG11, Joh17, Kap12, KK14a, KV19, KSN+10, KYH+13b, LVdSdM14, LWL+12, LB19, Luz12, MR12, MPRB+10, Mos14, MC18b, NSN17, NNSN17, OS10b, PBR18, Pon19, Qu13, RS12a, RLZ12, SR12, SRASZ16, SSP+17b, SBD+16, TÁ10, TD11, WH12, Yos20, Yur13, Yur15, ZSQ+10]. **spin-dependent** [DM16, NSN17, NNSN17]. **Spin-free** [Kle11, Luz11a, Luz12]. **spin-Hamiltonian** [TD11]. **Spin-inversion** [NKWT19]. **Spin-orbit** [MLK17, Ash18, CYL+18, KV19, MC18b, RS12a]. **spin-projection** [KYH+13b]. **spin-restricted** [KYH+13b]. **spin-spin** [CCP18, CFGC11]. **spinless** [NF11]. **spiro** [LLLB13]. **spiro-heterocyclic** [LLLB13]. **spiroborate** [QCW+12, WTZ+11]. **spiroiminodihydantoin** [SM13]. **spline** [HZS14]. **split** [GRD11, WLS+19]. **split-graph** [GRD11]. **splitting** [GWM11, HYH+10, SYK+12, SSK+12, Tan13, WTP+19, YYI+12]. **Spontaneous** [CCM08]. **spread** [BEM12]. **square** [LGHL11]. **squaric** [DLM+11]. **squeezed** [PSGK17]. **SR** [MC18b, MPD+15, MGP16, Oni10]. **Sr-doped** [Oni10]. **SrBi** [HLMO11]. **Src** [ZFW+13]. **SrH** [HMI+15]. **SrTiO** [OH13, WCL+17, OH12]. **SS** [SZZ+12]. **SSH** [DTFK15]. **stabilities** [AF16, MS17, SFW12, SUL+11, SM14c, ZYL+13, dAVdM17]. **Stability** [GV11, KZA+17, Kry11b, LWL19, MC12, PMEP19, TLC+17, USL+13, BMX+19, Boe12, CCC19, CYL+19, CWSZ13, DVC14, FBRBR12, GJ18, GB13, GAMM10, GWJ12, HLB19, Ire12, KK11b, Kry12b, LGHL11, LCZ15, LGS+16,

structure-stability [DVC14]. **structured** [Kim18]. **Structures** [CdAFS+12, GLT13, GCD13, IA13, JL12a, KBF+13, LFP+19, LHL+15, MS17, ONK+13, SM16, YWH+12c, ACMRN10, ALK18, ALK19, BMB10, Brä11a, BSO16, DWGX12, DM16, GR11, GLF+12, GZ14, GWJ12, HWL16, HWWW18, HM10a, JMPP19, Kim13, KSSK16, KYLC19, KMM16, Lad14, LL11, LWL+12, MZB+13, MK10a, MLW10, MUNZVR12, MUPC10, MJSC18, MM13, NH18, NZAVR10, OCGM+19, Puz16, QJ13, SSK+12, SLS+14, SIS+08, SACA18, SZZZ11, SKY+13, SCZG12, TSKN12, TYN13, TBB+19, VSN+11, WGLX10, WDS19, WJL+10, XTLA13, XTLA14, XWC10, XF19, YYI+13, YZL+10, YZL+11, YZW+15a, YC13, ZLLS10, ZZR+12, ZL12, ZQXP17, dHLdS12]. **Structuring** [KRG+13]. **studied** [AMMK11, BL10, CK17, DCHC11, FBO+11, SJZ+18, TTM16, ZL10, dSdS13b]. **Studies** [PCF+18, Roy13, ACF+11, AMK10, AVG19b, BD12, Buc11b, CJBMMAPR19, CCA+12, ÇAS13, CYLL11, CTW12, CWB+13, CSVCB12, CSSK+12, DSWL11, DSZB18, DB15, EAK+10b, EAK+10a, EI11, For12, GGD12, GKT+12, GZBH18, HTM10, HNBG15, Hop15, HWL16, JL12b, KDÇ12, KMM+18, KA13, KSY+11, KAOB11, Les12, LWL+12, LSR+13, LBY+14, LGZC15, LWJL10, LKLW11, MANP17, MLPT10, MAP+10, MMM+12, MSAB19, NTCK13, ONBP11, ÖEDB11, PBM10, PTD+12, PETB18, PAPCMM+16, RJY+10, RJA+10, RGTS11, RNdA+10, Ril10, Riv11, RGS+13, RGR12, Roy14, SMK+12, SD16a, SC12a, SJZL12, SIS+08, SK12b, SZ15, SSB+12b, TIKN11, TOSN12, TYN13, TAY11, Tan12, TIN13, TXL10, THSR13, UJSJ13, VGGPdL19, VPOG19, WZX11, WTH+11, Wan13, WZM+13, WYWL13, WLH+19, WHM14, Wit18, WWGW18, XS18, XFW+14, YZL+10, YZW+15a, YB11, ZZL+11, ZZX10, ZYZ+11, ZQJW13, ZLWY13, ZLZ+14]. **studies** [ZWL18, ZSZ14, dAGNJT12, YWY+12]. **Study** [Bar11, BWB+18, CH17, CYL+18, IFT13, IFT14, SGL+16, SS19b, ZCP11, AC19, AFC+10, lAyL14, AM12, AASU+17, AEAS+19, ATM17, AKC10, ASW13, AVG19a, ASD14, AMAC12, AG19, BMK+14, BD14, BF11, BCGC12, BDF+16, BDF+18, Bas11, BAMA12, BLB+18, BLR12, BS11, BEM11, BZBZ13, Ber13a, BL11, BLRdA+10, BHAH+18, BS14, BSSS19, BZZ15, yBZfC18, BXZ+19, BDG17, BLdV19, BMF13, Bon17, BGJSM+18, BDR12, BCF+11, BPSM12, BLM+12, BJ17, BJdlMAV12, BTH18, Buc10, BO11, BVRM10, BCS+12, BB16, BSV12, BSPK11, CRB+12, CMR13, CAZ+11, CLXZ12, CCL+13, Cao17, CPL15, CPF12, CCBR+12, CHM+14, CHH+19, CG12, CW16, CM12, CCL+10, Che12, CCS13, CWW+16, CZLD17, CLY12, CS13, CWS15, CZCW19, CK13, CFGC11, CGIAI12, CAPL12, CPAT11, CJOOW11, CD12, CS18, DWJZ11, DCBB11, DIOG12]. **study** [DMAB12, DAR+11, DSD18, DKS11, DPK18, DS12, DCDD10, DSRGD12, DPRK12, DPDR11, DTEMK11, DZ11a, DLO16, DG19, DMS+10, DCdG10, DDF+12, DdG+11, DQZF12, DWGX12, DSH+13, DCR10, DSFT17, DFF+13, EG10, ESDO16, ELC08, EAH13, EFO11, EO11, ETGLMJ+19, EBH11, EA12, ENV15, ES17, Esr18, EM19, ESBVJY12, FSQ+11, FZX18, FFF10, FO10, FM16, FTB11, FRNM12, FDNR10, Fin14a, FT15, FPRGMHGB12, FBU+11,

Gag11, GBS17, GWM11, Gao12, GLF+12, GGJD13, GZW16, GHGF12, GK12, GLXL18, GIO12, GFB12b, GC18, GP13b, GMT16, GMT18, GS11, GLOGM+11, GHCMCMQ17, GB18, GWME18, GD11, GSB10, GT13, GTSC+19, GGP13, GLPA10, GCZ+14, HNH+12, HMA+19, HK11, HDC+11, HLJZ11, HLZ+14, HZZ+19, HFD11, HHL12a, HHL14, HM12, HM10a, HKLW13, HZZW11, HFL+17, HHL+12b, HhGqZZ17, IIW+11, Iku17, IGMK11]. **study**
[IM15, JPPA10, JN13, Jal10, Jan10, JB18, JS17, JCCZ12, JSLH14, JLZ+17, JB11, JWG+12, JFDD10, KM12a, KS11, KWC10, KWC11, KP11, KBF+13, KKM+12, KI15, KI12, KK14b, KSAK17, KZZ13a, KZZ13b, KUTS10, KKT13, KKT14, KG08, KO12, KMU+13, KK11d, KBMM10, Lan10, LLF+12, LGM+18, LLM13, LKOS17, LJK+18, LVdSdM14, LPOP12, LZB10, LCL+11, LJL+11, LW11, LJW+11, LYW11, LGP+11, LMZ+11, LGP+12, LLP+13, LWX+14, LLL16, LYR+17, LLF17, LD17, LZW+18, LTL18, LFTL18, LLW+11, LLC+11, LGW11, LCZ15, LL19, LCCH10, LLZZ10, LCCH11, LJSS12, LXW+12, LWZ+14, LL17, LLW+12, Lu10, LWC+10, LCS+11a, LCH+11, LCS+11b, LXLL11, LLLB13, LW13, DVMC19, LKZ+16, MYZ+10, MLW+14, Ma14, MY17, MAD12, MBKH19, MSG16, MZB+13, MFB11, MK10b, MK12, MLC+11, MCP10, MMR+10, MCC12, MVG18, MP12, MTL+12, MSC10, MMW19, MOY13, MMWA11, MMC+19, MUNZVR12]. **study** [MUPC10, MDNDO+16, Men10, MFZ+18, MCL11, MKSG13, MS17, MHHPR+17, MM11, MSK+12, MPL+11, MGD11, MTS15, MPRCEG12, MMRRA10, MML+11a, MLB+12, MBBT+12, Mor11, MM13, MG10, MMF+13, MSRn+11, MSOV13, MCRS16, MOH+12, ND11, NS10a, NHG+12, NDH10, NBL12, NAK+17, NTNL10, NL11, NFQ+11, NHB12, NRGS11, NRS+11, NRP+11, NRHJ11, NJA+12, NIT16, NZAVR10, NEEV15, OAC17, OPC17, OAA19, OH12, OH13, OCB+10, OPP+14, OMÐ13a, OM13b, OD12, OD16, POLV12, PS13a, PEA+12, PTS+11, PWP+18, PDNC14, PMH+16, PE11, PWL+10, PSKV19, PK13b, PKK14, PRG+10, PAD+10, PRPU+13, PM17, Puz10, QHS11, QCW+12, Qu13, RYM12, RFN+12, RGPZD13, RRVJ10, RS12b, RSN12, RSM12, RCM+19, RD14, RRRV19, RGST12, RDB19, RYW+15, RI19, RCM10, RJLPGH+13, RDM+11, RBVAG18, RNE10, RNB+10]. **study**
[RS11b, RRB12, SF13, SB18, SSB19, SIT+12, SK14, SD16b, SBEH11, SSK11, SVRGV12, SB10a, SKHN13, Sat11b, Sch12a, SK17b, Ser11a, Ser11b, SLS+14, SKS11, SHL+13, SLSZ13, SHE10, Shi13, Shi18, SL10, SKM11, SM13, SR13, SSTÖ11, SLA12, SK11, SR18, SSA18, SSP+17b, ŚKB18, SMA11, SZ11, SBB16, SZZZ11, SZZ+12, SLZH12, SHW+13, Sri18, SMGZ13, SK10, STU19, SYQ+10, SWS12, SWS+14, SZL+14, SZL+15, SGL19, SYY16, SCZH16, SS13, TK16a, TV13, Tav11, Tav12, TM13, TT10, TDOD17, TU10, TYL10, TSL11, TFZ+15, TJS17, TFA10, TSH17, TFB11, TCCI10, TGA+11, Tug13, TWR15, TPT+13, TPT19, UKF+11, UMS13, VF13b, VPGC12, VFCSC17, Var11, VHTEG15, VVN+16, VLM+10, Ven12, VSMK13, VSMK15, VV12, VV13, Vie17, Vik13, VKF+19, VDG13, VS19, VO11]. **study**

LXW+14, LGZC15, LD17, LLC+11, LWJL10]. **Theoretical** [LDW+11, LXW+12, LWZ+14, LZZ+17, LLW+12, LWH+12, Lu10, LWC+10, LMCZ11, LCZL11, LCS+11a, LCH+11, LCS+11b, LXLL11, LW13, LYD+18, MLW10, MWH15, Mas10, MOY13, MDNDO+16, Men10, MAP+10, MMCNV19, MSK11, MJ14, MMV+19, MHHPR+17, MGD11, MBBT+12, Mor11, NYA+13, NL11, NMIP14, NFD+10, NFQ+11, NH11, NHB12, NIT16, OT14, ONK+13, PEA+12, PWP+18, Pan16, PMEP19, PSKV19, PKK14, PMC11, RFN+12, RMLPGGGH16, RI19, RCM10, Riv11, RGS+13, SK12a, SRASZ16, SLS+14, SLSZ13, SSA18, SZZZ11, SLZH12, SM14d, SK12b, SK10, SLS+15, SZL+15, SCZH16, TYN13, TWHZ14, TM13, TYL10, TXL10, TSH17, TFB11, TGA+11, TPT+13, TPT19, UKF+11, VF13b, WXB+11, WLL11, WLG+11, WTH+11, WLZ+12b, WHS+13, WHY+14, WTW+15, WWQG17, WHM14, WZZL10, WLL19, WJ11, WSL+11, WWGW18, XGH18a, XZL+12, XWC11b, XXbX+13, XCY15, XLZ+19, YZ13, YZL+10, YJ17, YHLC15, YC13]. **Theoretical** [Zha10, ZZX10, ZLLS10, ZYZ+11, ZZR+12, ZSHL14, Zha14, ZQW+17, ZYSW17, ZSQ+10, ZFS+11, ZL12, ZSS+13, ZTC11, dSdSPG11, dARAV12, dOdONM12, AZD+11, ASD14, AG19, BLL+13, BLB+18, BLRdA+10, BG13, yBZfC18, BPSM12, Buc10, CZJZ12, Cao17, CHH+19, CG12, CYLL11, Che12, CLH14, CZCW19, CGIAI12, CPAT11, DDÇY12, DPRK12, DTEMK11, DZ11a, DQZF12, DC12, EI11, EMED+12, ENV15, FMP+17, Fri12, GLF+12, GHGF12, GLXL18, GT13, GGP13, HYZ13, HSS18, Iku17, Jal10, Jia15, KO14, Kim16, KC19b, KO12, LS17, Lan10, LRP+11, LL11, LS19, LCZ15, LMC19, LLZZ10, LXD13, LW15, LdAA+11, MNP19, MCP10, MMR+10, MPTR12, MLPT10, MUPC10, MEF+15, MEEA+13, MSRn+11, MSOV13, MMSC19, ND11, NHG+12, NBL12, Ném14, NRGS11, NRS+11, OKR12, OAA19, OH12, OH13, OMÐ13a, ORJ18, POLV12, PM17, Puz10, RGR12, SF13]. **theoretical** [SA18, SFL+10, SSK11, SC12b, SKS11, SSTÖ11, SACA18, SRA+11, SYQ+10, Tch16, TK16b, VATPR11, VFCSC17, VLM+10, VSMK13, VKF+19, VO11, WGLX10, Wan11, WLZ+12a, WZM+13, WWB+14, XF19, YM12, YZZH15, YLW+13, ZAE10, ZWWY10, ZR13, ZKWZ17, ZPB12, ZW15, ZLWZ16, ZMB+17, dLRR11, dOR10, dOdCMUdALR11, DJB10, DC10, HHL14, LEU+11, Sit15]. **theoretical/computational** [Ném14]. **theoretically** [Jeo18, VMC11]. **theories** [Cam10, JNZ+14, Li15, Luz08, ZT13]. **Theory** [Ano13-49, BHA19, Buc12b, DCZ17, HKLW13, ISN13, IKN13, Koc13b, Kri13, Kut13, LMZY15, MIN13, NS13, SSI+10, SSK+12, SIS+08, SKY+13, TKN13, TH13, YSS+10, YKN13, YH14b, AC19, ABM+19, AM13b, AGPDZ13, BVP13, BAX+19, BGBV12, BLKB11, BJdlMAV12, Cam12, CCL+13, Car19, CEFMK12, Cha11, CH17, CM12, CZLD17, CC19, CK17, CF14, CTDOLA10, CSTA16, DWJZ11, DCBB11, DKS11, DLRMFY10, DB11, DMWY11, DGR+16, DG19, DCHC11, DSZB18, FZX18, Fin17, FA17, FMMD+10, Fri12, FSST16, GFPAV19, GCK+17, GM11, GEL18, GS11, GCZ+14, HMA+19, HR19, HLZ+14, HZZ+19, HMH10a, HMH10b, HKIH13, HYD11, HMA+18, IN15, IROW10, JR12, JPP+11, JHSG18, JMX+15, JW18, KAR12a, KCDC15,

KC18, Kar13, KKL+16, KSAK17, Kit14, KM12c, KYLC19, KdSM+10, KJ14, KMU+13, KFJ+18, KLE+19, Lar12, Lat13]. **theory** [LPO+12, LCL+10b, LW11, LWL+12, LPG+12, LBY+14, LHX+19, LLW+11, Lin14, LDZG16, LLZ+12, Lya14, LKd+16, MYZ+10, MLW+14, MJ16a, Mam14, MLC+11, MFK+12, Mas14, MW16, MLK17, MLB+12, MBBT+12, Mor13, MJM19, MCRS16, Mur12, Nag15, Nag17, NSN17, NNSN17, Nal13, NS10b, NAK+17, NTNL10, NL11, NMIP14, OK16, OD16, PS10b, PS14, PK13a, PABSK16, PP16, Pat15, PTH11, PR10b, PBB15, PU14, PM16, PJP10, PMAP12, PI16, PC13, QBRA18, RGPZD13, RCM+19, RB18, RMG+19, RMC19, RAMB18, RS09, RS11a, Rud12, SVRGV12, SLC+18, SN15, SN12, Sha18, SZS+10, SLZ+11c, SLS+11, SHL+13, SJZ+18, SM12, Sto18, SK12b, SD13c, SS13, TFBG14, TIN13, Tan13, TTD13, TH12, TDOD17, TG16, TXK+19, TLC+17, UV18a, VPGC12, Var11, VUC13, VBO+15, WKE17, WJL+11, WW11, WJY15, WB17, WDJ+17, WTZ+11]. **theory** [Wit18, XNL+14, XGH+18b, YKM+15, YLH+19, YWH12a, YWH12b, ZS11, ZQCJ10, ZLWY13, ZCX+16, ZBG+19, ZMZ13, ZSZ14, ZZ18, Zho18, dCSDdMC13, dSTH17, BM10, SP19]. **theory-based** [KSAK17, WJY15]. **there** [GI11f, SMR14, TKSK17]. **Thermal** [CEV10, FBM+10, NG11, AFM+10, AMMB+18, Chu12, Liu15a, MVC13, MCC12, Mar13, MOSK10, MML+11a, MB13, PP19b, RRRV19, YZ13]. **thermalization** [Nes11]. **thermalized** [PFdM13]. **thermally** [GMM+18]. **Thermochemical** [Kim19, Rus14]. **Thermochemistry** [ABTW14, ŞBAT16, AK11, BYAT13, ÇT14, HZG12, Rus14, WZX15b]. **Thermodynamic** [JAB12, VOAH18, XNL+14, COCF+14, DWGX12, Kim13, LZZ+13, OSJ+12, Pan19, PP19a, RMLPGGGH16, Tav11, TSH17, dOLdlV13]. **Thermodynamical** [Nag17]. **Thermodynamics** [MLW16, PK16, BvWG14, Bra19, DP11, PD11, PRFR17, RTG+19, WSCL11]. **thermoelectric** [KG17]. **thermostats** [GVPCK10]. **these** [MMM19, Ril10]. **THF** [HHL12a, HHL14, AG10b, RTT10]. **thiadiazole** [VMC11]. **thiazol** [DDÇY12, SC12a, SC12b]. **thiazolidine** [MBBT+12]. **thiazoximic** [LBM11]. **thieno** [ZWZK19]. **thieno-expanded** [ZWZK19]. **thienyl** [WDS19]. **thietane** [HL19]. **thiirane** [HL19, LCS+11b]. **thin** [ATS15, JK12]. **thio** [LKOS17, SF13]. **thioamides** [RMP+14]. **thioaminoacrolein** [NRP+11]. **thiocarbonyl** [BH10a, PJP08, dCSDdMC13]. **Thiocyanate** [LGS+16]. **Thiocyanate-free** [LGS+16]. **thioethers** [HL19]. **Thioflavin** [BBM17]. **thioguanine** [SS18a]. **thioketones** [MMW19]. **thiol** [JS17, KV11, OD16]. **thiol-functionalized** [OD16]. **thiolate** [MC18b, OPF11, ZZC15]. **thiolate-protected** [MC18b]. **thiols** [KV11]. **thione** [JS17, KKG12]. **thionucleobases** [CL18]. **thiophene** [BSSS19, CZLD17, MSG16, WDS19, YWR+18]. **thiophene-vinyl-thiophene** [BSSS19]. **thiophenols** [dSNBG08]. **thiosemicarbazone** [LWH+12]. **thiourea** [LCM+11]. **third** [KWC11, MMF+13, NKF+13, RS09, RS11a, WLZ+12a]. **third-order** [MMF+13, NKF+13, WLZ+12a]. **third-row** [KWC11]. **Thoughts**

[EMSB15]. **triatomic** [BCHN16, SA11a]. **triazides** [CWS15]. **triazine** [CLH14, MJ11, TJS17]. **triazol** [CLY12]. **triazole** [LLW+11, THSR13]. **triazolin** [IK14]. **tricarbon** [ZJC+13]. **tricarbonyl** [YZW+15a]. **trichelates** [LOHB13]. **trichloroacetyl** [SKS11]. **tricks** [SCB+14]. **tricyclic** [ZWZK19]. **tridiagonal** [HFZ12]. **tridiagonalization** [ZHF12]. **triel** [CDL+19]. **trifluoride** [DWGX12, For12, LQ13]. **trifluoroacetylacetone** [NRGS11]. **trifluoroethylene** [OCB+10]. **trifluoromethylphenyl** [SAHAA16]. **trifluromethyl** [DPRK12]. **trifluromethyl-phenyl** [DPRK12]. **trigonometric** [HR12]. **trihalomethanes** [MNV+17]. **triiodide** [VVY18]. **trimer** [PMMGL+11]. **trimers** [LJW+11, MZLM17]. **trimethyl** [Owe17]. **trimethylamine** [SC18]. **trimethylnaphthalenes** [OMÐ13a]. **trimethylxanthines** [SMGZ13]. **trinitrate** [LL17]. **trinitro** [CLH14, Men10, MJ11, TJS17]. **trioxide** [SQ10]. **tripeptide** [ScBsR+10]. **triphenylamine** [ZZR+12]. **triphenylphosphonium** [AG10b]. **triphosphate** [YTY19]. **triple** [ABG12, KKC14, KC16, KC18, MPT11, NZ13, Tob19]. **triples** [PCV19]. **triplet** [BMF13, GLOGM+11, Kim16, LSL+08, MGD11, RMJ11, YSS+10]. **triply** [GCD13]. **tris** [AC19, FO10]. **tRNA** [ST15]. **tropolone** [PS13a]. **Tropospheric** [dlLIAI+12]. **Tropsch** [MJ16a]. **TrR** [CDL+19]. **truncated** [MSNP18]. **Trypanosoma** [SLA12]. **tryptophan** [BSV12]. **Tsallis** [Gra08, OH19]. **TSSCDS** [KMNSP19]. **tuberculosis** [ST15]. **TUHC** [LSW19]. **Tunable** [ZX12]. **tuned** [MIN13, WDJ+17, ZZ18]. **tungsten** [Yam10]. **Tuning** [DWZZ15, GMT16, GMM+18]. **Tunneling** [HZW18, KC18, Xu19, CW13b, MVC13, TCG17, WZX+15a, XDM+10, XZJ+16, Xu16, ZLWY13]. **Tutorial** [AB16a, Bae16, BC15, Beh15, BBB16, BM16, BW13b, IN15, JW18, Laz14, LSP+16, Liu15b, LKd+16, MW16, Mos14, Nym14, OWD18, PSMD16, Per18, PI16, Rup15b, SMMT13, SBD+16, SPM+15, Val13, ZP16, vL13, AHC+18, BC16, Liu16, LC19]. **twinning** [GE12a]. **twisted** [FSBA12, LXW+12]. **Two** [Cho15, GSaY11, VOK+18, ART08, BKM15, BCF+11, CFP+10, ČW13a, CG12, CH17, CK17, CF17, DTF+11, Dw13, DSSM18, GW13, GI11e, GN19, HV11, JWJ+12, KWLS15, KYLC19, KAOB11, LMZ+11, LWJL10, Mam13, Mar12, MBA+13, MLDP10, MAN15, NZ13, Pir13, QB15, RP11a, RD14, RPVM10, RDB19, RNC+14, RAGM10, SDS19, SDS20, SBMM11, SBM16, SN15, SSAM13, TC12, WLZ+12b, Yak11, Yam11, YM14, YWR+18, ZWLC12, Zil14, ZJS13]. **Two-** [GSaY11, CG12, WLZ+12b]. **two-component** [SN15]. **Two-dimensional** [Cho15, ART08, Dw13, Mam13, MLDP10, RNC+14, SSAM13]. **two-dimensionally** [Yam11]. **two-electron** [BKM15, ČW13a, CH17, DSSM18, KWLS15, Pir13, RAGM10, SDS19, SDS20, SBM16, YM14, ZJS13]. **two-particle** [DTF+11]. **two-photon** [YWR+18]. **two-range** [GW13]. **two-stage** [KYLC19]. **two-state** [JWJ+12]. **Type** [TBRIS12, AGJ12, AY15, BPG+10, Boe12, GMGRMP12, GZF13, GZF14, GW13, GE12b, HITU16, Hog10, Hog13, IIS+17, JH15, LSS19, cLqFtW+14, Mat02, Mat10, Mit11c, PS10a, PP19a, PGMGRM15, RVO+14, TBRIS10,

[AG19]. **Zintl** [TZD+19]. **zirconia** [MCRS16]. **Zn** [ASHF13, DD17, JL12a, PAKA15, VO12, XZZ+10, XWC11a, YL11, Bal16, CRB+12, DSD18, MC17, MRT11, ZSASS13, dCDC+11]. **ZnO** [ESDO16, BRBRS11, KA13, LPO+12, MTL+12, RZC13]. **ZnO-based** [LPO+12]. **ZO** [EAV16]. **zone** [BG11a]. **Zr** [Bou11, Kim19, WJL+11]. **ZrF** [BLKB11]. **ZrN** [RMLPGGGH16]. **ZSM** [JLL11, SZ11]. **ZSM-5** [JLL11, SZ11]. **zündel** [MNC12]. **zwitterionic** [KRG+13, RFMC19, YZZ15, ZZ18].

References

Afaq:2011:CPR

[AA11] A. Afaq and Iftikhar Ahmad. Classification of partially reflecting surfaces using photodetached electron spectrum. *International Journal of Quantum Chemistry*, 111(15): 4067–4071, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avery:2015:REM

[AA15] John Scales Avery and James Emil Avery. Rapid evaluation of molecular integrals with ETOs. *International Journal of Quantum Chemistry*, 115(15):930–936, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arif:2012:TIH

[AAA12] Suneela Arif, Iftikhar Ahmad, and Bin Amin. Theoretical investigation of half-metallicity in Co/Ni substituted AlN. *International Journal of Quantum Chemistry*, 112(3):882–888, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arif:2012:RHM

[AAAM12] S. Arif, Iftikhar Ahmad, B. Amin, and M. Maqbool. Robust half-metallicity of AlCoN and AlNiN. *International Journal of Quantum Chemistry*, 112(14):2668–2674, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abdelmonem:2016:DSI

[AAHN16] Mohamed S. Abdelmonem, Afaf Abdel-Hady, and Ibraheem Nasser. Dealing with the shifted and inverted Tietz–Hua oscillator potential using the J-matrix method. *Inter-*

national Journal of Quantum Chemistry, 116(12):897–907, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Almatarneh:2017:CMS

[AASU+17] Mansour H. Almatarneh, Abd Al-Aziz A. Abu-Saleh, Kabir M. Uddin, Raymond A. Poirier, and Peter L. Warburton. A computational mechanistic study of the deamination reaction of melamine. *International Journal of Quantum Chemistry*, 117(3):180–189, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abarenkov:2016:TRW

[AB16a] I. V. Abarenkov and M. A. Boyko. Tutorial reviews: Wavefunction-based embedding potential for ion-covalent crystals. *International Journal of Quantum Chemistry*, 116(3): 211–236, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abbat:2016:ESC

[AB16b] Sheenu Abbat and Prasad V. Bharatam. Electronic structure and conformational analysis of P218: an antimalarial drug candidate. *International Journal of Quantum Chemistry*, 116(18):1362–1369, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alipour:2018:ITA

[AB18] Mojtaba Alipour and Zeinab Badooei. Information theoretic approach provides a reliable description for kinetic component of correlation energy density functional. *International Journal of Quantum Chemistry*, 118(23): e25791:1–e25791:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Avci:2011:EDB

[ABA11] Davut Avci, Adııl Başoğlu, and Yusuf Atalay. Effects of different basis sets and donor-acceptor groups on linear and second-order nonlinear optical properties and molecular frontier orbital energies. *International Journal of Quantum Chemistry*, 111(1):130–147, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adamo:2012:P

[ABC12] Carlo Adamo, Vincenzo Barone, and Gilberte Chambaud. Preface. *International Journal of Quantum Chemistry*, 112 (9):2031, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angelotti:2012:VTI

[ABG12] W. F. D. Angelotti, W. R. Batista, and A. C. Granato. Vertical triple ionization with diffusion quantum Monte Carlo. *International Journal of Quantum Chemistry*, 112 (20):3371–3373, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alhameedi:2018:PPF

[ABKJ18] Khidhir Alhameedi, Björn Bohman, Amir Karton, and Dylan Jayatilaka. Predicting the primary fragments in mass spectrometry using ab initio Roby–Gould bond indices. *International Journal of Quantum Chemistry*, 118(15): e25603:1–e25603:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2011:DAF

[ABLT11] Diego R. Alcoba, Roberto C. Bochicchio, Luis Lain, and Alicia Torre. Domain-averaged Fermi hole and domain-restricted reduced density matrices: a critical comparison. *International Journal of Quantum Chemistry*, 111(2):256–262, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adjieufack:2019:HEB

[ABM+19] Abel I. Adjieufack, Maraf Mbah Bake, Joseph Ketcha Mbadcam, Ibrahim Mbouombouo Ndassa, Juan Andrés, Mónica Oliva, and Vicent S. Safont. How effectively bonding evolution theory retrieves and visualizes curly arrows: the cycloaddition reaction of cyclic nitrones. *International Journal of Quantum Chemistry*, 119(19):e25985:1–e25985:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antonov:2013:VSD

[ABP13] Vladislav Antonov, Dobrina Borisova, and Ana Proykova. Vacancy spatial distribution causes different magnetism in

graphene. *International Journal of Quantum Chemistry*, 113(6):792–796, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abarenkov:2011:EAO

[ABS11] I. V. Abarenkov, M. A. Boyko, and P. V. Sushko. Embedding and atomic orbitals hybridization. *International Journal of Quantum Chemistry*, 111(11):2602–2619, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abarenkov:2013:LDO

[ABS13] Igor V. Abarenkov, Maksim A. Boyko, and Peter V. Sushko. Localized directed orbitals representing chemical bonds in ion-covalent crystals. *International Journal of Quantum Chemistry*, 113(14):1868–1876, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Altun:2014:THC

[ABTW14] Zikri Altun, Erdi A. Bleda, Carl Trindle, and Jason Wang. Thermochemistry of N-heterocyclic carbenes with 5-, 4-, 3-, and 2-membered rings. *International Journal of Quantum Chemistry*, 114(10):675–687, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2011:DRS

[AC11] S. A. Alexander and R. L. Coldwell. Decay rates of select magnetic quadrupole transitions in helium. *International Journal of Quantum Chemistry*, 111(12):2820–2824, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexander:2012:VEH

[AC12] Steven A. Alexander and Robert L. Coldwell. Vibrational energies of H_2^+ using fully nonadiabatic wavefunctions. *International Journal of Quantum Chemistry*, 112(23):3703–3705, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adeniyi:2019:EED

[AC19] Adebayo A. Adeniyi and Jeanet Conradie. Electronic effect of β-diketonato ligands on the redox potential of fac

and mer tris(β-diketonato) iron(III) complexes: a density functional theory study and molecular electrostatic potential analysis. *International Journal of Quantum Chemistry*, 119(24):e26036:1–e26036:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ai:2011:ECE

[ACF+11] Yue-Jie Ai, Gang-Long Cui, Qiu Fang, Wei-Hai Fang, and Yi Luo. Exploring concerted effects of base pairing and stacking on the excited-state nature of DNA oligonucleotides by DFT and TD–DFT studies. *International Journal of Quantum Chemistry*, 111(10):2366–2377, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adamo:2010:P

[ACL10] Carlo Adamo, Henry Chermette, and David Loffreda. Preface. *International Journal of Quantum Chemistry*, 110(12): 2101, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amusia:2012:GOS

[ACL12] M. Ya. Amusia, L. V. Chernysheva, and E. Z. Liverts. Generalized oscillator strength of endohedral molecules. *International Journal of Quantum Chemistry*, 112(18):3119–3130, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alves:2010:TCS

[ACMRN10] Marcel M. Alves, Edson F. V. Carvalho, Francisco B. C. Machado, and Orlando Roberto-Neto. Theoretical calculations of structures, energetics, and kinetics of O(^{3}P) + CH_3OH reactions. *International Journal of Quantum Chemistry*, 110(11):2037–2046, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arockiaraj:2019:MIC

[ACT19] Micheal Arockiaraj, Joseph Clement, and Niko Tratnik. Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems. *International Journal of Quantum Chemistry*, 119(24):e26043:1–e26043:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ali:2017:DBA

[AD17] Akbar Ali and Zhibin Du. On the difference between atom-bond connectivity index and Randić index of binary and chemical trees. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Almora-Diaz:2010:NCC

[ADB10] César X. Almora-Díaz and Carlos F. Bunge. Nonrelativistic CI calculations for B^+, B, and B^- ground states. *International Journal of Quantum Chemistry*, 110(15):2982–2988, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alberto:2018:DMI

[ADR+18] Marta Erminia Alberto, Stefania Di Tommaso, Chiara Ricca, Ilaria Ciofini, and Carlo Adamo. Dioxygenation of metal(II)-cysteinato complexes in CDO biomimetic models: Can ruthenium and osmium reach iron performances? *International Journal of Quantum Chemistry*, 118(9):e25525:1–e25525:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Almatarneh:2019:GPO

[AEAS+19] Mansour H. Almatarneh, Ismael A. Elayan, Abd Al-Aziz A. Abu-Saleh, Mohammednoor Altarawneh, and Parisa A. Ariya. The gas-phase ozonolysis reaction of methylbutenol: a mechanistic study. *International Journal of Quantum Chemistry*, 119(10):e25888:1–e25888:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Abu-Eittah:2012:SCA

[AEKGZ12] Rafie H. Abu-Eittah, M. K. Khedr, M. Goma, and W. Zordok. The structure of cinnamic acid and cinnamoyl azides, a unique localized π system: The electronic spectra and DFT-treatment. *International Journal of Quantum Chemistry*, 112(5):1256–1272, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amzallag:2012:IEE

[AEM+12] E. Amzallag, D. Ehinon, H. Martinez, M. Rérat, and I. Baraille. Ab initio electron energy-loss spectra and depolarization effects: Application to carbon nanotubes. *International Journal of Quantum Chemistry*, 112(9):2171–2184, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akdemir:2012:NAE

[AEÖ12] S. Ö. Akdemir, S. D. Eryilmaz, and E. Öztekin. New analytical expressions, symmetry relations and numerical solutions for the rotational overlap integrals. *International Journal of Quantum Chemistry*, 112(6):1585–1591, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alipour:2016:OSW

[AF16] Mojtaba Alipour and Parisa Fallahzadeh. Order of stabilities in water nanoclusters: Insight from some recent double-hybrid functionals. *International Journal of Quantum Chemistry*, 116(15):1173–1178, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Agbaglo:2019:PEC

[AF19a] Donatus Agbaglo and Ryan C. Fortenberry. The performance of explicitly correlated methods for the computation of anharmonic vibrational frequencies. *International Journal of Quantum Chemistry*, 119(11):e25899:1–e25899:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andreussi:2019:CEC

[AF19b] Oliviero Andreussi and Giuseppe Fisicaro. Continuum embeddings in condensed-matter simulations. *International Journal of Quantum Chemistry*, 119(1):e25725:1–e25725:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aliabad:2013:OPK

[AFA13] Hossein Asghar Rahnamaye Aliabad, Marjan Fathabadi, and Iftikhar Ahmad. Optoelectronic properties of KDP by

first principle calculations. *International Journal of Quantum Chemistry*, 113(6):865–872, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Adrover:2010:IIF

[AFC+10] Miquel Adrover, Juan Frau, Catalina Caldés, Bartolomé Vilanova, Josefa Donoso, and Francisco Muñoz. Impact of the ionic forms on the UV–Vis spectra 2-hydroxybenzylamine. A TD–DFT study. *International Journal of Quantum Chemistry*, 110(12):2179–2191, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Antunes:2010:DPT

[AFM+10] Adoniel W. S. Antunes, Wiliam Ferreira Da Cunha, Geraldo Magela E Silva, João B. L. Martins, and Ricardo Gargano. Dynamical properties and thermal rate coefficients for the Na + HF reaction using genetic algorithm. *International Journal of Quantum Chemistry*, 110(5):1070–1079, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alvarez-Falcon:2012:DMC

[ÁFV12] Leny Álvarez-Falcón and Luis Vicente. Dynamic Monte Carlo simulations of NO decomposition on Pt(100): Temperature-programmed desorption spectra. *International Journal of Quantum Chemistry*, 112(7):1803–1809, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alagona:2010:DWR

[AG10a] Giuliano Alagona and Caterina Ghio. Dependence of the Wittig reaction mechanism on the environment and on the substituents at the aldehyde group and at the phosphonium ylide. *International Journal of Quantum Chemistry*, 110 (3):765–776, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alagona:2010:FEL

[AG10b] Giuliano Alagona and Caterina Ghio. Free energy landscapes in THF for the Wittig reaction of acetaldehyde and triphenylphosphonium ylide. *International Journal*

of Quantum Chemistry, 110(13):2509–2521, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ayala:2019:TSB

[AG19] Regla Ayala and Agustín Galindo. A theoretical study of the bonding capabilities of the zinc-zinc double bond. *International Journal of Quantum Chemistry*, 119(5):e25823:1–e25823:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Agboola:2012:BSD

[Agb12] D. Agboola. Bound-states of diatomic molecules in the Dirac equation with the q-deformed Morse potential. *International Journal of Quantum Chemistry*, 112(4):1029–1035, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexandrou:2019:EFD

[AGB19] Eleni I. Alexandrou, Axel Groß, and Naoum C. Bacalis. Electronic factors determining the methane bond breaking process on small aluminum clusters. *International Journal of Quantum Chemistry*, 119(21):e26003:1–e26003:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aguilera-Granja:2015:SMV

[AGCVG15] Faustino Aguilera-Granja, Jesús Carrete, Andrés Vega, and Luis J. Gallego. Structural, magnetic, and vibrational properties of stoichiometric clusters of CrN. *International Journal of Quantum Chemistry*, 115(8):523–528, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andres:2018:FAN

[AGG+18] Juan Andrés, Amanda Fernandes Gouveia, Lourdes Gracia, Elson Longo, Giovani Manzeppi Faccin, Edison Zacarias da Silva, Douglas Henrique Pereira, and Miguel Angel San-Miguel. Formation of Ag nanoparticles under electron beam irradiation: Atomistic origins from first-principles calculations. *International Journal of Quantum Chemistry*, 118(9):e25551:1–e25551:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anne:2012:CRP

[AGJ12] Frédéric B. Anne, Nicolas Galland, and Denis Jacquemin. Computing redox potentials for dyes used in p-type dye-sensitized solar cells. *International Journal of Quantum Chemistry*, 112(24):3763–3768, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andres:2014:RUR

[AGNS14] Juan Andrés, Patricio González-Navarrete, and Vicent Sixte Safont. Reviews: Unraveling reaction mechanisms by means of Quantum Chemical Topology Analysis. *International Journal of Quantum Chemistry*, 114(19): 1239–1252, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aguilar-Galindo:2018:ECE

[AGOP18] Fernando Aguilar-Galindo, Pilar Ocón, and José Manuel L. Poyato. Exploring the catalytic efficiency of X-doped (X = B, N, P) graphene in oxygen reduction reaction: Influence of solvent and border effects. *International Journal of Quantum Chemistry*, 118(14):e25579:1–e25579:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Andjelkovic:2013:CEC

[AGPDZ13] Ljubica Andjelković, Maja Gruden-Pavlović, Claude Daul, and Matija Zlatar. The choice of the exchange-correlation functional for the determination of the Jahn–Teller parameters by the density functional theory. *International Journal of Quantum Chemistry*, 113(6):859–864, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aparicio:2012:SSI

[AGRI$^+$12] Felipe Aparicio, Nelly González-Rivas, Joel Ireta, Arturo Rojo, Laura I. Escobar, Andrés Cedillo, and Marcelo Galván. Soft–soft interactions in the protein–protein recognition process: the K^+ channel-charybdotoxin case. *International Journal of Quantum Chemistry*, 112(22):3618–3623, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alexeev:2019:SIE

[AH19] Yuri Alexeev and Robert Harrison. Special issue on emerging architectures in computational chemistry. *International Journal of Quantum Chemistry*, 119(12):e25959:1–e25959:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ahmadi:2018:MME

[AHC+18] Shideh Ahmadi, Lizandra Barrios Herrera, Morteza Chehelamirani, Jirí Hostas, Said Jalife, and Dennis R. Salahub. Multiscale modeling of enzymes: QM-cluster, QM/MM, and QM/MM/MD: a tutorial review. *International Journal of Quantum Chemistry*, 118(9):e25558:1–e25558:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angelotti:2012:GCM

[AHT12] W. F. D. Angelotti, R. L. A. Haiduke, and M. Trsic. The generator coordinate method in the unrestricted Hartree–Fock formalism. *International Journal of Quantum Chemistry*, 112(4):941–947, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alvarez-Idaboy:2012:SIM

[ÁIGVZW12] J. Raúl Álvarez-Idaboy, Marcelo Galván, Alberto Vela, and Claudio M. Zicovich-Wilson. Special Issue: Mexican Theoretical Physical Chemistry Meetings. *International Journal of Quantum Chemistry*, 112(21):3439–3440, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arbuznikov:2011:ALH

[AK11] Alexei V. Arbuznikov and Martin Kaupp. Advances in local hybrid exchange-correlation functionals: from thermochemistry to magnetic-resonance parameters and hyperpolarizabilities. *International Journal of Quantum Chemistry*, 111(11):2625–2638, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alharbi:2017:KED

[AK17] Fahhad H. Alharbi and Sabre Kais. Kinetic energy density for orbital-free density functional calculations by axiomatic

approach. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Amme:2010:CCP

[AKC10] Matthew J. Amme, Abul B. Kazi, and Thomas R. Cundari. Copper-catalyzed phosphinidene transfer to ethylene, acetylene, and carbon monoxide: a computational study. *International Journal of Quantum Chemistry*, 110(9):1702–1711, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ahmed:2013:SCH

[AKHS13] Ashour A. Ahmed, Oliver Kühn, Rifaat H. Hilal, and Mohamed F. Shibl. Structure and cooperativity of the hydrogen bonds in sodium dihydrogen triacetate. *International Journal of Quantum Chemistry*, 113(9):1394–1400, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azami:2012:LAM

[AKR12] S. M. Azami, M. Kheirmand, and G. Rezaei. Local angular momentum as ring strain descriptor. *International Journal of Quantum Chemistry*, 112(14):2623–2626, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Auvinen:2015:UTS

[ALA15] Sami Auvinen, Matti Lahti, and Matti Alatalo. Unoccupied titanium $3d$ states due to subcluster formation in stoichiometric TiO_2 nanoparticles. *International Journal of Quantum Chemistry*, 115(17):1175–1180, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aysin:2018:ASC

[ALB18] Rinat R. Aysin, Larissa A. Leites, and Sergey S. Bukalov. Aromaticity of some carbenes and their heavier analogs in light of gauge-including magnetically induced current approach as a new magnetic criterium. *International Journal of Quantum Chemistry*, 118(22):e25759:1–e25759:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alemany:2013:PAE

[Ale13] Pere Alemany. Perspective: Analyzing the electronic structure of molecules using continuous symmetry measures. *International Journal of Quantum Chemistry*, 113(14):1814–1820, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arvanitidis:2018:VBE

[ALHC18] Athanasios G. Arvanitidis, Kie Zen Lim, Remco W. A. Havenith, and Arnout Ceulemans. Valence bonds in elongated boron clusters. *International Journal of Quantum Chemistry*, 118(13):e25575:1–e25575:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alipour:2014:TDD

[Ali14] Mojtaba Alipour. Theoretical determination of the differential polarizability and anisotropy of alkaline earth oxide nanoclusters $(BeO)_n$ [n = 2–9]: the basis set and electron correlation effects. *International Journal of Quantum Chemistry*, 114(4):255–260, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alipour:2019:OES

[Ali19a] Mojtaba Alipour. Oxidation energies of shuttle molecules candidates in lithium-ion batteries from double-hybrid models. *International Journal of Quantum Chemistry*, 119(20):e25950:1–e25950:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alipour:2019:TPV

[Ali19b] Mojtaba Alipour. Theoretical prediction of valence and Rydberg excited states: Minnesota exchange–correlation functionals vs symmetry adapted cluster-configuration interaction. *International Journal of Quantum Chemistry*, 119 (11):e25898:1–e25898:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Attia:2018:APH

[ALK18] Amr A. A. Attia, Alexandru Lupan, and Robert Bruce King. Aluminum-poor hexacarbalane structures: the transition from localized organoaluminum structures to delocal-

ized polyhedra. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Attia:2019:STU

[ALK19] Amr A. A. Attia, Alexandru Lupan, and R. Bruce King. Segregation of tetracarbon units in low-energy tetracarbindane structures: Major differences from their aluminum and gallium analogs. *International Journal of Quantum Chemistry*, 119(15):e25934:1–e25934:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arslancan:2018:CBC

[ALMY18] Serra Arslancan, Al Mokhtar Lamsabhi, Otilia Mó, and Manuel Yáñez. Complexes between cyclopentene and cyclopentyne derivatives with HCu and FCu: the importance of cyclization effects. *International Journal of Quantum Chemistry*, 118(9):e25489:1–e25489:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angulo:2010:EIR

[ALRA10] J. C. Angulo, S. López-Rosa, and J. Antolín. Effect of the interelectronic repulsion on the information content of position and momentum atomic densities. *International Journal of Quantum Chemistry*, 110(9):1738–1747, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angulo:2011:GJD

[ALRAE11] J. C. Angulo, S. López-Rosa, J. Antolín, and R. O. Esquivel. Generalized Jensen divergence analysis of atomic electron densities in conjugated spaces. *International Journal of Quantum Chemistry*, 111(2):297–306, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ayuela:2010:MMT

[AM10] A. Ayuela and N. H. March. The magnetic moments and their long-range ordering for Fe atoms in a wide variety of metallic environments. *International Journal of Quantum*

Chemistry, 110(15):2725–2733, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alaa:2012:TSR

[AM12] Hamdan Alaa and Korek Mahmoud. Theoretical study with rovibrational and dipole moment calculation of sextet states of the CrCl molecule. *International Journal of Quantum Chemistry*, 112(5):1235–1242, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ahlstrom:2013:CBB

[AM13a] Logan S. Ahlstrom and Osamu Miyashita. Computational biochemistry and biophysics: Comparison of a simulated λ Cro dimer conformational ensemble to its NMR models. *International Journal of Quantum Chemistry*, 113(4):518–524, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alipour:2013:APD

[AM13b] Mojtaba Alipour and Afshan Mohajeri. Assessing the performance of density functional theory for the dynamic polarizabilities of amino acids: Treatment of correlation and role of exact exchange. *International Journal of Quantum Chemistry*, 113(13):1803–1811, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ariyarathna:2018:DBV

[AM18] Isuru R. Ariyarathna and Evangelos Miliordos. Dative bonds versus electron solvation in tri-coordinated beryllium complexes: $Be(CX)_3$ [X = O, S, Se, Te, Po] and $Be(PH_3)_3$ versus $Be(NH_3)_3$. *International Journal of Quantum Chemistry*, 118(18):e25673:1–e25673:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ayadi:2012:TSP

[AMAC12] Sameh Ayadi, Pierre Mignon, Manef Abderrabba, and Henry Chermette. Theoretical study of the polymerization of *p*-tert-butyl-anisol. *International Journal of Quantum Chemistry*, 112(9):2154–2159, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aucar:2018:RFL

[AMAM18] Gustavo A. Aucar, Juan I. Melo, Ignacio Agustín Aucar, and Alejandro F. Maldonado. Reviews: Foundations of the LRESC model for response properties and some applications. *International Journal of Quantum Chemistry*, 118 (1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arlund:2010:CSO

[AMK10] David Arlund, David A. Micha, and Dmitri S. Kilin. Computational studies of the optical properties of silicon compounds bonding to silver atoms and with group III and V substituents. *International Journal of Quantum Chemistry*, 110(15):3086–3094, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azizi:2018:VBR

[AMMB+18] Alireza Azizi, Roya Momen, Alejandro Morales-Bayuelo, Tianlv Xu, Steven R. Kirk, and Samantha Jenkins. A vector-based representation of the chemical bond for predicting competitive and noncompetitive torquoselectivity of thermal ring-opening reactions. *International Journal of Quantum Chemistry*, 118(20):e25707:1–e25707:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aucar:2019:TDA

[AMMC19] Gustavo A. Aucar, Alejandro F. Maldonado, Marcos D. A. Montero, and Teresita Santa Cruz. Theoretical developments and applications of polarization propagators. *International Journal of Quantum Chemistry*, 119(2):e25722:1–e25722:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aidas:2011:FPA

[AMMK11] Kestutis Aidas, Kurt V. Mikkelsen, Benedetta Mennucci, and Jacob Kongsted. Fluorescence and phosphorescence of acetone in neat liquid and aqueous solution studied by QM/MM and PCM approaches. *International Journal of Quantum Chemistry*, 111(7–8):1511–1520, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arruda:2015:MAB

[ANC+15] Priscilla Mendes Arruda, Antônio Canal Neto, Mauro Cesar Martins Campos, Henrique Raulino Coelho da Cruz, and Fábio Alves dos Santos. Molecule-adapted basis sets optimized with a quantum Monte Carlo method. *International Journal of Quantum Chemistry*, 115(2):77–83, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Angeli:2010:ADP

[Ang10] Celestino Angeli. An analysis of the dynamic σ polarization in the V state of ethene. *International Journal of Quantum Chemistry*, 110(13):2436–2447, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2010:LPa

[Ano10a] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 110(1):5–10, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2010:LPb

[Ano10b] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 110(12):2102–2116, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2010:LPc

[Ano10c] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 110(13):2332–2341, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2010:LPd

[Ano10d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 110(15):2722–2724, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2011:BCV

[Ano11a] Anonymous. Brief curriculum vitae [Sylvio Canuto]. *International Journal of Quantum Chemistry*, 111(7–8):1251,

June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2011:DMBb

[Ano11b] Anonymous. David M. Bishop. *International Journal of Quantum Chemistry*, 111(4):726–735, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2011:DMBa

[Ano11c] Anonymous. David M. Bishop curriculum vitae. *International Journal of Quantum Chemistry*, 111(4):725, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2011:LPa

[Ano11d] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 111(2):205–212, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2011:LPb

[Ano11e] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 111(6):1128–1130, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVa

[Ano12a] Anonymous. Cover image, volume 112, issue 17. *International Journal of Quantum Chemistry*, 112(17):i–ii, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVb

[Ano12b] Anonymous. Cover image, volume 112, issue 18. *International Journal of Quantum Chemistry*, 112(18):i–ii, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVc

[Ano12c] Anonymous. Cover image, volume 112, issue 19. *International Journal of Quantum Chemistry*, 112(19):i–ii, Octo-

ber 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVd

[Ano12d] Anonymous. Cover image, volume 112, issue 20. *International Journal of Quantum Chemistry*, 112(20):i–ii, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVe

[Ano12e] Anonymous. Cover image, volume 112, issue 21. *International Journal of Quantum Chemistry*, 112(21):i–ii, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVf

[Ano12f] Anonymous. Cover image, volume 112, issue 22. *International Journal of Quantum Chemistry*, 112(22):i–ii, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVg

[Ano12g] Anonymous. Cover image, volume 112, issue 23. *International Journal of Quantum Chemistry*, 112(23):i–ii, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:CIVh

[Ano12h] Anonymous. Cover image, volume 112, issue 24. *International Journal of Quantum Chemistry*, 112(24):i–ii, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVa

[Ano12i] Anonymous. Inside cover, volume 112, issue 17. *International Journal of Quantum Chemistry*, 112(17):iii–iv, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVb

[Ano12j] Anonymous. Inside cover, volume 112, issue 18. *International Journal of Quantum Chemistry*, 112(18):iii–iv,

September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVc

[Ano12k] Anonymous. Inside cover, volume 112, issue 19. *International Journal of Quantum Chemistry*, 112(19):iii–iv, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVd

[Ano12l] Anonymous. Inside cover, volume 112, issue 20. *International Journal of Quantum Chemistry*, 112(20):iii–iv, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVe

[Ano12m] Anonymous. Inside cover, volume 112, issue 21. *International Journal of Quantum Chemistry*, 112(21):iii–iv, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVf

[Ano12n] Anonymous. Inside cover, volume 112, issue 22. *International Journal of Quantum Chemistry*, 112(22):iii–iv, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:ICVg

[Ano12o] Anonymous. Inside Cover, Volume 112, Issue 24. *International Journal of Quantum Chemistry*, 112(24):iii–iv, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:LCa

[Ano12p] Anonymous. List of contributors. *International Journal of Quantum Chemistry*, 112(1):2–4, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:LCb

[Ano12q] Anonymous. List of contributors. *International Journal of Quantum Chemistry*, 112(8):1860–1861, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2012:LP

[Ano12r] Anonymous. List of participants. *International Journal of Quantum Chemistry*, 112(7):1760–1767, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIi

[Ano13a] Anonymous. Cover image: Inside cover, volume 113, issue 10. *International Journal of Quantum Chemistry*, 113(10): iii–iv, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIj

[Ano13b] Anonymous. Cover image: Inside cover, volume 113, issue 11. *International Journal of Quantum Chemistry*, 113(11): iii–iv, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIk

[Ano13c] Anonymous. Cover image: Inside cover, volume 113, issue 12. *International Journal of Quantum Chemistry*, 113(12): iii–iv, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIl

[Ano13d] Anonymous. Cover image: Inside cover, volume 113, issue 13. *International Journal of Quantum Chemistry*, 113(13): iii–iv, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIm

[Ano13e] Anonymous. Cover image: Inside cover, volume 113, issue 14. *International Journal of Quantum Chemistry*, 113(14): iii–iv, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIn

[Ano13f] Anonymous. Cover image: Inside cover, volume 113, issue 15. *International Journal of Quantum Chemistry*, 113(15): iii–iv, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIo

[Ano13g] Anonymous. Cover image: Inside cover, volume 113, issue 16. *International Journal of Quantum Chemistry*, 113(16): iii–iv, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIp

[Ano13h] Anonymous. Cover image: Inside cover, volume 113, issue 17. *International Journal of Quantum Chemistry*, 113(17): iii–iv, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIq

[Ano13i] Anonymous. Cover image: Inside cover, volume 113, issue 18. *International Journal of Quantum Chemistry*, 113(18): iii–iv, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIr

[Ano13j] Anonymous. Cover image: Inside cover, volume 113, issue 19. *International Journal of Quantum Chemistry*, 113(19): iii–iv, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIa

[Ano13k] Anonymous. Cover image: Inside cover, volume 113, issue 2. *International Journal of Quantum Chemistry*, 113(2):iii–iv, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIs

[Ano13l] Anonymous. Cover image: Inside cover, volume 113, issue 20. *International Journal of Quantum Chemistry*, 113(20): iii–iv, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIt

[Ano13m] Anonymous. Cover image: Inside cover, volume 113, issue 21. *International Journal of Quantum Chemistry*, 113(21): iii–iv, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIu

[Ano13n] Anonymous. Cover image: Inside cover, volume 113, issue 22. *International Journal of Quantum Chemistry*, 113(22): iii–iv, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIv

[Ano13o] Anonymous. Cover image: Inside cover, volume 113, issue 23. *International Journal of Quantum Chemistry*, 113(23): iii–iv, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIw

[Ano13p] Anonymous. Cover image: Inside cover, volume 113, issue 24. *International Journal of Quantum Chemistry*, 113(24): iii–iv, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIb

[Ano13q] Anonymous. Cover image: Inside cover, volume 113, issue 3. *International Journal of Quantum Chemistry*, 113(3):iii–iv, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIc

[Ano13r] Anonymous. Cover image: Inside cover, volume 113, issue 4. *International Journal of Quantum Chemistry*, 113(4):iii–iv, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIId

[Ano13s] Anonymous. Cover image: Inside cover, volume 113, issue 5. *International Journal of Quantum Chemistry*, 113(5): iii–iv, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIe

[Ano13t] Anonymous. Cover image: Inside cover, volume 113, issue 6. *International Journal of Quantum Chemistry*, 113(6): iii–iv, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIf

[Ano13u] Anonymous. Cover image: Inside cover, volume 113, issue 7. *International Journal of Quantum Chemistry*, 113(7): iii–iv, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIg

[Ano13v] Anonymous. Cover image: Inside cover, volume 113, issue 8. *International Journal of Quantum Chemistry*, 113(8): iii–iv, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIIh

[Ano13w] Anonymous. Cover image: Inside cover, volume 113, issue 9. *International Journal of Quantum Chemistry*, 113(9): iii–iv, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVa

[Ano13x] Anonymous. Cover image, volume 113, issue 1. *International Journal of Quantum Chemistry*, 113(1):i–ii, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVj

[Ano13y] Anonymous. Cover image, volume 113, issue 10. *International Journal of Quantum Chemistry*, 113(10):i–ii, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVk

[Ano13z] Anonymous. Cover image, volume 113, issue 11. *International Journal of Quantum Chemistry*, 113(11):i–ii, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVl

[Ano13-27] Anonymous. Cover image, volume 113, issue 12. *International Journal of Quantum Chemistry*, 113(12):i–ii, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVm

[Ano13-28] Anonymous. Cover image, volume 113, issue 13. *International Journal of Quantum Chemistry*, 113(13):i–ii, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVn

[Ano13-29] Anonymous. Cover image, volume 113, issue 14. *International Journal of Quantum Chemistry*, 113(14):i–ii, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVo

[Ano13-30] Anonymous. Cover image, volume 113, issue 15. *International Journal of Quantum Chemistry*, 113(15):i–ii, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVp

[Ano13-31] Anonymous. Cover image, volume 113, issue 16. *International Journal of Quantum Chemistry*, 113(16):i–ii, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVq

[Ano13-32] Anonymous. Cover image, volume 113, issue 17. *International Journal of Quantum Chemistry*, 113(17):i–ii, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVr

[Ano13-33] Anonymous. Cover image, volume 113, issue 18. *International Journal of Quantum Chemistry*, 113(18):i–ii, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVs

[Ano13-34] Anonymous. Cover image, volume 113, issue 19. *International Journal of Quantum Chemistry*, 113(19):i–ii, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVb

[Ano13-35] Anonymous. Cover image, volume 113, issue 2. *International Journal of Quantum Chemistry*, 113(2):i–ii, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVt

[Ano13-36] Anonymous. Cover image, volume 113, issue 20. *International Journal of Quantum Chemistry*, 113(20):i–ii, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVu

[Ano13-37] Anonymous. Cover image, volume 113, issue 21. *International Journal of Quantum Chemistry*, 113(21):i–ii, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVv

[Ano13-38] Anonymous. Cover image, volume 113, issue 22. *International Journal of Quantum Chemistry*, 113(22):i–ii, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVw

[Ano13-39] Anonymous. Cover image, volume 113, issue 23. *International Journal of Quantum Chemistry*, 113(23):i–ii, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVx

[Ano13-40] Anonymous. Cover image, volume 113, issue 24. *International Journal of Quantum Chemistry*, 113(24):i–ii, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVc

[Ano13-41] Anonymous. Cover image, volume 113, issue 3. *International Journal of Quantum Chemistry*, 113(3):i–ii, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVd

[Ano13-42] Anonymous. Cover image, volume 113, issue 4. *International Journal of Quantum Chemistry*, 113(4):i–ii, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVe

[Ano13-43] Anonymous. Cover image, volume 113, issue 5. *International Journal of Quantum Chemistry*, 113(5):i–ii, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVf

[Ano13-44] Anonymous. Cover image, volume 113, issue 6. *International Journal of Quantum Chemistry*, 113(6):i–ii, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVg

[Ano13-45] Anonymous. Cover image, volume 113, issue 7. *International Journal of Quantum Chemistry*, 113(7):i–ii, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVh

[Ano13-46] Anonymous. Cover image, volume 113, issue 8. *International Journal of Quantum Chemistry*, 113(8):i–ii, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:CIVi

[Ano13-47] Anonymous. Cover image, volume 113, issue 9. *International Journal of Quantum Chemistry*, 113(9):i–ii, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:ICV

[Ano13-48] Anonymous. Inside cover, volume 113, issue 1. *International Journal of Quantum Chemistry*, 113(1):iii–iv, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2013:PWI

[Ano13-49] Anonymous. Preface: Welcome to the 14th International Density Functional Theory Conference. *International Journal of Quantum Chemistry*, 113(5):619, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIC

[Ano14a] Anonymous. Cover image: Cover, volume 114, issue 3. *International Journal of Quantum Chemistry*, 114(3):i–ii, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIa

[Ano14b] Anonymous. Cover image: Inside cover, volume 114, issue 1. *International Journal of Quantum Chemistry*, 114(1): iii–iv, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIj

[Ano14c] Anonymous. Cover image: Inside cover, volume 114, issue 10. *International Journal of Quantum Chemistry*, 114(10): iii–iv, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIk

[Ano14d] Anonymous. Cover image: Inside cover, volume 114, issue 11. *International Journal of Quantum Chemistry*, 114(11): iii–iv, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIl

[Ano14e] Anonymous. Cover image: Inside cover, volume 114, issue 12. *International Journal of Quantum Chemistry*, 114(12): iii–iv, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIm

[Ano14f] Anonymous. Cover image: Inside cover, volume 114, issue 13. *International Journal of Quantum Chemistry*, 114(13): iii–iv, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIn

[Ano14g] Anonymous. Cover image: Inside cover, volume 114, issue 14. *International Journal of Quantum Chemistry*, 114(14): iii–iv, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIo

[Ano14h] Anonymous. Cover image: Inside cover, volume 114, issue 15. *International Journal of Quantum Chemistry*, 114(15): iii–iv, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIp

[Ano14i] Anonymous. Cover image: Inside cover, volume 114, issue 16. *International Journal of Quantum Chemistry*, 114(16): i–ii, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIq

[Ano14j] Anonymous. Cover image: Inside cover, volume 114, issue 16. *International Journal of Quantum Chemistry*, 114 (16):iii–iv, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIr

[Ano14k] Anonymous. Cover image: Inside cover, volume 114, issue 17. *International Journal of Quantum Chemistry*, 114 (17):iii–iv, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIs

[Ano14l] Anonymous. Cover image: Inside cover, volume 114, issue 18. *International Journal of Quantum Chemistry*, 114 (18):iii–iv, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIt

[Ano14m] Anonymous. Cover image: Inside cover, volume 114, issue 19. *International Journal of Quantum Chemistry*, 114 (19):iii–iv, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIb

[Ano14n] Anonymous. Cover image: Inside cover, volume 114, issue 2. *International Journal of Quantum Chemistry*, 114(2):iii–iv, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIu

[Ano14o] Anonymous. Cover image: Inside cover, volume 114, issue 20. *International Journal of Quantum Chemistry*, 114(20): iii–iv, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIv

[Ano14p] Anonymous. Cover image: Inside cover, volume 114, issue 21. *International Journal of Quantum Chemistry*, 114(21): iii–iv, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIw

[Ano14q] Anonymous. Cover image: Inside cover, volume 114, issue 22. *International Journal of Quantum Chemistry*, 114(22): iii–iv, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIx

[Ano14r] Anonymous. Cover image: Inside cover, volume 114, issue 23. *International Journal of Quantum Chemistry*, 114(23): iii–iv, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIy

[Ano14s] Anonymous. Cover image: Inside cover, volume 114, issue 24. *International Journal of Quantum Chemistry*, 114(24): iii–iv, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIc

[Ano14t] Anonymous. Cover image: Inside cover, volume 114, issue 3. *International Journal of Quantum Chemistry*, 114(3):iii–iv, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIId

[Ano14u] Anonymous. Cover image: Inside cover, volume 114, issue 4. *International Journal of Quantum Chemistry*, 114(4):iii–iv, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIe

[Ano14v] Anonymous. Cover image: Inside cover, volume 114, issue 5. *International Journal of Quantum Chemistry*, 114(5): iii–iv, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIf

[Ano14w] Anonymous. Cover image: Inside cover, volume 114, issue 6. *International Journal of Quantum Chemistry*, 114(6): iii–iv, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIg

[Ano14x] Anonymous. Cover image: Inside cover, volume 114, issue 7. *International Journal of Quantum Chemistry*, 114(7): iii–iv, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIh

[Ano14y] Anonymous. Cover image: Inside cover, volume 114, issue 8. *International Journal of Quantum Chemistry*, 114(8): iii–iv, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIIi

[Ano14z] Anonymous. Cover image: Inside cover, volume 114, issue 9. *International Journal of Quantum Chemistry*, 114(9): iii–iv, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVa

[Ano14-27] Anonymous. Cover image, volume 114, issue 1. *International Journal of Quantum Chemistry*, 114(1):i–ii, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVi

[Ano14-28] Anonymous. Cover image, volume 114, issue 10. *International Journal of Quantum Chemistry*, 114(10):i–ii, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVj

[Ano14-29] Anonymous. Cover image, volume 114, issue 11. *International Journal of Quantum Chemistry*, 114(11):i–ii, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVk

[Ano14-30] Anonymous. Cover image, volume 114, issue 12. *International Journal of Quantum Chemistry*, 114(12):i–ii, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVl

[Ano14-31] Anonymous. Cover image, volume 114, issue 13. *International Journal of Quantum Chemistry*, 114(13):i–ii, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVm

[Ano14-32] Anonymous. Cover image, volume 114, issue 14. *International Journal of Quantum Chemistry*, 114(14):i–ii, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVn

[Ano14-33] Anonymous. Cover image, volume 114, issue 15. *International Journal of Quantum Chemistry*, 114(15):i–ii, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVo

[Ano14-34] Anonymous. Cover image, volume 114, issue 17. *International Journal of Quantum Chemistry*, 114(17):i–ii, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVp

[Ano14-35] Anonymous. Cover image, volume 114, issue 18. *International Journal of Quantum Chemistry*, 114(18):i–ii, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVq

[Ano14-36] Anonymous. Cover image, volume 114, issue 19. *International Journal of Quantum Chemistry*, 114(19):i–ii, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVb

[Ano14-37] Anonymous. Cover image, volume 114, issue 2. *International Journal of Quantum Chemistry*, 114(2):i–ii, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVr

[Ano14-38] Anonymous. Cover image, volume 114, issue 20. *International Journal of Quantum Chemistry*, 114(20):i–ii, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVs

[Ano14-39] Anonymous. Cover image, volume 114, issue 21. *International Journal of Quantum Chemistry*, 114(21):i–ii, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVt

[Ano14-40] Anonymous. Cover image, volume 114, issue 22. *International Journal of Quantum Chemistry*, 114(22):i–ii, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVu

[Ano14-41] Anonymous. Cover image, volume 114, issue 23. *International Journal of Quantum Chemistry*, 114(23):i–ii, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVv

[Ano14-42] Anonymous. Cover image, volume 114, issue 24. *International Journal of Quantum Chemistry*, 114(24):i–ii, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVc

[Ano14-43] Anonymous. Cover image, volume 114, issue 4. *International Journal of Quantum Chemistry*, 114(4):i–ii, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVd

[Ano14-44] Anonymous. Cover image, volume 114, issue 5. *International Journal of Quantum Chemistry*, 114(5):i–ii, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVe

[Ano14-45] Anonymous. Cover image, volume 114, issue 6. *International Journal of Quantum Chemistry*, 114(6):i–ii, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVf

[Ano14-46] Anonymous. Cover image, volume 114, issue 7. *International Journal of Quantum Chemistry*, 114(7):i–ii, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVg

[Ano14-47] Anonymous. Cover image, volume 114, issue 8. *International Journal of Quantum Chemistry*, 114(8):i–ii, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2014:CIVh

[Ano14-48] Anonymous. Cover image, volume 114, issue 9. *International Journal of Quantum Chemistry*, 114(9):i–ii, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIIa

[Ano15a] Anonymous. Cover image: Inside cover, volume 115, issue 2. *International Journal of Quantum Chemistry*, 115(2):iii–iv, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIIb

[Ano15b] Anonymous. Cover image: Inside cover, volume 115, issue 3. *International Journal of Quantum Chemistry*, 115(3):iii–iv, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIIc

[Ano15c] Anonymous. Cover image: Inside cover, volume 115, issue 4. *International Journal of Quantum Chemistry*, 115(4):iii–iv, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIId

[Ano15d] Anonymous. Cover image: Inside cover, volume 115, issue 5. *International Journal of Quantum Chemistry*, 115(5): iii–iv, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIIe

[Ano15e] Anonymous. Cover image: Inside cover, volume 115, issue 6. *International Journal of Quantum Chemistry*, 115(6): iii–iv, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVj

[Ano15f] Anonymous. Cover image, volume 115, issue 10. *International Journal of Quantum Chemistry*, 115(10):i–ii, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVk

[Ano15g] Anonymous. Cover image, volume 115, issue 10. *International Journal of Quantum Chemistry*, 115(10):iii–iv, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVl

[Ano15h] Anonymous. Cover image, volume 115, issue 11. *International Journal of Quantum Chemistry*, 115(11):i–ii, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVm

[Ano15i] Anonymous. Cover image, volume 115, issue 12. *International Journal of Quantum Chemistry*, 115(12):i–ii, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVn

[Ano15j] Anonymous. Cover image, volume 115, issue 13. *International Journal of Quantum Chemistry*, 115(13):i–ii, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVo

[Ano15k] Anonymous. Cover image, volume 115, issue 14. *International Journal of Quantum Chemistry*, 115(14):i–ii, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVp

[Ano15l] Anonymous. Cover image, volume 115, issue 15. *International Journal of Quantum Chemistry*, 115(15):i–ii, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVq

[Ano15m] Anonymous. Cover image, volume 115, issue 16. *International Journal of Quantum Chemistry*, 115(16):i–ii, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVr

[Ano15n] Anonymous. Cover image, volume 115, issue 16. *International Journal of Quantum Chemistry*, 115(16):iii–iv, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVs

[Ano15o] Anonymous. Cover image, volume 115, issue 16. *International Journal of Quantum Chemistry*, 115(16):v–vi, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVt

[Ano15p] Anonymous. Cover image, volume 115, issue 17. *International Journal of Quantum Chemistry*, 115(17):i–ii, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVu

[Ano15q] Anonymous. Cover image, volume 115, issue 18. *International Journal of Quantum Chemistry*, 115(18):i–ii, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVv

[Ano15r] Anonymous. Cover image, volume 115, issue 19. *International Journal of Quantum Chemistry*, 115(19):i–ii, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVw

[Ano15s] Anonymous. Cover image, volume 115, issue 19. *International Journal of Quantum Chemistry*, 115(19):iii–iv, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVa

[Ano15t] Anonymous. Cover image, volume 115, issue 2. *International Journal of Quantum Chemistry*, 115(2):i–ii, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVx

[Ano15u] Anonymous. Cover image, volume 115, issue 20. *International Journal of Quantum Chemistry*, 115(20):i–ii, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVy

[Ano15v] Anonymous. Cover image, volume 115, issue 21. *International Journal of Quantum Chemistry*, 115(21):i–ii, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVz

[Ano15w] Anonymous. Cover image, volume 115, issue 22. *International Journal of Quantum Chemistry*, 115(22):i–ii, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVaa

[Ano15x] Anonymous. Cover image, volume 115, issue 23. *International Journal of Quantum Chemistry*, 115(23):i–ii, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVab

[Ano15y] Anonymous. Cover image, volume 115, issue 23. *International Journal of Quantum Chemistry*, 115(23):iii–iv, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVac

[Ano15z] Anonymous. Cover image, volume 115, issue 24. *International Journal of Quantum Chemistry*, 115(24):i–ii, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVb

[Ano15-27] Anonymous. Cover image, volume 115, issue 3. *International Journal of Quantum Chemistry*, 115(3):i–ii, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVc

[Ano15-28] Anonymous. Cover image, volume 115, issue 4. *International Journal of Quantum Chemistry*, 115(4):i–ii, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVd

[Ano15-29] Anonymous. Cover image, volume 115, issue 5. *International Journal of Quantum Chemistry*, 115(5):i–ii, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVe

[Ano15-30] Anonymous. Cover image, volume 115, issue 6. *International Journal of Quantum Chemistry*, 115(6):i–ii, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVf

[Ano15-31] Anonymous. Cover image, volume 115, issue 7. *International Journal of Quantum Chemistry*, 115(7):i–ii, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVg

[Ano15-32] Anonymous. Cover image, volume 115, issue 8. *International Journal of Quantum Chemistry*, 115(8):i–ii, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVh

[Ano15-33] Anonymous. Cover image, volume 115, issue 9. *International Journal of Quantum Chemistry*, 115(9):i–ii, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:CIVi

[Ano15-34] Anonymous. Cover image, volume 115, issue 9. *International Journal of Quantum Chemistry*, 115(9):iii–iv, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIa

[Ano15-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(1):i–v, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIb

[Ano15-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(2):v–viii, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIc

[Ano15-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(3):v–viii, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IId

[Ano15-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(4):v–viii, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIe

[Ano15-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(5):v–ix, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIf

[Ano15-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(6):v–viii, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIg

[Ano15-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(7):iii–vi, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIh

[Ano15-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(8):iii–vi, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIi

[Ano15-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(9):v–viii, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIj

[Ano15-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(10):v–viii, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIk

[Ano15-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(11):iii–vii, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIl

[Ano15-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(12):iii–vi, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIm

[Ano15-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(13):iii–vi, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIn

[Ano15-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(14):iii–vi, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIo

[Ano15-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(15):iii–vi, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIp

[Ano15-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(16):vii–xii, August 15, 2015. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIq

[Ano15-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(17):iii–vi, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIr

[Ano15-52] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(18):iii–vii, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIs

[Ano15-53] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(19):v–x, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIt

[Ano15-54] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(20):iii–vii, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIu

[Ano15-55] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(21):iii–vi, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIv

[Ano15-56] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(22):iii–vi, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIw

[Ano15-57] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(23):v–viii, December 5, 2015.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2015:IIx

[Ano15-58] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 115(24):iii–vi, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVa

[Ano16a] Anonymous. Cover image, volume 116, issue 1. *International Journal of Quantum Chemistry*, 116(1):i, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVk

[Ano16b] Anonymous. Cover image, volume 116, issue 10. *International Journal of Quantum Chemistry*, 116(10):i, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVl

[Ano16c] Anonymous. Cover image, volume 116, issue 10. *International Journal of Quantum Chemistry*, 116(10):i, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVm

[Ano16d] Anonymous. Cover image, volume 116, issue 11. *International Journal of Quantum Chemistry*, 116(11):i, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVn

[Ano16e] Anonymous. Cover image, volume 116, issue 12. *International Journal of Quantum Chemistry*, 116(12):i, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVo

[Ano16f] Anonymous. Cover image, volume 116, issue 12. *International Journal of Quantum Chemistry*, 116(12):ii, June

15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVp

[Ano16g] Anonymous. Cover image, volume 116, issue 13. *International Journal of Quantum Chemistry*, 116(13):i, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVq

[Ano16h] Anonymous. Cover image, volume 116, issue 14. *International Journal of Quantum Chemistry*, 116(14):i, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVr

[Ano16i] Anonymous. Cover image, volume 116, issue 15. *International Journal of Quantum Chemistry*, 116(15):i, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVs

[Ano16j] Anonymous. Cover image, volume 116, issue 16. *International Journal of Quantum Chemistry*, 116(16):i, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVt

[Ano16k] Anonymous. Cover image, volume 116, issue 17. *International Journal of Quantum Chemistry*, 116(17):i, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVu

[Ano16l] Anonymous. Cover image, volume 116, issue 18. *International Journal of Quantum Chemistry*, 116(18):i, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVv

[Ano16m] Anonymous. Cover image, volume 116, issue 19. *International Journal of Quantum Chemistry*, 116(19):i, October

5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVb

[Ano16n] Anonymous. Cover image, volume 116, issue 2. *International Journal of Quantum Chemistry*, 116(2):i, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVw

[Ano16o] Anonymous. Cover image, volume 116, issue 20. *International Journal of Quantum Chemistry*, 116(20):i, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVx

[Ano16p] Anonymous. Cover image, volume 116, issue 21. *International Journal of Quantum Chemistry*, 116(21):i, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVy

[Ano16q] Anonymous. Cover image, volume 116, issue 22. *International Journal of Quantum Chemistry*, 116(22):i, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVz

[Ano16r] Anonymous. Cover image, volume 116, issue 23. *International Journal of Quantum Chemistry*, 116(23):i, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVaa

[Ano16s] Anonymous. Cover image, volume 116, issue 23. *International Journal of Quantum Chemistry*, 116(23):ii, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVab

[Ano16t] Anonymous. Cover image, volume 116, issue 24. *International Journal of Quantum Chemistry*, 116(24):i, December

15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVc

[Ano16u] Anonymous. Cover image, volume 116, issue 3. *International Journal of Quantum Chemistry*, 116(3):i, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVd

[Ano16v] Anonymous. Cover image, volume 116, issue 4. *International Journal of Quantum Chemistry*, 116(4):i, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVe

[Ano16w] Anonymous. Cover image, volume 116, issue 5. *International Journal of Quantum Chemistry*, 116(5):i, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVf

[Ano16x] Anonymous. Cover image, volume 116, issue 6. *International Journal of Quantum Chemistry*, 116(6):i, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVg

[Ano16y] Anonymous. Cover image, volume 116, issue 7. *International Journal of Quantum Chemistry*, 116(7):i, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVh

[Ano16z] Anonymous. Cover image, volume 116, issue 8. *International Journal of Quantum Chemistry*, 116(8):i, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVi

[Ano16-27] Anonymous. Cover image, volume 116, issue 8. *International Journal of Quantum Chemistry*, 116(8):ii, April 15,

2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:CIVj

[Ano16-28] Anonymous. Cover image, volume 116, issue 9. *International Journal of Quantum Chemistry*, 116(9):i, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIa

[Ano16-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(1):ii–vi, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIb

[Ano16-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(2):61–66, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIc

[Ano16-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(3):131–136, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IId

[Ano16-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(4):253–257, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIe

[Ano16-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(5):333–337, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIf

[Ano16-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(6):405–409, March 15, 2016. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIg

[Ano16-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(7):483–488, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIh

[Ano16-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(8):555–560, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIi

[Ano16-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(9):657–662, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIj

[Ano16-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(10):731–736, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIk

[Ano16-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(10):731–736, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIl

[Ano16-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(11):795–800, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIm

[Ano16-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(12):891–896, June 15, 2016. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIn

[Ano16-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(13):973–978, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIo

[Ano16-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(14):1051–1056, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIp

[Ano16-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(15):1133–1137, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIq

[Ano16-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(16):1191–1195, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIr

[Ano16-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(17):1269–1273, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIs

[Ano16-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(18):1323–1327, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIt

[Ano16-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(19):1383–1387, October 5, 2016.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIu

[Ano16-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(20):1437–1441, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIv

[Ano16-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(21):1493–1498, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIw

[Ano16-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(22):1613–1617, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIx

[Ano16-52] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(23):1747–1751, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2016:IIy

[Ano16-53] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 116(24):1823–1828, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVa

[Ano17a] Anonymous. Cover image, volume 117, issue 1. *International Journal of Quantum Chemistry*, 117(1):i, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVb

[Ano17b] Anonymous. Cover image, volume 117, issue 1. *International Journal of Quantum Chemistry*, 117(1):ii, January

5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVl

[Ano17c] Anonymous. Cover image, volume 117, issue 10. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVm

[Ano17d] Anonymous. Cover image, volume 117, issue 11. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVn

[Ano17e] Anonymous. Cover image, volume 117, issue 12. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVo

[Ano17f] Anonymous. Cover image, volume 117, issue 13. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVp

[Ano17g] Anonymous. Cover image, volume 117, issue 14. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVq

[Ano17h] Anonymous. Cover image, volume 117, issue 15. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVr

[Ano17i] Anonymous. Cover image, volume 117, issue 16. *International Journal of Quantum Chemistry*, 117(16):??, August

15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVs

[Ano17j] Anonymous. Cover image, volume 117, issue 17. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVt

[Ano17k] Anonymous. Cover image, volume 117, issue 18. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVu

[Ano17l] Anonymous. Cover image, volume 117, issue 19. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVc

[Ano17m] Anonymous. Cover image, volume 117, issue 2. *International Journal of Quantum Chemistry*, 117(2):i, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVd

[Ano17n] Anonymous. Cover image, volume 117, issue 2. *International Journal of Quantum Chemistry*, 117(2):ii, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVv

[Ano17o] Anonymous. Cover image, volume 117, issue 20. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVw

[Ano17p] Anonymous. Cover image, volume 117, issue 21. *International Journal of Quantum Chemistry*, 117(21):??, Novem-

ber 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVx

[Ano17q] Anonymous. Cover image, volume 117, issue 22. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVy

[Ano17r] Anonymous. Cover image, volume 117, issue 23. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVz

[Ano17s] Anonymous. Cover image, volume 117, issue 24. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVe

[Ano17t] Anonymous. Cover image, volume 117, issue 3. *International Journal of Quantum Chemistry*, 117(3):i, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVf

[Ano17u] Anonymous. Cover image, volume 117, issue 4. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVg

[Ano17v] Anonymous. Cover image, volume 117, issue 5. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVh

[Ano17w] Anonymous. Cover image, volume 117, issue 6. *International Journal of Quantum Chemistry*, 117(6):??, March

15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVi

[Ano17x] Anonymous. Cover image, volume 117, issue 7. *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVj

[Ano17y] Anonymous. Cover image, volume 117, issue 8. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:CIVk

[Ano17z] Anonymous. Cover image, volume 117, issue 9. *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIa

[Ano17-27] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(1):1–5, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIb

[Ano17-28] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(2):75–79, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIc

[Ano17-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(3):151–156, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IId

[Ano17-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIe

[Ano17-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIf

[Ano17-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIg

[Ano17-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIh

[Ano17-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIi

[Ano17-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIj

[Ano17-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIk

[Ano17-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIl

[Ano17-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIm

[Ano17-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIn

[Ano17-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIo

[Ano17-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIp

[Ano17-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIq

[Ano17-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIr

[Ano17-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIs

[Ano17-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIt

[Ano17-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIu

[Ano17-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIv

[Ano17-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIw

[Ano17-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2017:IIx

[Ano17-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVa

[Ano18a] Anonymous. Cover image, volume 118, issue 1. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVb

[Ano18b] Anonymous. Cover image, volume 118, issue 1. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVm

[Ano18c] Anonymous. Cover image, volume 118, issue 10. *International Journal of Quantum Chemistry*, 118(10):e25636:1–e25636:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVn

[Ano18d] Anonymous. Cover image, volume 118, issue 11. *International Journal of Quantum Chemistry*, 118(11):e25642:1–e25642:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVo

[Ano18e] Anonymous. Cover image, volume 118, issue 12. *International Journal of Quantum Chemistry*, 118(12):e25652:1–e25652:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVp

[Ano18f] Anonymous. Cover image, volume 118, issue 13. *International Journal of Quantum Chemistry*, 118(13):e25668:1–e25668:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVq

[Ano18g] Anonymous. Cover image, volume 118, issue 14. *International Journal of Quantum Chemistry*, 118(14):e25701:1–e25701:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVr

[Ano18h] Anonymous. Cover image, volume 118, issue 15. *International Journal of Quantum Chemistry*, 118(15):e25702:1–e25702:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVs

[Ano18i] Anonymous. Cover image, volume 118, issue 16. *International Journal of Quantum Chemistry*, 118(16):e25790:1–e25790:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVt

[Ano18j] Anonymous. Cover image, volume 118, issue 16. *International Journal of Quantum Chemistry*, 118(16):e25803:1–e25803:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVu

[Ano18k] Anonymous. Cover image, volume 118, issue 17. *International Journal of Quantum Chemistry*, 118(17):e25804:1–e25804:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVv

[Ano18l] Anonymous. Cover image, volume 118, issue 18. *International Journal of Quantum Chemistry*, 118(18):e25805:1–e25805:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVw

[Ano18m] Anonymous. Cover image, volume 118, issue 18. *International Journal of Quantum Chemistry*, 118(18):e25810:1–e25810:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVx

[Ano18n] Anonymous. Cover image, volume 118, issue 19. *International Journal of Quantum Chemistry*, 118(19):e25815:1–e25815:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVc

[Ano18o] Anonymous. Cover image, volume 118, issue 2. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVy

[Ano18p] Anonymous. Cover image, volume 118, issue 20. *International Journal of Quantum Chemistry*, 118(20):e25828:1–e25828:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVz

[Ano18q] Anonymous. Cover image, volume 118, issue 21. *International Journal of Quantum Chemistry*, 118(21):e25829:1–e25829:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVaa

[Ano18r] Anonymous. Cover image, volume 118, issue 22. *International Journal of Quantum Chemistry*, 118(22):e25830:1–e25830:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVab

[Ano18s] Anonymous. Cover image, volume 118, issue 23. *International Journal of Quantum Chemistry*, 118(23):e25832:1–e25832:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVac

[Ano18t] Anonymous. Cover image, volume 118, issue 24. *International Journal of Quantum Chemistry*, 118(24):e25833:1–e25833:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVd

[Ano18u] Anonymous. Cover image, volume 118, issue 3. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVe

[Ano18v] Anonymous. Cover image, volume 118, issue 4. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVf

[Ano18w] Anonymous. Cover image, volume 118, issue 5. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVg

[Ano18x] Anonymous. Cover image, volume 118, issue 6. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVh

[Ano18y] Anonymous. Cover image, volume 118, issue 7. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVi

[Ano18z] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25628:1–e25628:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVj

[Ano18-27] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25631:1–e25631:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVk

[Ano18-28] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25632:1–e25632:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:CIVl

[Ano18-29] Anonymous. Cover image, volume 118, issue 9. *International Journal of Quantum Chemistry*, 118(9):e25633:1–e25633:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:E

[Ano18-30] Anonymous. Editorial. *International Journal of Quantum Chemistry*, 118(9):e25615:1–e25615:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIa

[Ano18-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIb

[Ano18-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIc

[Ano18-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IId

[Ano18-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIe

[Ano18-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIf

[Ano18-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIg

[Ano18-37] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIh

[Ano18-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(9):e25471:1–e25471:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIi

[Ano18-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(10):e25472:1–e25472:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIj

[Ano18-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(11):e25473:1–e25473:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIk

[Ano18-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(12):e25474:1–e25474:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIl

[Ano18-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(13):e25475:1–e25475:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIm

[Ano18-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(14):e25476:1–e25476:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIn

[Ano18-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(15):e25477:1–e25477:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIo

[Ano18-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(16):e25478:1–e25478:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIp

[Ano18-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(17):e25479:1–e25479:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIq

[Ano18-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(18):e25480:1–e25480:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIr

[Ano18-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(19):e25481:1–e25481:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIs

[Ano18-49] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(20):e25482:1–e25482:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIt

[Ano18-50] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(21):e25483:1–e25483:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIu

[Ano18-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(22):e25484:1–e25484:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIv

[Ano18-52] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(23):e25485:1–e25485:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2018:IIw

[Ano18-53] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 118(24):e25486:1–e25486:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVa

[Ano19a] Anonymous. Cover image, volume 119, issue 1. *International Journal of Quantum Chemistry*, 119(1):e25840:1–e25840:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVb

[Ano19b] Anonymous. Cover image, volume 119, issue 1. *International Journal of Quantum Chemistry*, 119(1):e25841:1–e25841:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVc

[Ano19c] Anonymous. Cover image, volume 119, issue 1. *International Journal of Quantum Chemistry*, 119(1):e25842:1–e25842:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVd

[Ano19d] Anonymous. Cover image, volume 119, issue 1. *International Journal of Quantum Chemistry*, 119(1):e25843:1–e25843:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVm

[Ano19e] Anonymous. Cover image, volume 119, issue 10. *International Journal of Quantum Chemistry*, 119(10):e25947:1–e25947:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVn

[Ano19f] Anonymous. Cover image, volume 119, issue 11. *International Journal of Quantum Chemistry*, 119(11):e25948:1–e25948:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVo

[Ano19g] Anonymous. Cover image, volume 119, issue 12. *International Journal of Quantum Chemistry*, 119(12):e25960:1–e25960:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVp

[Ano19h] Anonymous. Cover image, volume 119, issue 13. *International Journal of Quantum Chemistry*, 119(13):e25970:1–e25970:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVq

[Ano19i] Anonymous. Cover image, volume 119, issue 14. *International Journal of Quantum Chemistry*, 119(14):e25988:1–e25988:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVr

[Ano19j] Anonymous. Cover image, volume 119, issue 15. *International Journal of Quantum Chemistry*, 119(15):e26002:1–e26002:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVs

[Ano19k] Anonymous. Cover image, volume 119, issue 16. *International Journal of Quantum Chemistry*, 119(16):e26011:1–e26011:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVt

[Ano19l] Anonymous. Cover image, volume 119, issue 17. *International Journal of Quantum Chemistry*, 119(17):e26023:1–e26023:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVu

[Ano19m] Anonymous. Cover image, volume 119, issue 18. *International Journal of Quantum Chemistry*, 119(18):e26024:1–e26024:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVv

[Ano19n] Anonymous. Cover image, volume 119, issue 19. *International Journal of Quantum Chemistry*, 119(19):e26031:1–e26031:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVe

[Ano19o] Anonymous. Cover image, volume 119, issue 2. *International Journal of Quantum Chemistry*, 119(2):e25879:1–e25879:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVw

[Ano19p] Anonymous. Cover image, volume 119, issue 20. *International Journal of Quantum Chemistry*, 119(20):e26049:1–e26049:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVx

[Ano19q] Anonymous. Cover image, volume 119, issue 21. *International Journal of Quantum Chemistry*, 119(21):e26050:1–e26050:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVy

[Ano19r] Anonymous. Cover image, volume 119, issue 22. *International Journal of Quantum Chemistry*, 119(22):e26063:1–e26063:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVz

[Ano19s] Anonymous. Cover image, volume 119, issue 23. *International Journal of Quantum Chemistry*, 119(23):e26064:1–e26064:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVaa

[Ano19t] Anonymous. Cover image, volume 119, issue 24. *International Journal of Quantum Chemistry*, 119(24):e26095:1–e26095:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVf

[Ano19u] Anonymous. Cover image, volume 119, issue 3. *International Journal of Quantum Chemistry*, 119(3):e25889:1–e25889:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVg

[Ano19v] Anonymous. Cover image, volume 119, issue 4. *International Journal of Quantum Chemistry*, 119(4):e25891:1–e25891:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVh

[Ano19w] Anonymous. Cover image, volume 119, issue 5. *International Journal of Quantum Chemistry*, 119(5):e25901:1–e25901:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVi

[Ano19x] Anonymous. Cover image, volume 119, issue 6. *International Journal of Quantum Chemistry*, 119(6):e25905:1–e25905:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVj

[Ano19y] Anonymous. Cover image, volume 119, issue 7. *International Journal of Quantum Chemistry*, 119(7):e25906:1–e25906:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVk

[Ano19z] Anonymous. Cover image, volume 119, issue 8. *International Journal of Quantum Chemistry*, 119(8):e25922:1–e25922:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:CIVl

[Ano19-27] Anonymous. Cover image, volume 119, issue 9. *International Journal of Quantum Chemistry*, 119(9):e25923:1–e25923:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIa

[Ano19-28] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(1):e25730:1–e25730:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIb

[Ano19-29] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(2):e25731:1–e25731:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIc

[Ano19-30] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(3):e25732:1–e25732:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IId

[Ano19-31] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(4):e25733:1–e25733:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIe

[Ano19-32] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(5):e25734:1–e25734:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIf

[Ano19-33] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(6):e25735:1–e25735:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIg

[Ano19-34] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(7):e25736:1–e25736:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIh

[Ano19-35] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(8):e25737:1–e25737:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIi

[Ano19-36] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(9):e25738:1–e25738:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIj

[Ano19-37] Anonymous. Issue Information. *International Journal of Quantum Chemistry*, 119(10):e25739:1–e25739:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIk

[Ano19-38] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(11):e25740:1–e25740:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIl

[Ano19-39] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(12):e25741:1–e25741:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIm

[Ano19-40] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(13):e25742:1–e25742:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIn

[Ano19-41] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(14):e25743:1–e25743:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIo

[Ano19-42] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(15):e25744:1–e25744:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIp

[Ano19-43] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(16):e25745:1–e25745:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIq

[Ano19-44] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(17):e25746:1–e25746:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIr

[Ano19-45] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(18):e25747:1–e25747:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIs

[Ano19-46] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(19):e25748:1–e25748:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIt

[Ano19-47] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(20):e25749:1–e25749:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIu

[Ano19-48] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(21):e25750:1–e25750:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIv

[Ano19-49] Anonymous. Issue Information. *International Journal of Quantum Chemistry*, 119(22):e25751:1–e25751:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIw

[Ano19-50] Anonymous. Issue Information. *International Journal of Quantum Chemistry*, 119(23):e25752:1–e25752:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Anonymous:2019:IIx

[Ano19-51] Anonymous. Issue information. *International Journal of Quantum Chemistry*, 119(24):e25753:1–e25753:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aburto:2012:HSO

[AO12a] Andrea Aburto and Emilio Orgaz. Hydrogen site occupation and electronic structure in the La_2Ni_2In intermetallic and hydrides. *International Journal of Quantum Chemistry*, 112(22):3606–3611, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Akdemir:2012:GFR

[AÖ12b] S. Ö. Akdemir and E. Öztekin. Generating function for rotation matrix elements. *International Journal of Quantum Chemistry*, 112(2):367–372, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alves:2012:DFP

[AOLB12] Márcio Oliveira Alves, Jessé Moreira Oliveira, Nelson Henrique Teixeira Lemes, and João Pedro Braga. From deflection function to potential energy: a Firsov approach critical analysis. *International Journal of Quantum Chemistry*, 112 (19):3141–3146, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2018:OLC

[AOT+18] Diego R. Alcoba, Ofelia B. Oña, Alicia Torre, Luis Lain, and William Tiznado. An orbital localization criterion based on the topological analysis of the electron localization function at correlated level. *International Journal of Quantum Chemistry*, 118(15):e25588:1–e25588:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ancarani:2011:CSC

[ARG11] L. U. Ancarani, K. V. Rodriguez, and G. Gasaneo. Correlated $n^{1,3}$ S states for Coulomb three-body systems. *International Journal of Quantum Chemistry*, 111(15):4255–4265, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arntsen:2013:DDC

[ARH+13] Christopher Arntsen, Randa Reslan, Samuel Hernandez, Yi Gao, and Daniel Neuhauser. Direct delocalization for calculating electron transfer in fullerenes. *International Journal of Quantum Chemistry*, 113(15):1885–1889, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arteca:2008:GED

[ART08] Gustavo A. Arteca, Jean Pierre Rank, and O. Tapia. Generalized electronic diabatic approach to structural similarity in two-dimensional potential energy surfaces of various topologies. *International Journal of Quantum Chemistry*, 108(4):651–666, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Albuquerque:2019:PMD

[AS19] Johnross Virgil Albuquerque and Rajendra Nivrutti Shirsat. Prelude to molecular dynamics: Topography-driven Gaussian charge models. *International Journal of Quantum Chemistry*, 119(6):e25835:1–e25835:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Attia:2014:TSR

[ASD14] Amr Ali Attia and Radu Silaghi-Dumitrescu. A theoretical study on the reaction pathways of peroxynitrite formation and decay at nonheme iron centers. *International Journal of Quantum Chemistry*, 114(10):652–665, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Attia:2018:NSI

[ASD18] Amr A. A. Attia and Radu Silaghi-Dumitrescu. Nickel-substituted iron-dependent cysteine dioxygenase: Implica-

tions for the dioxygenation activity of nickel model compounds. *International Journal of Quantum Chemistry*, 118 (13):e25564:1–e25564:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Asher:2018:AVO

[Ash18] James R. Asher. An animated visualization of orbital angular momentum and spin-orbit coupling. *International Journal of Quantum Chemistry*, 118(18):e25683:1–e25683:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ahlstrand:2013:IEB

[ASHF13] Emma Ahlstrand, Daniel Spångberg, Kersti Hermansson, and Ran Friedman. Interaction energies between metal ions (Zn^{2+} and Cd^{2+}) and biologically relevant ligands. *International Journal of Quantum Chemistry*, 113(23):2554–2562, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Azadi:2015:RVB

[ASK15] Sam Azadi, Ranber Singh, and Thoms D. Kühne. Resonating valence bond quantum Monte Carlo: Application to the ozone molecule. *International Journal of Quantum Chemistry*, 115(23):1673–1677, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ahubelem:2015:FBC

[ASMP15] Nwakamma Ahubelem, Kalpit Shah, Behdad Moghtaderi, and Alister J. Page. Formation of benzofuran and chlorobenzofuran from 1,3-dichloropropene: a quantum chemical investigation. *International Journal of Quantum Chemistry*, 115(24):1739–1745, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Astakhov:2016:PIA

[AST16] Andrey A. Astakhov, Adam I. Stash, and Vladimir G. Tsirelson. Perspective: Improving approximate determination of the noninteracting electronic kinetic energy density from electron density. *International Journal of Quantum Chemistry*, 116(3):237–246, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Artyukova:2019:AHP

[AST19] Svetlana Artyukova, Konstantin Sveshnikov, and Andrey Tolokonnikov. Atomic H over plane: Effective potential and level reconstruction. *International Journal of Quantum Chemistry*, 119(17):e25965:1–e25965:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Arriagada:2013:RCU

[ASW13] Diego Cortés Arriagada, Luís Sanhueza, and Kerry Wrighton. Removal of 4-chlorophenol using graphene, graphene oxide, and A-doped graphene ($A = N, B$): a computational study. *International Journal of Quantum Chemistry*, 113(15):1931–1939, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Astakhov:2018:SRC

[AT18] Andrey A. Astakhov and Vladimir G. Tsirelson. Spatially resolved characterization of electron localization and delocalization in molecules: Extending the Kohn–Resta approach. *International Journal of Quantum Chemistry*, 118 (15):e25600:1–e25600:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2014:DHE

[ATL+14] Diego R. Alcoba, Alicia Torre, Luis Lain, Ofelia B. Oña, and Josep M. Oliva. Determination of Heisenberg exchange coupling constants in clusters with magnetic sites: a local spin approach. *International Journal of Quantum Chemistry*, 114(14):952–958, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alvarez-Thon:2017:IAH

[ATM17] Luis Alvarez-Thon and Liliana Mammino. An investigation of aromaticity in hydroxybenzenes based on the study of magnetically induced current density. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Alcoba:2011:CCE

[ATPRV11] D. R. Alcoba, L. M. Tel, E. Pérez-Romero, and C. Valdemoro. Convergence and computational efficiency enhancements in the iterative solution of the G-particle-hole hypervirial equation. *International Journal of Quantum Chemistry*, 111(5):937–949, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aquino:2011:FCB

[ATS+11] Adélia J. A. Aquino, Daniel Tunega, Gabriele E. Schaumann, Georg Haberhauer, Martin H. Gerzabek, and Hans Lischka. The functionality of cation bridges for binding polar groups in soil aggregates. *International Journal of Quantum Chemistry*, 111(7–8):1531–1542, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aschauer:2015:ISS

[ATS15] Ulrich Johannes Aschauer, Antonio Tilocca, and Annabella Selloni. Ab initio simulations of the structure of thin water layers on defective anatase TiO_2 (101) surfaces. *International Journal of Quantum Chemistry*, 115(18):1250–1257, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Afonin:2019:BCI

[AV19] Andrei V. Afonin and Alexander V. Vashchenko. Benchmark calculations of intramolecular hydrogen bond energy based on molecular tailoring and function-based approaches: Developing hybrid approach. *International Journal of Quantum Chemistry*, 119(21):e26001:1–e26001:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Asha:2019:PBI

[AVG19a] Suseeladevi Asha, Kunduchi P. Vijayalakshmi, and Benny K. George. Pyrrolidinium-based ionic liquids as electrolytes for lithium batteries: a computational study. *International Journal of Quantum Chemistry*, 119(22): e26014:1–e26014:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Asha:2019:ESS

[AVG19b] Suseeladevi Asha, Kunduchi Periya Vijayalakshmi, and Benny K. George. Electronic structural studies of pyrrolidinium-based ionic liquids for electrochemical application. *International Journal of Quantum Chemistry*, 119(17):e25972:1–e25972:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aydogdu:2015:BSS

[AY15] Oktay Aydoğdu and Hilmi Yanar. Bound and scattering states for a hyperbolic-type potential in view of a new developed approximation. *International Journal of Quantum Chemistry*, 115(8):529–534, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Aschi:2011:EEB

[AZD+11] Massimiliano Aschi, Romina Zappacosta, Paolo De Maria, Gabriella Siani, Antonella Fontana, and Andrea Amadei. Entropy–energy balance in base catalyzed keto-enol interconversion: a joint theoretical and experimental investigation. *International Journal of Quantum Chemistry*, 111 (7–8):1293–1305, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boyko:2013:CBS

[BA13] Maksim A. Boyko and Igor V. Abarenkov. Crystal band structure from the embedded cluster. *International Journal of Quantum Chemistry*, 113(14):1877–1883, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bertini:2018:PFE

[BAA+18] Luca Bertini, Marta Erminia Alberto, Federica Arrigoni, Jacopo Vertemara, Piercarlo Fantucci, Maurizio Bruschi, Giuseppe Zampella, and Luca De Gioia. On the photochemistry of Fe_2 (edt)$(CO)_4$ $(PMe_3)_2$, a [FeFe]-hydrogenase model: a DFT/TDDFT investigation. *International Journal of Quantum Chemistry*, 118(9):e25537:1–e25537:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Breuza:2018:MSZ

[BAB+18] Emanuele Breuza, Giuseppe Antinucci, Peter H. M. Budzelaar, Vincenzo Busico, Andrea Correa, and Christian Ehm. $MgCl_2$-supported Ziegler–Natta catalysts: a DFT-D 'flexible-cluster' approach. $TiCl_4$ and probe donor adducts. *International Journal of Quantum Chemistry*, 118(21): e25721:1–e25721:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baer:2014:TDM

[Bae14] Michael Baer. Time-dependent molecular fields created by the interaction of an external electromagnetic field with a molecular system. *International Journal of Quantum Chemistry*, 114(24):1645–1659, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baeck:2016:TRB

[Bae16] Kyoung Koo Baeck. Tutorial reviews: Basics of the time-dependent wave-packet propagation for photodissociations of polyatomic systems. *International Journal of Quantum Chemistry*, 116(8):634–643, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balasubramanian:2016:QCI

[Bal16] Krishnan Balasubramanian. Quantum chemical insights into Alzheimer's disease: Curcumin's chelation with Cu(II), Zn(II), and Pd(II) as a mechanism for its prevention. *International Journal of Quantum Chemistry*, 116 (14):1107–1119, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Batiha:2012:TSR

[BAMA12] Marwan Batiha, Ala'a H. Al-Muhtaseb, and Mohammednoor Altarawneh. Theoretical study on the reaction of the phenoxy radical with O_2, OH, and NO_2. *International Journal of Quantum Chemistry*, 112(3):848–857, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandrauk:2012:BRA

[Ban12] Andre D. Bandrauk. Book review: *Advances in quantum chemistry: Unstable states in the continuous spectra. Part 1*, edited by C. A. Nicolaides and E. Brändas. *International Journal of Quantum Chemistry*, 112(15):2763, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barreto:2012:PES

[BAP12] Patrícia R. P. Barreto, Alessandra F. Albernaz, and Federico Palazzetti. Potential energy surfaces for van der Waals complexes of rare gases with H_2S and H_2S_2: Extension to xenon interactions and hyperspherical harmonics representation. *International Journal of Quantum Chemistry*, 112 (3):834–847, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borisova:2013:HSA

[BAP13] Dobrina Borisova, Vladislav Antonov, and Ana Proykova. Hydrogen sulfide adsorption on a defective graphene. *International Journal of Quantum Chemistry*, 113(6):786–791, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrera:2011:SOH

[Bar11] Mauricio Barrera. Study of the orbital hardness and the Kohn–Sham radius on single monoatomic anions. *International Journal of Quantum Chemistry*, 111(12):3097–3111, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barone:2016:ETC

[Bar16] Vincenzo Barone. Editorial: Theoretical and computational chemistry in Italy. *International Journal of Quantum Chemistry*, 116(21):1499–1500, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Basiuk:2011:ESD

[Bas11] Vladimir A. Basiuk. Electron smearing in DFT calculations: a case study of doxorubicin interaction with single-walled carbon nanotubes. *International Journal of Quan-*

tum Chemistry, 111(15):4197–4205, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bin:2019:NGQ

[BAX+19] Xin Bin, Alireza Azizi, Tianlv Xu, Steven R. Kirk, Michael Filatov, and Samantha Jenkins. Next-generation quantum theory of atoms in molecules for the photochemical ring-opening reactions of oxirane. *International Journal of Quantum Chemistry*, 119(16):e25957:1–e25957:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baye:2019:CHA

[Bay19] Daniel Baye. Confinement of hydrogen atom with Dirac equation. *International Journal of Quantum Chemistry*, 119(24):e26034:1–e26034:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:2010:QSM

[BB10] Edward A. Boudreaux and Eric C. Baxter. QR-SCMEH-MO calculations on inner-transition metal diatomic molecules having 12 valence electrons-Nd_2 and U_2. *International Journal of Quantum Chemistry*, 110(15): 2860–2864, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bushnell:2016:ISD

[BB16] Eric A. C. Bushnell and Russell J. Boyd. Identifying similarities and differences between analogous bisdithiolene and bisdiselenolene complexes: a computational study. *International Journal of Quantum Chemistry*, 116(5):369–376, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bruschi:2016:RCA

[BBA+16] Maurizio Bruschi, Raffaella Breglia, Federica Arrigoni, Piercarlo Fantucci, and Luca De Gioia. Reviews: Computational approaches to the prediction of the redox potentials of iron and copper bioinorganic systems. *International Journal of Quantum Chemistry*, 116(22):1695–1705, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borges:2012:ESN

[BBAL12] Itamar Borges Jr., Mario Barbatti, Adélia J. A. Aquino, and Hans Lischka. Electronic spectra of nitroethylene. *International Journal of Quantum Chemistry*, 112(4):1225–1232, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barone:2012:TAC

[BBB+12a] Vincenzo Barone, Małgorzata Biczysko, Julien Bloino, Monika Borkowska-Panek, Ivan Carnimeo, and Pawel Panek. Toward anharmonic computations of vibrational spectra for large molecular systems. *International Journal of Quantum Chemistry*, 112(9):2185–2200, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bordat:2012:ISS

[BBB+12b] P. Bordat, D. Bégué, R. Brown, A. Marbeuf, H. Cardy, and I. Baraille. The IR spectrum of supercritical water: Combined molecular dynamics/quantum mechanics strategy and force field for cluster sampling. *International Journal of Quantum Chemistry*, 112(13):2578–2584, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bloino:2016:TRA

[BBB16] Julien Bloino, Alberto Baiardi, and Małgorzata Biczysko. Tutorial reviews: Aiming at an accurate prediction of vibrational and electronic spectra for medium-to-large molecules: an overview. *International Journal of Quantum Chemistry*, 116(21):1543–1574, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balaban:2016:ECA

[BBKO16] Alexandru T. Balaban, Debojit Bhattacharya, Douglas J. Klein, and Yenni P. Ortiz. Energies for cyclic and acyclic aggregations of adamantane and diamantane units sharing vertices, edges, or six-membered rings. *International Journal of Quantum Chemistry*, 116(2):113–122, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benguria:2012:NEI

[BBL12] Rafael D. Benguria, Gonzalo A. Bley, and Michael Loss. A new estimate on the indirect Coulomb energy. *International Journal of Quantum Chemistry*, 112(6):1579–1584, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Biancardi:2017:FDC

[BBM17] Alessandro Biancardi, Tarita Biver, and Benedetta Mennucci. Fluorescent dyes in the context of DNA-binding: the case of Thioflavin T. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhusal:2018:ESC

[BBYZ18] Shusil Bhusal, Tunna Baruah, Yoh Yamamoto, and Rajendra R. Zope. Electronic structure calculation of vanadium- and scandium-based endohedral fullerenes $VSc_2N@C_{2n}$ ($2n = 70, 76, 78, 80$). *International Journal of Quantum Chemistry*, 118(24):e25785:1–e25785:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bartok:2015:TRG

[BC15] Albert P. Bartók and Gábor Csányi. Tutorial reviews: Gaussian approximation potentials: a brief tutorial introduction. *International Journal of Quantum Chemistry*, 115 (16):1051–1057, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [BC16].

Bartok:2016:EGA

[BC16] Albert P. Bartók and Gábor Csányi. Erratum: Gaussian approximation potentials: a brief tutorial introduction. *International Journal of Quantum Chemistry*, 116(13):1049, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BC15].

Bras:2011:CST

[BCF+11] Natércia F. Brás, Luís Cruz, Pedro A. Fernandes, Victor De Freitas, and Maria João Ramos. Conformational study of two diasteroisomers of vinylcatechin dimers in a methanol

solution. *International Journal of Quantum Chemistry*, 111 (7–8):1498–1510, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bandaru:2012:TAS

[BCGC12] Sateesh Bandaru, Arindam Chakraborty, Santanab Giri, and Pratim K. Chattaraj. Toward analyzing some neutral and cationic boron–lithium clusters (B_xLi_y, $x = 2$–$6; y = 1, 2$) as effective hydrogen storage materials: a conceptual density functional study. *International Journal of Quantum Chemistry*, 112(3):695–702, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrow:2016:PTC

[BCHN16] Joshua Barrow, Ken Caviness, Ray Hefferlin, and Devin Nash. Periodic trends in constants of triatomic molecules. *International Journal of Quantum Chemistry*, 116(14): 1071–1083, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barysz:2019:RCA

[BCK19] Maria Barysz, Ivan Cernusák, and Vladimir Kellö. Relativistic calculations of $AuSi^+$ and $AuSi^-$. *International Journal of Quantum Chemistry*, 119(16):e25951:1–e25951:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bolivar:2018:FMT

[BCNR18] Juan Carlos Bolívar, Nicolas A. Cordero, Ágnes Nagy, and Elvira Romera. Fidelity as a marker of topological phase transitions in 2D Dirac materials. *International Journal of Quantum Chemistry*, 118(17):e25674:1–e25674:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bastos:2010:RVB

[BCP10] Cristiano C. Bastos, Marconi B. S. Costa, and Antonio C. Pavão. Resonating valence-bond mechanism for the superconductivity in K_3 C_{60}. *International Journal of Quantum Chemistry*, 110(11):2088–2093, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burrell:2012:CSH

[BCS+12] Emily Burrell, Jared C. Clark, Mathew Snow, Heidi Dumais, Seong cheol Lee, Brad J. Nielson, Derek Osborne, Lucia Salamanca-cardona, Logan Zemp, Ryan S. Dabell, and Jaron C. Hansen. Computational study of hexanal peroxy radical–water complexes. *International Journal of Quantum Chemistry*, 112(8):1936–1944, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Banerjee:2012:TSS

[BD12] Amartya Banerjee and Kalyan Kumar Das. Theoretical spectroscopic studies of InI and InI^+. *International Journal of Quantum Chemistry*, 112(2):453–469, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baishya:2014:CAA

[BD14] Subhi Baishya and Ramesh C. Deka. Catalytic activities of Au_6, Au_6^-, and Au_6^+ clusters for CO oxidation: a density functional study. *International Journal of Quantum Chemistry*, 114(22):1559–1566, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baseggio:2016:SNU

[BDF+16] Oscar Baseggio, Martina De Vetta, Giovanna Fronzoni, Mauro Stener, and Alessandro Fortunelli. Software news & updates: a new time-dependent density-functional method for molecular plasmonics: Formalism, implementation, and the Au_{144} $(SH)_{60}$ case study. *International Journal of Quantum Chemistry*, 116(21):1603–1611, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baseggio:2018:TDD

[BDF+18] Oscar Baseggio, Martina De Vetta, Giovanna Fronzoni, Daniele Toffoli, Mauro Stener, Luca Sementa, and Alessandro Fortunelli. Time-dependent density-functional study of the photoabsorption spectrum of Au_25 $(SC_2H_4C_6H_5)_18$ anion: Validation of the computational protocol. *International Journal of Quantum Chemistry*, 118(22):e25769:1–

e25769:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barone:2010:CCA

[BDFM10] Giampaolo Barone, Dario Duca, Francesco Ferrante, and Gianfranco La Manna. CASSCF/CASPT2 analysis of the fragmentation of H_2 on a Pd_4 cluster. *International Journal of Quantum Chemistry*, 110(3):558–562, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Biswas:2017:INI

[BDG17] Abul Kalam Biswas, Amitava Das, and Bishwajit Ganguly. The influence of noncovalent interactions in metal-free organic dye molecules to augment the efficiency of dye sensitized solar cells: a computational study. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brouder:2012:RSP

[BDPT12] Christian Brouder, Gérard H. E. Duchamp, Frédéric Patras, and Gábor Z. Tóth. The Rayleigh–Schrödinger perturbation series of quasi-degenerate systems. *International Journal of Quantum Chemistry*, 112(10):2256–2266, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brahim:2012:SOA

[BDR12] Houari Brahim, Chantal Daniel, and Ali Rahmouni. Spin–orbit absorption spectroscopy of transition metal hydrides: A TD–DFT and MS-CASPT2 study of $HM(CO)_5$ (M = Mn, Re). *International Journal of Quantum Chemistry*, 112(9):2085–2097, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bargueno:2011:MSW

[BdTG11] Pedro Bargueño, Ricardo Pérez de Tudela, and Isabel Gonzalo. Mikheev–Smirnov–Wolfenstein effect in chiral molecules. *International Journal of Quantum Chemistry*, 111(2):430–434, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Behler:2015:TRC

[Beh15] Jörg Behler. Tutorial reviews: Constructing high-dimensional neural network potentials: a tutorial review. *International Journal of Quantum Chemistry*, 115(16): 1032–1050, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bendazzoli:2011:FCI

[BEM11] Gian Luigi Bendazzoli, Stefano Evangelisti, and Antonio Monari. Full-configuration-interaction study of the metal-insulator transition in a model system: H_n linear chains n =4, 6,..., 16. *International Journal of Quantum Chemistry*, 111(13):3416–3423, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bendazzoli:2012:AAL

[BEM12] Gian Luigi Bendazzoli, Stefano Evangelisti, and Antonio Monari. Asymptotic analysis of the localization spread and polarizability of 1-D noninteracting electrons. *International Journal of Quantum Chemistry*, 112(3):653–664, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brizhik:2010:DSZ

[BEPZ10a] Larissa Brizhik, Alexander Eremko, Bernard Piette, and Wojtek Zakrzewski. Davydov's solitons in zigzag carbon nanotubes. *International Journal of Quantum Chemistry*, 110(1):11–24, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brizhik:2010:RED

[BEPZ10b] Larissa Brizhik, Alexander Eremko, Bernard Piette, and Wojtek Zakrzewski. Ratchet effect of Davydov's solitons in nonlinear low-dimensional nanosystems. *International Journal of Quantum Chemistry*, 110(1):25–37, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berriche:2013:OEP

[Ber13a] H. Berriche. One-electron pseudopotential study of the alkali hydride cation NaH^+: Structure, spectroscopy, transition dipole moments, and radiative lifetimes. *International*

Journal of Quantum Chemistry, 113(7):1003–1009, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berriche:2013:ESS

[Ber13b] Hamid Berriche. Electronic, spectra, and spin orbit interaction for FrAr van der Waals system. *International Journal of Quantum Chemistry*, 113(9):1349–1357, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berriche:2013:PED

[Ber13c] Hamid Berriche. Potential energy and dipole moment of the Na_2^+ ionic molecule. *International Journal of Quantum Chemistry*, 113(21):2405–2412, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balakina:2011:QCS

[BF11] Marina Yu. Balakina and Olga D. Fominykh. The quantum-chemical study of organic octupolar chromophore triaminotrinitrobenzene and the dimer: Topological analysis and nonlinear optical characteristics. *International Journal of Quantum Chemistry*, 111(11):2677–2687, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bjorkman:2011:ASB

[BG11a] Torbjörn Björkman and Oscar Grånäs. Adaptive smearing for Brillouin zone integration. *International Journal of Quantum Chemistry*, 111(5):1025–1030, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borin:2011:ESC

[BG11b] Antonio Carlos Borin and João Paulo Gobbo. Electronic structure and chemical bonding in the ground and low-lying electronic states of Ta_2. *International Journal of Quantum Chemistry*, 111(7–8):1306–1315, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borin:2011:ESG

[BG11c] Antonio Carlos Borin and João Paulo Gobbo. Electronic structure of the ground and low-lying electronic states

of MoB and MoB^+. *International Journal of Quantum Chemistry*, 111(13):3362–3370, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhavaraju:2013:TAS

[BG13] Manikanthan Bhavaraju and Steven R. Gwaltney. A theoretical analysis of substituted aromatic compounds. *International Journal of Quantum Chemistry*, 113(8):1171–1179, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blanchard:2012:DFT

[BGBV12] Philippe Blanchard, José M. Gracia-Bondía, and Joseph C. Várilly. Density functional theory on phase space. *International Journal of Quantum Chemistry*, 112(4):1134–1164, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bertini:2014:TMC

[BGFD14] Luca Bertini, Claudio Greco, Piercarlo Fantucci, and Luca De Gioia. TDDFT modeling of the CO-photolysis of $Fe_2(S_2C_3H_6)(CO)_6$, a model of the [FeFe]-hydrogenase catalytic site. *International Journal of Quantum Chemistry*, 114(13):851–861, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bordes:2018:CSP

[BGJSM+18] Isabel Bordes, Eduardo García-Junceda, Israel Sánchez-Moreno, Raquel Castillo, and Vicent Moliner. Computational study of the phosphoryl donor activity of dihydroxyacetone kinase from ATP to inorganic polyphosphate. *International Journal of Quantum Chemistry*, 118 (9):e25520:1–e25520:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boes:2016:NNR

[BGKK16] Jacob R. Boes, Mitchell C. Groenenboom, John A. Keith, and John R. Kitchin. Neural network and ReaxFF comparison for Au properties. *International Journal of Quantum Chemistry*, 116(13):979–987, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bo:2016:EQS

[BGL+16] Maolin Bo, Yongling Guo, Yonghui Liu, Cheng Peng, Yongli Huang, and Chang Q. Sun. Enhanced quantum size effect in Li and Na clusters via rare gas doping. *International Journal of Quantum Chemistry*, 116(24):1829–1835, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Begum:2015:TIN

[BGMD15] Pakiza Begum, Pranjal Gogoi, Bhupesh Kumar Mishra, and Ramesh Chandra Deka. Theoretical insight of nitric oxide adsorption on neutral and charged Pd_n ($n = 1$–5) clusters. *International Journal of Quantum Chemistry*, 115 (13):837–845, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Braida:2010:ESE

[BH10a] Benoît Braïda and Philippe C. Hiberty. Explicit solvation effects on the conventional resonance model for protonated imine, carbonyl, and thiocarbonyl compounds. *International Journal of Quantum Chemistry*, 110(3):571–577, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burke:2010:SPP

[BH10b] Luke A. Burke and Fenton Heirtzler. Spectroscopic and photophysical properties of dicopper(I) metallocyclophanes. *International Journal of Quantum Chemistry*, 110 (15):3061–3071, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bugeanu:2019:PRM

[BH19] Monica Bugeanu and Helmut Harbrecht. Parametric representation of molecular surfaces. *International Journal of Quantum Chemistry*, 119(1):e25695:1–e25695:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

BenAissa:2019:TDF

[BHA19] Mohamed Ali Ben Aissa, Sabri Hassen, and Youssef Arfaoui. Theoretical density functional theory insights into the nature of chalcogen bonding between CX_2 (X = S,

Se, Te) and diazine from monomer to supramolecular complexes. *International Journal of Quantum Chemistry*, 119 (6):e25837:1–e25837:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhandari:2018:RDS

[BHAH+18] Aashka S. Bhandari, Walid M. I. Hassan, Nessreen Al-Hashimi, Mohamed F. Shibl, Sunil R. Patil, and Amit Verma. Role of doping and sheet size in tailoring optoelectronic properties of germanene: a TDDFT study. *International Journal of Quantum Chemistry*, 118(19):e25700:1–e25700:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bochevarov:2013:SNU

[BHH+13] Art D. Bochevarov, Edward Harder, Thomas F. Hughes, Jeremy R. Greenwood, Dale A. Braden, Dean M. Philipp, David Rinaldo, Mathew D. Halls, Jing Zhang, and Richard A. Friesner. Software news & updates: Jaguar: a high-performance quantum chemistry software program with strengths in life and materials sciences. *International Journal of Quantum Chemistry*, 113(18):2110–2142, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Banerjee:2019:SEN

[BHMN19] Paramita Banerjee, Kaushik Hatua, Avijit Mondal, and Prasanta K. Nandi. Substituent effects at nitrogen/phosphorus atoms of dialkaline earth metal complexes: Excess electron and large second-hyperpolarizability. *International Journal of Quantum Chemistry*, 119(15):e25939:1–e25939:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bene:2011:ITC

[BHV+11] E. Bene, G. J. Halász, Á. Vibók, L. F. Errea, L. Méndez, I. Rabadán, and M. C. Bacchus-Montabonel. Ab initio treatment of charge exchange in $H^+ + CH$ collisions. *International Journal of Quantum Chemistry*, 111(2):487–492, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bibak:2013:NST

[Bib13] Khodakhast Bibak. The number of spanning trees in an (r, s)-semiregular graph and its line graph. *International Journal of Quantum Chemistry*, 113(8):1209–1212, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brzyska:2012:CCD

[BJ12] Agnieszka Brzyska and Michał Jaszuński. Coupled cluster and DFT calculations of ^{14}N nuclear quadrupole coupling constants. *International Journal of Quantum Chemistry*, 112(10):2281–2286, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bridle:2017:CSF

[BJ17] Mark J. Bridle and Benjamin G. Janesko. Computational study of fluoroquinolone binding to $Mg(H_2O)N^{2+}$ and its applicability to future drug design. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Briones-Jurado:2012:DFT

[BJdlMAV12] Claudia Briones-Jurado, Pablo de la Mora, and Esther Agacino-Valdés. Density functional theory study of Au_n ($n = 1$–5) clusters supported on montmorillonite. *International Journal of Quantum Chemistry*, 112(22):3646–3654, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bodoor:2015:NSP

[BKM15] Khaled Bodoor, Jacek Kobus, and John Morrison. A numerical solution of the pair equation of a model two-electron diatomic system. *International Journal of Quantum Chemistry*, 115(14):868–874, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berski:2010:QCT

[BL10] Sławomir Berski and Zdzisław Latajka. Quantum chemical topology: The electronic structure of the alkaline nitrites MONO (M = Li, Na, K) studied by means of topological analysis of the electron localization function. *International*

Journal of Quantum Chemistry, 110(10):1890–1900, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Berski:2011:MDC

[BL11] Slawomir Berski and Zdzislaw Latajka. A mechanism of the 1,3-dipolar cycloaddition between the hydrogen nitryl HNO_2 and acetylene HCCH: The electron localization function study on evolution of the chemical bonds. *International Journal of Quantum Chemistry*, 111(10):2378–2389, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brites:2012:CFI

[BL12] Vincent Brites and Céline Léonard. CCSD(T)-F12 investigations on HBNH and its isotopologues. *International Journal of Quantum Chemistry*, 112(9):2051–2061, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baranowska-Laczkowska:2016:EPB

[BŁ16] Angelika Baranowska-Łaczkowska. Efficient polarized basis sets for evaluation of static and dynamic molecular electric properties. *International Journal of Quantum Chemistry*, 116(14):1084–1089, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barquera-Lozada:2019:VCD

[BL19] José Enrique Barquera-Lozada. The vorticity of the current density tensor and 3D-aromaticity. *International Journal of Quantum Chemistry*, 119(8):e25848:1–e25848:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blanquart:2015:ESC

[Bla15] Guillaume Blanquart. Effects of spin contamination on estimating bond dissociation energies of polycyclic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 115(12):796–801, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Battaglia:2018:TSC

[BLB+18] Stefano Battaglia, Hai-Anh Le, Gian Luigi Bendazzoli, Noelia Faginas-Lago, Thierry Leininger, and Stefano Evangelisti. A theoretical study on cyclacenes: Analytical tight-binding approach. *International Journal of Quantum Chemistry*, 118(12):e25569:1–e25569:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bochicchio:2019:DAI

[BLdV19] Roberto C. Bochicchio, Rosana M. Lobayan, and Carlos Pérez del Valle. Donor–acceptor interactions: Transition metal carbonyl group ligand $[\mathrm{TM}(\mathrm{CO})_6]^q$ complexes. A case study at correlated level from the topological density point of view. *International Journal of Quantum Chemistry*, 119(9):e25876:1–e25876:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Branken:2011:DFT

[BLKB11] D. J. Branken, G. Lachmann, H. M. Krieg, and O. S. L. Bruinsma. A density-functional theory approach to the separation of $K_2\ ZrF_6$ and $K_2\ HfF_6$ via fractional crystallization. *International Journal of Quantum Chemistry*, 111(3):682–693, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bai:2013:MMM

[BLL+13] Xiangbin Bai, Qingzhong Li, Ran Li, Jianbo Cheng, and Wenzuo Li. Is a MH (M = Be and Mg) radical a better electron donor in halogen-hydride interaction?: a theoretical comparison with HMH. *International Journal of Quantum Chemistry*, 113(9):1293–1298, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brea:2012:TSM

[BLM+12] Oriana Brea, Marcos Loroño, Edgar Marquez, Jose R. Mora, Tania Cordova, and Gabriel Chuchani. Theoretical study of methoxy group influence in the gas-phase elimination kinetics of methoxyalkyl chlorides. *International Journal of Quantum Chemistry*, 112(12):2504–2514, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blomberg:2015:PHQ

[Blo15] Margareta R. A. Blomberg. Perspectives: How quantum chemistry can solve fundamental problems in bioenergetics. *International Journal of Quantum Chemistry*, 115(18): 1197–1201, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Belarmino:2012:HBB

[BLR12] M. K. D. L. Belarmino, N. B. D. Lima, and M. N. Ramos. Hydrogen bonds between acetylene and formic acid: an ab initio study. *International Journal of Quantum Chemistry*, 112(19):3246–3251, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bertin:2010:CTS

[BLRdA+10] V. Bertin, R. Lopez-Rendón, G. del Angel, E. Poulain, R. Avilés, and V. Uc-Rosas. Comparative theoretical study of small Rh_n nanoparticles ($2 \leq n \leq 8$) using DFT methods. *International Journal of Quantum Chemistry*, 110(6): 1152–1164, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2017:IRM

[BLWJ17] Cheng Bian, Yu Li, Shujuan Wang, and Xinli Jing. Initial reaction mechanism between HO· and bisphenol-F: Conformational dependence and the role of nonbond interactions. *International Journal of Quantum Chemistry*, 117 (6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bryk:2010:NCP

[BM10] Taras Bryk and Ihor Mryglod. Nonhydrodynamic collective processes in molten salts: Theory and ab initio simulations. *International Journal of Quantum Chemistry*, 110 (1):38–45, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonfanti:2016:TRC

[BM16] Matteo Bonfanti and Rocco Martinazzo. Tutorial reviews: Classical and quantum dynamics at surfaces: Basic concepts from simple models. *International Journal of Quantum Chemistry*, 116(21):1575–1602, November 5,

2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bohorquez:2010:LED

[BMB10] Hugo J. Bohórquez, Chérif F. Matta, and Russell J. Boyd. The localized electrons detector as an ab initio representation of molecular structures. *International Journal of Quantum Chemistry*, 110(13):2418–2425, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Borges:2012:IPI

[BMB12] E. Borges, D. C. Menezes, and J. P. Braga. An ill-posed inverse problem in enzymatic kinetics: Jack-Bean urease denaturation by an anionic surfactant. *International Journal of Quantum Chemistry*, 112(19):3240–3245, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bucinsky:2016:AKP

[BMB16] Lukáš Bučinský, Michal Malček, and Stanislav Biskupič. Additivity in Kramers pairs symmetry: Multiplets with up to four unpaired electrons. *International Journal of Quantum Chemistry*, 116(13):1040–1048, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharyya:2010:SDC

[BMBD10] I. Bhattacharyya, B. Mondal, N. C. Bera, and A. K. Das. Structure and dissociation of cyanogen halides BrCN and ICN. *International Journal of Quantum Chemistry*, 110(6): 1165–1171, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bondarchuk:2013:TST

[BMF13] Sergey V. Bondarchuk, Boris F. Minaev, and Alexander Yu. Fesak. Theoretical study of the triplet state aryl cations recombination: a possible route to unusually stable doubly charged biphenyl cations. *International Journal of Quantum Chemistry*, 113(24):2580–2588, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhatt:2014:NRP

[BMF+14] Jayesh S. Bhatt, Peter J. McDonald, David A. Faux, Nicholas C. Howlett, and Sergey V. Churakov. NMR relaxation parameters from molecular simulations of hydrated inorganic nanopores. *International Journal of Quantum Chemistry*, 114(18):1220–1228, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baba:2014:DFS

[BMK+14] Takeshi Baba, Toru Matsui, Katsumasa Kamiya, Masayoshi Nakano, and Yasuteru Shigeta. A density functional study on the pK_a of small polyprotic molecules. *International Journal of Quantum Chemistry*, 114(17):1128–1134, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Baggioli:2013:ICI

[BMR+13] Alberto Baggioli, Stefano V. Meille, Guido Raos, Riccardo Po, Martin Brinkmann, and Antonino Famulari. Intramolecular CH/π interactions in alkylaromatics: Monomer conformations for poly(3-alkylthiophene) atomistic models. *International Journal of Quantum Chemistry*, 113(18):2154–2162, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barrientos:2019:NII

[BMRM19] Lorena Barrientos, Sebatian Miranda-Rojas, and Fernando Mendizabal. Noncovalent interactions in inorganic supramolecular chemistry based in heavy metals. Quantum chemistry point of view. *International Journal of Quantum Chemistry*, 119(2):e25675:1–e25675:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bacchus-Montabonel:2011:AEC

[BMTT11] M. C. Bacchus-Montabonel, Y. S. Tergiman, and D. Talbi. Anisotropic effect in collisions of ions with biomolecules. *International Journal of Quantum Chemistry*, 111(2):520–527, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bin:2019:DBP

[BMX+19] Xin Bin, Roya Momen, Tianlv Xu, Steven R. Kirk, Michael Filatov, and Samantha Jenkins. A 3-D bonding perspective of the factors influencing the relative stability of the S_1 / S_0 conical intersections of the penta-2,4-dieniminium cation (PSB3). *International Journal of Quantum Chemistry*, 119 (11):e25903:1–e25903:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burileanu:2011:LFD

[BN11] L. M. Burileanu and E. C. Niculescu. Laser field dependence of intersubband transition in inverse V-shaped quantum wells. *International Journal of Quantum Chemistry*, 111(5):1108–1114, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barbatti:2012:DHH

[BN12] Mario Barbatti and Marco Antonio Chaer Nascimento. Does the H_5^+ hydrogen cluster exist in dense interstellar clouds? *International Journal of Quantum Chemistry*, 112 (19):3169–3173, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Budyka:2011:CSD

[BO11] Mikhayl F. Budyka and Ilia V. Oshkin. Comparative semiempirical and DFT study of styrylnaphthalenes and styrylquinolines and their photocyclization products. *International Journal of Quantum Chemistry*, 111(14):3673–3680, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bochicchio:2017:SFM

[Boc17] Roberto C. Bochicchio. Structure of Fukui matrices. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boettger:2012:TCZ

[Boe12] Jonathan C. Boettger. Theoretical calculation of the zero-temperature isotherm and phase stability of silver up to 2 Gbar using the linear combinations of Gaussian type orbitals method. *International Journal of Quantum Chem-*

istry, 112(24):3822–3828, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bondarchuk:2017:ISC

[Bon17] Sergey V. Bondarchuk. Impact sensitivity of crystalline phenyl diazonium salts: a first-principles study of solid-state properties determining the phenomenon. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouazza:2011:SHS

[Bou11] Safa Bouazza. Semiempirical hyperfine structure and ab initio isotope shift predictions in Zr II. *International Journal of Quantum Chemistry*, 111(12):3000–3007, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bouazza:2012:IHS

[Bou12a] Safa Bouazza. Investigations of hyperfine structure and isotope shift predictions in Hf II. *International Journal of Quantum Chemistry*, 112(2):470–477, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boudreaux:2012:QSM

[Bou12b] Edward A. Boudreaux. QR–SCMEH–MO calculations on the complex $[Pt(SnCl_3)_5]^{3-}$: Electronic structure, UV-visible spectrum, magnetic properties, and bond energy. *International Journal of Quantum Chemistry*, 112(16):2801–2807, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barragan:2013:DBP

[BP13] Patricia Barragán and Rita Prosmiti. A DFT-based potential energy surface for the H cluster. *International Journal of Quantum Chemistry*, 113(5):651–655, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barreto:2010:RSI

[BPG+10] Patrícia R. P. Barreto, F. Palazzetti, G. Grossi, A. Lombardi, G. S. Maciel, and A. F. A. Vilela. Range and strength

of intermolecular forces for van der Waals complexes of the type H_2X_n-Rg, with X = O, S and $n = 1, 2$. *International Journal of Quantum Chemistry*, 110(3):777–786, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buglak:2019:PAS

[BPK19] Andrey A. Buglak, Vladimir A. Pomogaev, and Alexei I. Kononov. Predicting absorption spectra of silver-ligand complexes. *International Journal of Quantum Chemistry*, 119(20):e25995:1–e25995:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Becerra:2013:NBO

[BPL13] Marcos Becerra, Víctor Posligua, and Eduardo V. Ludeña. Non-Born–Oppenheimer nuclear and electronic densities for a Hooke–Coulomb model for a four-particle system. *International Journal of Quantum Chemistry*, 113(10):1584–1590, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bravo-Perez:2012:TSC

[BPSM12] Graciela Bravo-Pérez and Humberto Saint-Martin. A theoretical study of the confinement of methane in water clusters. *International Journal of Quantum Chemistry*, 112 (22):3655–3660, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barsukov:2012:CZM

[BPT12] Yu. V. Barsukov, V. V. Porsev, and A. V. Tulub. Comparison of zinc and magnesium clusters in their reaction with organochlorides: Toward a molecular picture of Grignard reagent formation. *International Journal of Quantum Chemistry*, 112(18):3002–3007, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barragan:2011:GPE

[BPVDB11] Patricia Barragán, Rita Prosmiti, Pablo Villarreal, and Gerardo Delgado-Barrio. Global potential energy surface for the ground electronic state of H: a DFT approach. *International Journal of Quantum Chemistry*, 111(2):368–374,

February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balaban:2008:RSB

[BR08] Alexandru T. Balaban and Milan Randić. Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. *International Journal of Quantum Chemistry*, 108(5):898–926, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [BR12a].

Bonnet:2010:DDE

[BR10] L. Bonnet and J.-C. Rayez. Dynamical derivation of Eyring equation and the second-order kinetic law. *International Journal of Quantum Chemistry*, 110(13):2355–2359, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Balaban:2012:ERS

[BR12a] Alexandru T. Balaban and Milan Randić. Erratum: Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. *International Journal of Quantum Chemistry*, 112(10):2342, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BR08].

Bogdanova:2012:RDV

[BR12b] Julia Bogdanova and Olga B. Rodimova. Role of diffusion in the violation of the long-wave approximation in line wings. *International Journal of Quantum Chemistry*, 112(17):2924–2931, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Botu:2015:AML

[BR15] Venkatesh Botu and Rampi Ramprasad. Adaptive machine learning framework to accelerate ab initio molecular dynamics. *International Journal of Quantum Chemistry*, 115 (16):1074–1083, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bonnet:2016:CCD

[BR16] L. Bonnet and J.-C. Rayez. Comment: Comment on "Dynamical derivation of Eyring equation and the second-order

kinetic law" [Int. J. Quantum Chem. 2010, 110, 2355]. *International Journal of Quantum Chemistry*, 116(16):1267, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bracken:2010:HSQ

[Bra10] Paul Bracken. Hamiltonian for the spin quantum Hall effect solution and derivation based on an $rmSU(2)$ gauge field. *International Journal of Quantum Chemistry*, 110(7): 1322–1326, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2011:GSS

[Brä11a] Erkki J. Brändas. Gödelian structures and self-organization in biological systems. *International Journal of Quantum Chemistry*, 111(7–8):1321–1332, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2011:SCP

[Brä11b] Erkki J. Brändas. Some comments on the problem of decoherence. *International Journal of Quantum Chemistry*, 111(2):215–224, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2012:BRN

[Brä12] Erkki J. Brändas. Book review: *Non-Hermitean quantum mechanics*, by Nimrod Moiseyev. *International Journal of Quantum Chemistry*, 112(15):2764–2765, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2013:CFM

[Brä13] Erkki J. Brändas. Concepts and fundamental methods in quantum chemistry: Arrows of time and fundamental symmetries in chemical physics. *International Journal of Quantum Chemistry*, 113(3):173–184, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2014:ESG

[Brä14] Erkki Brändas. Editorial: The statement of goals of the International Society for Theoretical Chemical Physics. *International Journal of Quantum Chemistry*, 114(15):961–

962, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bracken:2019:QMT

[Bra19] Paul Bracken. Quantum measurements and thermodynamics. *International Journal of Quantum Chemistry*, 119(23): e26037:1–e26037:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Blanca-Romero:2011:KLR

[BRBRS11] A. Blanca-Romero, M. Berrondo, and J. F. Rivas-Silva. Kondo-like resonance in ZnO:Eu. *International Journal of Quantum Chemistry*, 111(14):3831–3840, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bentarcurt:2010:MFM

[BRS10] Yenner Bentarcurt, Fernando Ruette, and Morella Sánchez. Modeling formation of molecules in the interstellar medium by radical reactions with polycyclic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 110 (13):2560–2572, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benassi:2011:TSS

[BS11] Enrico Benassi and Peter S. Sherin. Theoretical study of solvent influence on the electronic absorption and emission spectra of kynurenine. *International Journal of Quantum Chemistry*, 111(14):3799–3804, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharjee:2014:DSR

[BS14] Kanika Bhattacharjee and Pradeep Kumar Shukla. A DFT study of reactions of methyldiazonium ion with DNA/RNA nucleosides: Investigating effect of sugar moiety on methylation pattern of bases. *International Journal of Quantum Chemistry*, 114(24):1637–1644, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barbatti:2016:EDI

[BS16] Mario Barbatti and Kakali Sen. Effects of different initial condition samplings on photodynamics and spectrum of pyrrole. *International Journal of Quantum Chemistry*, 116(10):762–771, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharya:2015:PNO

[BSM+15] Debojit Bhattacharya, Suranjan Shil, Anirban Misra, Laimutis Bytautas, and Douglas J. Klein. Photomagnetic and nonlinear optical properties in cis-trans green fluoroprotein chromophore coupled bis-imino nitroxide diradicals. *International Journal of Quantum Chemistry*, 115(21):1561–1572, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bulusheva:2011:SSN

[BSO11] Lyubov G. Bulusheva, Olga V. Sedelnikova, and Alexander V. Okotrub. Substitutional sites of nitrogen atoms in carbon nanotubes and their influence on field-emission characteristics. *International Journal of Quantum Chemistry*, 111(11):2696–2704, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bulusheva:2016:RMB

[BSO16] L. G. Bulusheva, O. V. Sedelnikova, and A. V. Okotrub. Reviews: Many-body effects in optical response of graphene-based structures. *International Journal of Quantum Chemistry*, 116(4):270–281, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buzko:2011:DSC

[BSPK11] Vladimir Buzko, Igor Sukhno, Alexey Polushin, and Denis Kashaev. DFT study of ceric subgroup $Ln(H_2\ O)_9^{3+}$ aqua ions. *International Journal of Quantum Chemistry*, 111 (11):2705–2711, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brandas:2014:P

[BSS14] Erkki Brändas, Ágnes Szabados, and Péter Surján. Preface. *International Journal of Quantum Chemistry*, 114(15):959–

960, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharya:2015:PBD

[BSS15] Barnali Bhattacharya, Ngangbam Bedamani Singh, and Utpal Sarkar. Pristine and BN doped graphyne derivatives for UV light protection. *International Journal of Quantum Chemistry*, 115(13):820–829, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bengtson:2016:QNE

[BSS16] Charlotta Bengtson, Michael Stenrup, and Erik Sjöqvist. Quantum nonlocality in the excitation energy transfer in the Fenna–Matthews–Olson complex. *International Journal of Quantum Chemistry*, 116(23):1763–1771, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharya:2019:EEW

[BSSS19] Labanya Bhattacharya, Smruti R. Sahoo, Sagar Sharma, and Sridhar Sahu. Effect of electron-withdrawing groups on photovoltaic performance of thiophene-vinyl-thiophene derivative and benzochalcogenadiazole based copolymers: a computational study. *International Journal of Quantum Chemistry*, 119(18):e25982:1–e25982:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Butchosa:2012:CDE

[BSV12] C. Butchosa, S. Simon, and A. A. Voityuk. Conformational dependence of the electronic coupling in guanine–tryptophan complexes: A DFT study. *International Journal of Quantum Chemistry*, 112(7):1838–1843, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Boguslawski:2015:POE

[BT15] Katharina Boguslawski and Paweł Tecmer. Perspectives: Orbital entanglement in quantum chemistry. *International Journal of Quantum Chemistry*, 115(19):1289–1295, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [BT17].

Boguslawski:2017:EOE

[BT17] Katharina Boguslawski and Paweł Tecmer. Erratum: Orbital entanglement in quantum chemistry. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BT15].

Brovarets:2018:UWR

[BTH18] Ol'ha O. Brovarets', Kostiantyn S. Tsiupa, and Dmytro M. Hovorun. Unexpected A·T(WC)<->A·T(rWC)/ A·T(rH) and A·T(H)<->A·T(rH)/ A·T(rWC) conformational transitions between the classical A·T DNA base pairs: a QM/ QTAIM comprehensive study. *International Journal of Quantum Chemistry*, 118(18):e25674:1–e25674:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2010:LTC

[Buc10] Henk M. Buck. A linear three-center four electron bonding identity nucleophilic substitution at carbon, boron, and phosphorus. A theoretical study in combination with van't Hoff modeling. *International Journal of Quantum Chemistry*, 110(7):1412–1424, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2011:MII

[Buc11a] Henk M. Buck. A model investigation of ab initio geometries for identity and nonidentity substitution with three-center four- and three-electron transition states. *International Journal of Quantum Chemistry*, 111(10):2242–2250, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2011:MMS

[Buc11b] Henk M. Buck. Molecular model studies based on ab initio calculations of nucleophilic and electrophilic addition-substitution reactions focused on carbon–halogen compounds. *International Journal of Quantum Chemistry*, 111 (15):4472–4482, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buchowiecki:2012:TDR

[Buc12a] Marcin Buchowiecki. Temperature dependence of the rate constant of ionic analogs of H + H_2 → H_2 + H reaction by quantum instanton method. *International Journal of Quantum Chemistry*, 112(4):1107–1113, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Buck:2012:MMI

[Buc12b] Henk M. Buck. Mechanistic models for the intramolecular hydroxycarbene–formaldehyde conversion and their intermolecular interactions: Theory and chemistry of radicals, mono-, and dications of hydroxycarbene and related configurations. *International Journal of Quantum Chemistry*, 112(23):3711–3719, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Budyka:2012:DOP

[Bud12] Mikhayl F. Budyka. Does one-photon photocyclization of trans-diarylethylenes involve adiabatic trans-to-cis photoisomerization? Potential energy surface calculations for 1-styrylnaphthalene. *International Journal of Quantum Chemistry*, 112(14):2643–2649, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bostrom:2014:AGS

[BVA+14] Jonas Boström, Valera Veryazov, Francesco Aquilante, Thomas Bondo Pedersen, and Roland Lindh. Analytical gradients of the second-order Møller–Plesset energy using Cholesky decompositions. *International Journal of Quantum Chemistry*, 114(5):321–327, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Barboza:2012:TDB

[BVCAP12] Cristina Aparecida Barboza, Pedro Antonio Muniz Vazquez, Desmond Mac-Leod Carey, and Ramiro Arratia-Perez. A TD–DFT basis set and density functional assessment for the calculation of electronic excitation energies of fluorene. *International Journal of Quantum Chemistry*, 112 (20):3434–3438, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharya:2013:FSM

[BVP13] Sumantra Bhattacharya, Nayana Vaval, and Sourav Pal. Fock space multireference coupled cluster theory: Study of shape resonance. *International Journal of Quantum Chemistry*, 113(12):1690–1695, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bhattacharya:2014:ETD

[BVP14] Debarati Bhattacharya, Nayana Vaval, and Sourav Pal. Electronic transition dipole moment: a semi-biorthogonal approach within valence universal coupled cluster framework. *International Journal of Quantum Chemistry*, 114 (18):1212–1219, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bulo:2010:BEM

[BVRM10] Rosa E. Bulo, Hans Van Schoot, Daniel Rohr, and Carine Michel. Bias-exchange metadynamics applied to the study of chemical reactivity. *International Journal of Quantum Chemistry*, 110(12):2299–2307, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Beret:2014:RCP

[BvWG14] Elizabeth C. Beret, Merel M. van Wijk, and Luca M. Ghiringhelli. Reaction cycles and poisoning in catalysis by gold clusters: a thermodynamics approach. *International Journal of Quantum Chemistry*, 114(1):57–65, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Burke:2013:EDN

[BW13a] Kieron Burke and Lucas O. Wagner. Erratum: DFT in a nutshell. *International Journal of Quantum Chemistry*, 113(10):1601, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [BW13b].

Burke:2013:TRD

[BW13b] Kieron Burke and Lucas O. Wagner. Tutorial reviews: DFT in a nutshell. *International Journal of Quantum Chemistry*, 113(2):96–101, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [BW13a].

Bielinska-Waz:2015:SMG

[BW15] Dorota Bielińska-Waż. Statistical method of generating envelopes of the electronic hot bands. *International Journal of Quantum Chemistry*, 115(24):1726–1732, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Banafsheh:2018:RNK

[BW18] Mojdeh Banafsheh and Tomasz Adam Wesolowski. Reviews: Nonadditive kinetic potentials from inverted Kohn–Sham problem. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Brela:2018:SHB

[BWB+18] Mateusz Z. Brela, Marek J. Wójcik, Marek Boczar, Erika Onishi, Harumi Sato, Takahito Nakajima, and Yukihiro Ozaki. Study of hydrogen bond dynamics in Nylon 6 crystals using IR spectroscopy and molecular dynamics focusing on the differences between α and γ crystal forms. *International Journal of Quantum Chemistry*, 118(14): e25595:1–e25595:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bruckner:2016:TII

[BWE16] Charlotte Brückner, Christof Walter, and Bernd Engels. Theoretical investigation of the interactions between the π-systems of molecular organic semiconductors and an analysis of the contributions of repulsion and electrostatics. *International Journal of Quantum Chemistry*, 116(15):1138–1152, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bagus:2010:IAM

[BWW10] P. S. Bagus, A. Wieckowski, and Ch. Wöll. Ionic adsorbates on metal surfaces. *International Journal of Quantum Chemistry*, 110(15):2844–2859, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bai:2013:FPI

[BXR+13] Jing Bai, Nan Xu, Jean-Marc Raulot, Claude Esling, Xiang Zhao, and Liang Zuo. First-principles investigation

of magnetic property and defect formation energy in Ni–Mn–Ga ferromagnetic shape memory alloy. *International Journal of Quantum Chemistry*, 113(6):847–851, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2019:TSA

[BXZ+19] He Bian, Bin Xu, Honghong Zhang, Qian Wang, Huiming Zhang, Shiguo Zhang, and Daohong Xia. Theoretical study on the atmospheric reaction of CH_3 SH with O_2. *International Journal of Quantum Chemistry*, 119(5):e25822:1–e25822:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bleda:2013:CTG

[BYAT13] Erdi A. Bleda, Ilhan Yavuz, Zikri Altun, and Carl Trindle. Computational thermochemistry of glycolaldehyde. *International Journal of Quantum Chemistry*, 113(8):1147–1154, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Benmachiche:2013:ESC

[BZBZ13] Akila Benmachiche, Saber-Mustapha Zendaoui, Salah-Eddine Bouaoud, and Bachir Zouchoune. Electronic structure and coordination chemistry of phenanthridine ligand in first-row transition metal complexes: a DFT study. *International Journal of Quantum Chemistry*, 113(7):985–996, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2015:TSA

[BZZ15] He Bian, Shiguo Zhang, and Huiming Zhang. Theoretical study on the atmospheric reaction of CH_3 O_2 with OH. *International Journal of Quantum Chemistry*, 115(17):1181–1186, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cortes-Arriagada:2017:APA

[CA17] Diego Cortés-Arriagada. Adsorption of polycyclic aromatic hydrocarbons onto graphyne: Comparisons with graphene. *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cavasotto:2019:CCD

[CAA19] Claudio N. Cavasotto, María Gabriela Aucar, and Natalia S. Adler. Computational chemistry in drug lead discovery and design. *International Journal of Quantum Chemistry*, 119(2):e25678:1–e25678:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castaneda-Arriaga:2012:IMD

[CAAI12] Romina Castañeda-Arriaga and J. Raul Alvarez-Idaboy. Influence of the methylation degree on the rate constants of the ˙OH addition to alkenes and its temperature dependence. *International Journal of Quantum Chemistry*, 112(21):3479–3483, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cortes-Arriagada:2018:ILP

[CADSG18] Diego Cortés-Arriagada, Paulina Dreyse, Felipe Salas, and Iván González. Insights into the luminescent properties of anionic cyclometalated iridium(III) complexes with ligands derived from natural products. *International Journal of Quantum Chemistry*, 118(17):e25664:1–e25664:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calvo:2010:ENM

[Cal10] Florent Calvo. Efficiency of nested Markov chain Monte Carlo for polarizable potentials and perturbed Hamiltonians. *International Journal of Quantum Chemistry*, 110(13): 2347–2354, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cammi:2010:CCT

[Cam10] R. Cammi. Coupled-cluster theories for the polarizable continuum model. II. Analytical gradients for excited states of molecular solutes by the equation of motion coupled-cluster method. *International Journal of Quantum Chemistry*, 110 (15):3040–3052, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cammi:2012:CCT

[Cam12] R. Cammi. Coupled-cluster theory for the polarizable continuum model. III. A response theory for molecules in solution. *International Journal of Quantum Chemistry*, 112 (13):2547–2560, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2017:TSE

[Cao17] Jun Cao. A theoretical study of the excited-state decay of acylhydrazones. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cortes-Arriagada:2018:EAC

[CAO18] Diego Cortés-Arriagada and Daniela E. Ortega. Effects on the aromatic character of DNA/ RNA nucleobases due to its adsorption onto graphene. *International Journal of Quantum Chemistry*, 118(19):e25699:1–e25699:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cappelli:2016:RIQ

[Cap16] Chiara Cappelli. Reviews: Integrated QM/polarizable MM/continuum approaches to model chiroptical properties of strongly interacting solute–solvent systems. *International Journal of Quantum Chemistry*, 116(21):1532–1542, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castaneda-Arriaga:2018:RPC

[CAPGAIG18] Romina Castañeda-Arriaga, Adriana Pérez-González, Juan Raúl Alvarez-Idaboy, and Annia Galano. Role of purines on the copper-catalyzed oxidative damage in biological systems: Protection versus promotion. *International Journal of Quantum Chemistry*, 118(9):e25527:1–e25527:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Costantini:2012:MDS

[CAPL12] Alessandro Costantini, Margarita Albertí, Fernando Pirani, and Antonio Laganà. A molecular dynamics study of sodium dodecyl sulfate-methane system in water using

the improved Lennard Jones formulation. *International Journal of Quantum Chemistry*, 112(7):1810–1817, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caricato:2019:CCT

[Car19] Marco Caricato. Coupled cluster theory with the polarizable continuum model of solvation. *International Journal of Quantum Chemistry*, 119(1):e25710:1–e25710:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Catikkas:2013:DFR

[ÇAS13] Berna Çatıkkaş, Ebru Aktan, and Zeynel Seferoğlu. DFT, FT-Raman, FTIR, NMR, and UV–Vis studies of a hetarylazo indole dye. *International Journal of Quantum Chemistry*, 113(5):683–689, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Casanova:2015:TIP

[Cas15] David Casanova. Theoretical investigations of the perylene electronic structure: Monomer, dimers, and excimers. *International Journal of Quantum Chemistry*, 115(7):442–452, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cavalleri:2013:QCR

[Cav13] Matteo Cavalleri. Quantum chemistry reloaded. *International Journal of Quantum Chemistry*, 113(1):1, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cavalleri:2017:ERR

[Cav17] Matteo Cavalleri. Editorial: Recognizing reviewers. *International Journal of Quantum Chemistry*, 117(1):6, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2011:TSI

[CAZ+11] Lu-Jie Cao, Hong-Qi Ai, Li-Ming Zheng, Su-Na Wang, Mei-Juan Zhou, Ji-Feng Liu, and Chong Zhang. Theoretical study on the interaction of neutral and charged

Ti_n ($n = 1--7$) clusters with one oxygen molecule. *International Journal of Quantum Chemistry*, 111(10):2416–2427, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Courcot:2010:WAC

[CB10] Blandine Courcot and Adam J. Bridgeman. Which atomic charges are best adapted to describe polyoxometalates? *International Journal of Quantum Chemistry*, 110(12):2155–2161, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Choluj:2019:EPM

[CB19] Marta Chołuj and Wojciech Bartkowiak. Electric properties of molecules confined by the spherical harmonic potential. *International Journal of Quantum Chemistry*, 119(20): e25997:1–e25997:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2011:FPI

[CC11a] Fang Chen and Xin-Lu Cheng. A first-principles investigation of the hydrogen bond interaction and the sensitive characters in *cis*-1,3,4,6-tetranitrooctahydroimidazo-[4,5-d]imidazole. *International Journal of Quantum Chemistry*, 111(15):4457–4464, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corongiu:2011:EDA

[CC11b] Giorgina Corongiu and Enrico Clementi. Energy and density analysis on the H_2 molecule from the united atom to dissociation: The Σ, Π, Δ, φ, and Γ manifolds. *International Journal of Quantum Chemistry*, 111(14):3517–3540, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Clementi:2012:NOH

[CC12] Enrico Clementi and Giorgina Corongiu. Nonorthogonal orbitals; the Hartree–Fock–Heitler–London method and preliminary applications. *International Journal of Quantum Chemistry*, 112(17):2940–2946, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chinini:2019:ACM

[CC19] Guilherme Luiz Chinini and Rogério Custodio. Assessment of a composite method based on selected density functional theory methods and complete basis set extrapolation formulas. *International Journal of Quantum Chemistry*, 119 (10):e25892:1–e25892:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carregal:2012:IVS

[CCA+12] Ana Paula Carregal, Moacyr Comar Jr., Stênio Nunes Alves, João Máximo de Siqueira, Luciana A. Lima, and Alex Gutterres Taranto. Inverse virtual screening studies of selected natural compounds from cerrado. *International Journal of Quantum Chemistry*, 112(20):3333–3340, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cassam-Chenai:2012:IER

[CCBR+12] P. Cassam-Chenaï, Y. Bouret, M. Rey, S. A. Tashkun, A. V. Nikitin, and Vl. G. Tyuterev. Ab initio effective rotational Hamiltonians: a comparative study. *International Journal of Quantum Chemistry*, 112(9):2201–2220, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coutinho:2011:I

[CCC11] Kaline Coutinho, Benedito J. Costa Cabral, and Rogério Custodio. Introduction. *International Journal of Quantum Chemistry*, 111(7–8):1249–1250, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cezar:2019:SES

[CCC19] Henrique M. Cezar, Sylvio Canuto, and Kaline Coutinho. Solvent effect on the syn/anti conformational stability: a comparison between conformational bias Monte Carlo and molecular dynamics methods. *International Journal of Quantum Chemistry*, 119(1):e25688:1–e25688:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calaminici:2012:SDP

[CCEGK12] Patrizia Calaminici, Javier Carmona-Espindola, Gerald Geudtner, and Andreas M. Köster. Static and dynamic polarizability of C_{540} fullerene. *International Journal of Quantum Chemistry*, 112(19):3252–3255, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2010:DSH

[CCL+10] Jin Can Chen, Lan Mei Chen, Si Yan Liao, Kang Cheng Zheng, and Liang Nian Ji. A DFT study on the hydrolysis mechanism of NH-tautomeric antitumors of [HL][trans-$RuCl_4$L(dmso-S)]. *International Journal of Quantum Chemistry*, 110(6):1252–1263, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2013:DFT

[CCL+13] Zhenfeng Cao, Qibin Chen, Yunxiang Lu, Honglai Liu, and Ying Hu. Density functional theory study on the interaction between metalloporphyrins and NH_3. *International Journal of Quantum Chemistry*, 113(8):1137–1146, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaquin:2016:ELB

[CCL+16] Patrick Chaquin, Yves Canac, Christine Lepetit, Davit Zargarian, and Remi Chauvin. Estimating local bonding/antibonding character of canonical molecular orbitals from their energy derivatives. The case of coordinating lone pair orbitals. *International Journal of Quantum Chemistry*, 116 (17):1285–1295, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Charro:2008:SRD

[CCM08] E. Charro, Z. Curiel, and I. Martín. Spontaneous radiative decay rates in Ga-like ions. *International Journal of Quantum Chemistry*, 108(4):744–753, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhuri:2018:NSS

[CCP18] Puspitapallab Chaudhuri, Sylvio Canuto, and Patricio F. Provasi. NMR spin-spin coupling constants in hydrogen-bonded glycine clusters. *International Journal of Quantum Chemistry*, 118(15):e25608:1–e25608:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2013:ISI

[CCS13] Long Chen, Fenglei Cao, and Huai Sun. Ab initio study of the π–π interactions between CO_2 and benzene, pyridine, and pyrrole. *International Journal of Quantum Chemistry*, 113(20):2261–2266, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Curotto:2012:DFS

[CD12] Verónica Ferraresi Curotto and Reinaldo Pis Diez. Density functional study on the geometric features and growing pattern of B_nP_m clusters with $n = 1$–4, $m = 1$–4, $n + m \leq 5$. *International Journal of Quantum Chemistry*, 112(19):3261–3268, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chatzidimitriou-Dreismann:2015:RQC

[CD15] C. A. Chatzidimitriou-Dreismann. Review: Quantumness of correlations and Maxwell's demon in molecular excitations created by neutron scattering. *International Journal of Quantum Chemistry*, 115(15):909–929, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbo-Dorca:2018:TUQ

[CD18] Ramon Carbó-Dorca. Toward a universal quantum QSPR operator. *International Journal of Quantum Chemistry*, 118(15):e25602:1–e25602:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardoso:2012:CRS

[CdAFS+12] Daniely Verônica Viana Cardoso, Luiz Fernando de Araújo Ferrão, Rene Felipe Keidel Spada, Orlando Roberto-Neto, and Francisco Bolivar Correto Machado. $O(^3P) + CH_3SH$ reactions: Structures, energetics, and kinetics. *International*

Journal of Quantum Chemistry, 112(19):3269–3275, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chi:2019:CTB

[CDL+19] Zongqing Chi, Wenbo Dong, Qingzhong Li, Xin Yang, Steve Scheiner, and Shufeng Liu. Carbene triel bonds between TrR_3 (Tr = B, Al) and N-heterocyclic carbenes. *International Journal of Quantum Chemistry*, 119 (8):e25867:1–e25867:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chakraborty:2018:EHB

[CdLdSC18] Sumana Chakraborty, Bonifácio Coelho de Lima, Arnaldo Machado da Silva, and Puspitapallab Chaudhuri. Effect of hydrogen-bonded interactions on the energetics and spectral properties of the astromolecule aminoacetonitrile. *International Journal of Quantum Chemistry*, 118(2): ??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chandra:2018:ECV

[CDS+18] Reet Chandra, Bibhas Dutta, Jayanta K. Saha, Sukhamoy Bhattacharyya, and Tapan K. Mukherjee. Explicitly correlated variational estimates of the energy levels of negative hydrogen ion under spatial confinement. *International Journal of Quantum Chemistry*, 118(15):e25597:1–e25597:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Calaminici:2012:CMG

[CDSK12] Patrizia Calaminici, Victor Daniel Domínguez-Soria, and Andreas M. Köster. Comparison of molecular graphs of Li_n, Na_n and Cu_n (n = 2–5) clusters obtained from the density and the molecular electrostatic potential. *International Journal of Quantum Chemistry*, 112(22):3624–3629, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Contreras:2012:CAT

[CDT12] Rubén H. Contreras, Lucas C. Ducati, and Cláudio F. Tormena. Critical analysis of the through-space transmission of NMR J_{FH} spin–spin coupling constants. *International*

Journal of Quantum Chemistry, 112(19):3158–3163, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carmona-Espindola:2012:SDF

[CEFMK12] Javier Carmona-Espíndola, Roberto Flores-Moreno, and Andreas M. Köster. Static and dynamic first hyperpolarizabilities from time-dependent auxiliary density perturbation theory. *International Journal of Quantum Chemistry*, 112(21):3461–3471, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carmona:2014:ERL

[CEM14] Angeles Carmona, Andres M. Encinas, and Margarida Mitjana. Effective resistances for ladder-like chains. *International Journal of Quantum Chemistry*, 114(24):1670–1677, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chetverikov:2010:TSS

[CEV10] Alexander P. Chetverikov, Werner Ebeling, and Manuel G. Velarde. Thermal solitons and solectrons in nonlinear conducting chains. *International Journal of Quantum Chemistry*, 110(1):46–61, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Centeno:2011:BBM

[CF11] Jesus Centeno and Patricio Fuentealba. Big bang methodology applied to atomic clusters. *International Journal of Quantum Chemistry*, 111(7–8):1419–1435, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cornaton:2014:DHD

[CF14] Yann Cornaton and Emmanuel Fromager. Double hybrid density-functional theory using the coulomb-attenuating method. *International Journal of Quantum Chemistry*, 114 (18):1199–1211, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Czapla:2017:UPB

[CF17] Marcin Czapla and Sylwia Freza. Uncatalyzed peptide bond formation between two double amino acid molecules

in the gas phase. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cukovicova:2011:AMB

[ČFČ11] Martina Čukovičová, Jozef Federič, and Ivan Černušák. Alkali metal borides MeB (Me = Li, Na, K, Rb, Cs, Fr): CASPT2 calculations. *International Journal of Quantum Chemistry*, 111(13):3438–3451, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Colherinhas:2011:IEC

[CFGC11] G. Colherinhas, T. L. Fonseca, H. C. Georg, and M. A. Castro. Isomerization effects on chemical shifts and spin-spin coupling constants of polyacetylene chains: A GIAO-DFT study. *International Journal of Quantum Chemistry*, 111(7–8):1616–1625, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Casasnovas:2010:SCQ

[CFOC+10] Rodrigo Casasnovas, Juan Frau, Joaquín Ortega-Castro, Antoni Salvà, Josefa Donoso, and Francisco Muñoz. Simplification of the CBS-QB3 method for predicting gas-phase deprotonation free energies. *International Journal of Quantum Chemistry*, 110(2):323–330, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carlotto:2010:IEF

[CFP+10] Silvia Carlotto, Camilla Ferrante, Antonino Polimeno, Caterina Benzi, and Vincenzo Barone. Interpretation of the emission fluorescence spectra of two fluoroionophores: DMABN-Crown4 and DMABN-Crown5. *International Journal of Quantum Chemistry*, 110(2):368–375, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaquin:2018:BAC

[CFV18] Patrick Chaquin, Franck Fuster, and François Volatron. Bonding/ antibonding character of "lone pair" molecular orbitals from their energy derivatives; consequences for experimental data. *International Journal of Quantum Chemistry*, 118(17):e25658:1–e25658:??, September 5, 2018. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaquin:2012:OTT

[CG12] Patrick Chaquin and Claudine Gutlé. One-, two-, and three-electron bonding: an "in vitro" theoretical study using noninteger nuclear charges evidences the crucial role of electronegativity in the strength of symmetrical bonds. *International Journal of Quantum Chemistry*, 112(15):2715–2723, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chakraborty:2018:EAB

[CGG18] Rahul Chakraborty, Paulami Ghosh, and Debashree Ghosh. Evolutionary algorithm based configuration interaction approach. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cordova-Gomez:2012:MRC

[CGIAI12] Moises Cordova-Gomez, Cristina Iuga, and Juan Raúl Alvarez-Idaboy. Mechanisms and rate constants in the atmospheric oxidation of saturated esters by hydroxyl radicals: a theoretical study. *International Journal of Quantum Chemistry*, 112(21):3508–3515, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castro:2012:BKI

[CGM12] Elton A. S. Castro, Ricardo Gargano, and João B. L. Martins. Benzene–kaolinite interaction properties. *International Journal of Quantum Chemistry*, 112(16):2828–2831, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chauhan:2017:SAC

[CH17] Rabeet Singh Chauhan and Manoj K. Harbola. Study of adiabatic connection in density functional theory with an accurate wavefunction for two-electron spherical systems. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2010:HBI

[Cha10] Ajay Chaudhari. Hydrogen bonding interaction between 1,4-dioxane and water. *International Journal of Quantum Chemistry*, 110(5):1092–1099, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chatterjee:2011:ESR

[Cha11] Abhijit Chatterjee. Excited state reactivity index theory application for small moieties. *International Journal of Quantum Chemistry*, 111(14):3821–3830, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2012:TSH

[Che12] Xiao-Xia Chen. A theoretical study of H — H σ bond activation catalyzed by VO_2^+ in gas phase. *International Journal of Quantum Chemistry*, 112(2):359–366, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2013:DST

[Che13] Xiang Chen. DNA sequencing with titanium nitride electrodes. *International Journal of Quantum Chemistry*, 113 (20):2295–2305, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chang:2019:TSP

[CHH+19] Jia-Lin Chang, Jung-Hang Hsieh, Yun-Jhu Huang, Chiing-Chang Chen, and Mu-Fong Chang. A theoretical study of the photoelectron spectra of dichloroketene with accurate computation of ionization energies via complete basis set limit extrapolation. *International Journal of Quantum Chemistry*, 119(8):e25866:1–e25866:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2019:SJD

[CHL+19] Wei-Hong Chen, Hui-Min He, Ying Li, Hui Yang, Jia-Yuan Liu, Dan Yu, Di Wu, Zhong-Jun Zhou, Wei-Ming Sun, Feng-Long Gu, and Zhi-Ru Li. Small Janus dimer as electric field manipulated molecular clam switch and electric

information storage unit. *International Journal of Quantum Chemistry*, 119(21):e26005:1–e26005:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaieb:2014:ISS

[CHM+14] Maha Chaieb, Héla Habli, Leila Mejrissi, Brahim Oujia, and Florent Xavier Gadéa. Ab initio spectroscopic study for the NaRb molecule in ground and excited states. *International Journal of Quantum Chemistry*, 114(11):731–747, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaieb:2017:DIN

[CHM+17] Maha Chaieb, Héla Habli, Leila Mejrissi, Attieh A. Al-Ghamdi, Brahim Oujia, and Florent Xavier Gadéa. Diabatic investigation for the NaRb molecule. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2015:TDR

[Cho15] Chia-Chun Chou. Two-dimensional reactive scattering with transmitted quantum trajectories. *International Journal of Quantum Chemistry*, 115(7):419–425, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2016:QCT

[Cho16] Chia-Chun Chou. Quantum-classical transition equation with complex trajectories. *International Journal of Quantum Chemistry*, 116(23):1752–1762, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2019:QCT

[Cho19] Chia-Chun Chou. Quantum-classical transition of the dissipative wave packet dynamics for barrier scattering. *International Journal of Quantum Chemistry*, 119(4):e25812:1–e25812:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Christophorov:2010:SOE

[Chr10] L. N. Christophorov. Self-organization effects in reactions of macromolecules. *International Journal of Quantum Chemistry*, 110(1):62–66, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chiba:2013:CRP

[CHSO13] Kouji Chiba, Toshiyuki Hirano, Fumitoshi Sato, and Masahiro Okamoto. Clarification of the role of protein in carbonmonoxy myoglobin by investigating electronic states. *International Journal of Quantum Chemistry*, 113 (21):2345–2354, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chun:2012:BTS

[Chu12] Paul W. Chun. Beyond the thermal set point: Significance of the compensatory temperatures of water vapor condensation in biological interactions. *International Journal of Quantum Chemistry*, 112(24):3782–3790, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Csehi:2014:MSP

[CHV14] András Csehi, Gábor J. Halász, and Ágnes Vibók. Molecular switch properties of 7-hydroxyquinoline compounds. *International Journal of Quantum Chemistry*, 114(17):1135–1145, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cinkir:2011:DCI

[Cin11a] Zubeyir Cinkir. Deletion and contraction identities for the resistance values and the Kirchhoff index. *International Journal of Quantum Chemistry*, 111(15):4030–4041, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cinkir:2011:GFI

[Cin11b] Zubeyir Cinkir. Generalized Foster's identities. *International Journal of Quantum Chemistry*, 111(10):2228–2233, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cinal:2020:CDI

[Cin20] Marek Cinal. Comment on "Depurated inversion method for orbital-specific exchange potentials". *International Journal of Quantum Chemistry*, 120(4):e26101:1–e26101:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See reply [MMM20].

Cardenas-Jiron:2019:QCS

[CJBMMAPR19] Gloria Cárdenas-Jirón, Merlys Borges-Martínez, Raúl Mera-Adasme, and Ricardo Pino-Rios. Quantum chemical studies of porphyrin- and expanded porphyrin-based systems and their potential applications in nanoscience. Latin America research review. *International Journal of Quantum Chemistry*, 119(2):e25821:1–e25821:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Correa:2012:EAC

[CJGTL12] José V. Correa, Pablo Jaque, Paul Geerlings, and Alejandro Toro-Labbé. Electronic activity in chelotropic and cycloaddition reactions. *International Journal of Quantum Chemistry*, 112(9):2142–2153, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Charistos:2019:ACC

[CJMC19] Nickolas D. Charistos, Peng Jin, and Alvaro Muñoz-Castro. Aromatic character of O_h-$C_{24}N_{24}$. A cavernous nitride fullerene bearing N_4-macrocycle motifs. *International Journal of Quantum Chemistry*, 119(13):e25919:1–e25919:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cundari:2011:FPS

[CJOOW11] Thomas R. Cundari, Smitha S. Janardan, Olayinka Olatunji-Ojo, and Brent R. Wilson. A first-principles study of diatomic NiAl: Ground state, structure, and spectroscopic constants. *International Journal of Quantum Chemistry*, 111(15):4303–4308, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardenas-Jiron:2011:QSP

[CJSNLM11] Gloria I. Cárdenas-Jirón, Mireya Santander-Nelli, Ramón López, and María Isabel Menéndez. Quantitative structure property relationships to evaluate the photosensitizing capability in porphyrins and chlorins. *International Journal of Quantum Chemistry*, 111(7–8):1570–1582, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chrysos:2013:LEC

[CK13] Michael Chrysos and David Kremer. Letters to the editor: Comment on "CCSD study of anharmonic Raman cross sections of fundamental, overtone, and combination transitions". *International Journal of Quantum Chemistry*, 113(24):2634–2636, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [VV12, VV13].

Chung:2017:DSO

[CK17] You Kyoung Chung and Seong Kyu Kim. Dissociation of sulfur oxoacids by two water molecules studied using ab initio and density functional theory calculations. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Choluj:2018:BDM

[CKB18] Marta Choluj, Justyna Kozlowska, and Wojciech Bartkowiak. Benchmarking DFT methods on linear and nonlinear electric properties of spatially confined molecules. *International Journal of Quantum Chemistry*, 118(17):e25666:1–e25666:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cardamone:2019:FPG

[CKB+19] Salvatore Cardamone, Jonathan R. R. Kimmitt, Hugh G. A. Burton, Timothy J. Todman, Shurui Li, Wayne Luk, and Alex J. W. Thom. Field-programmable gate arrays and quantum Monte Carlo: Power efficient coprocessing for scalable high-performance computing. *International Journal of Quantum Chemistry*, 119(12):e25853:1–e25853:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cho:2016:RQC

[CKL16] Daeheum Cho, Kyoung Chul Ko, and Jin Yong Lee. Reviews: Quantum chemical approaches for controlling and evaluating intramolecular magnetic interactions in organic diradicals. *International Journal of Quantum Chemistry*, 116(8):578–597, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Choi:2018:AHF

[CKYR18] Sunghwan Choi, Woo Youn Kim, Min Sun Yeom, and Hoon Ryu. On the achievement of high fidelity and scalability for large-scale diagonalizations in grid-based DFT simulations. *International Journal of Quantum Chemistry*, 118(16):e25622:1–e25622:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Curteanu:2008:OSB

[CL08] Silvia Curteanu and Florin Leon. Optimization strategy based on genetic algorithms and neural networks applied to a polymerization process. *International Journal of Quantum Chemistry*, 108(4):617–630, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caputo:2011:GDB

[CL11] M. C. Caputo and P. Lazzeretti. Geometry distortion of the benzene molecule in a strong magnetic field. *International Journal of Quantum Chemistry*, 111(4):772–779, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2018:SCE

[CL18] Hsiu-Yao Cheng and Cheng-Jung Lin. Shape and core-excited resonances of thionucleobases. *International Journal of Quantum Chemistry*, 118(16):e25634:1–e25634:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2010:GRD

[CLC10] Zhi Cao, Renfa Li, and Weiyang Chen. A 3D graphical representation of DNA sequence based on numerical coding method. *International Journal of Quantum Chemistry*, 110

(5):975–980, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2014:CTS

[CLH14] Ken-Fa Cheng, Min-Hsien Liu, and Pang-Hsing Ho. Comparative theoretical synthesis of high-energy density materials 2,4,6-trinitro-1,3,5-triazine. *International Journal of Quantum Chemistry*, 114(21):1457–1465, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caccin:2015:FML

[CLKD15] Marco Caccin, Zhenwei Li, James R. Kermode, and Alessandro De Vita. A framework for machine-learning-augmented multiscale atomistic simulations on parallel supercomputers. *International Journal of Quantum Chemistry*, 115(16):1129–1139, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2011:RSS

[CLL+11] Zhi Cao, Bo Liao, Renfa Li, Jiawei Luo, and Wen Zhu. RNA secondary structure alignment based on an extended binary coding method. *International Journal of Quantum Chemistry*, 111(5):978–982, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Corral:2012:ISC

[CLMY12] Inés Corral, Al Mokhtar Lamsabhi, Otilia Mó, and Manuel Yáñez. Infrared spectra of charge-solvated versus salt-bridge conformations of glycine-, serine-, and cysteine-Ca^{2+} complexes. *International Journal of Quantum Chemistry*, 112(9):2126–2134, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:DHP

[cLqFtW+14] Yuan chao Li, Ya qing Feng, Ya ting Wang, Chen cheng Fan, Xiu jun Liu, Xiang gao Li, and Bao Zhang. Design of high-performance chlorine type dyes for dye-sensitized solar cells. *International Journal of Quantum Chemistry*, 114(3):222–232, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chu:2015:RVC

[CLXD15] Tianshu Chu, Dongyue Liang, Jinmei Xu, and Shunle Dong. Review: The validities of centrifugal sudden approximations in chemical reaction dynamics. *International Journal of Quantum Chemistry*, 115(13):803–816, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2012:CSR

[CLXZ12] Li Juan Cao, An Yong Li, Li Xu, and Ying Zhang. A computational study on the ring stretching modes of halogen-substituted pyridine involved in H-bonding. *International Journal of Quantum Chemistry*, 112(2):498–508, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2012:CSC

[CLY12] Ken-Fa Cheng, Min-Hsien Liu, and Ping-Hua Yang. Computational study of the catalytic synthesis of 5-nitro-1,2,4-triazol-3-one. *International Journal of Quantum Chemistry*, 112(3):703–712, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chemouri:2012:DFT

[CM12] Hafida Chemouri and Sidi Mohamed Mekelleche. Density functional theory study of the regio- and stereoselectivity of Diels–Alder reactions of 5-Aryl-2-pyrones. *International Journal of Quantum Chemistry*, 112(10):2294–2300, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chakraborty:2015:RSO

[CM15] Romit Chakraborty and David A. Mazziotti. Reviews: Structure of the one-electron reduced density matrix from the generalized Pauli exclusion principle. *International Journal of Quantum Chemistry*, 115(19):1305–1310, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chakraborty:2016:RGP

[CM16] Romit Chakraborty and David A. Mazziotti. Role of the generalized Pauli constraints in the quantum chemistry of

excited states. *International Journal of Quantum Chemistry*, 116(10):784–790, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Candian:2017:PAI

[CM17] Alessandra Candian and Cameron J. Mackie. Perspective: Anharmonic interstellar PAH molecules. *International Journal of Quantum Chemistry*, 117(2):146–150, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Castro:2011:ANM

[CMCN11] M. E. Castro, C. Muñoz-Caro, and A. Niño. Analysis of the nitrile and methyl torsional vibrations of n-propyl cyanide in its S_0 electronic state. *International Journal of Quantum Chemistry*, 111(14):3681–3694, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coccia:2016:GCB

[CML+16] Emanuele Coccia, Bastien Mussard, Marie Labeye, Jérémie Caillat, Richard Taïeb, Julien Toulouse, and Eleonora Luppi. Gaussian continuum basis functions for calculating high-harmonic generation spectra. *International Journal of Quantum Chemistry*, 116(14):1120–1131, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caicedo:2013:TSN

[CMR13] Carolina Caicedo, Ana Martínez, and Ernesto Rivera. Theoretical study of novel porphyrins bearing electron donor–acceptor groups. *International Journal of Quantum Chemistry*, 113(9):1376–1383, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cristea:2012:CSD

[CN12] M. Cristea and E. C. Niculescu. Off-center shallow donors in a spherical Si quantum dot with dielectric border. *International Journal of Quantum Chemistry*, 112(6):1737–1745, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carmona-Novillo:2011:DDI

[CNBPR+11] Estela Carmona-Novillo, Massimiliano Bartolomei, Jesús Pérez-Ríos, José Campos-Martínez, and Marta I. Hernández. Diatom–diatom interactions: Building potential energy surfaces and effect of intramolecular vibrations. *International Journal of Quantum Chemistry*, 111(2):333–341, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chaudhari:2011:TIM

[CNSK11] Ajay Chaudhari, Mahadevappa Naganathappa, M. N. Shinde, and A. C. Kumbharkhane. Theoretical investigation of molecular interactions in dioxane and water using hydrogen bonding model and density functional method. *International Journal of Quantum Chemistry*, 111(12): 2972–2979, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Casasnovas:2014:RTP

[COCF+14] Rodrigo Casasnovas, Joaquin Ortega-Castro, Juan Frau, Josefa Donoso, and Francisco Muñoz. Reviews: Theoretical pK_a calculations with continuum model solvents, alternative protocols to thermodynamic cycles. *International Journal of Quantum Chemistry*, 114(20):1350–1363, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carvalho:2011:CIK

[COdF+11] Alexandre R. F. Carvalho, Joana Oliveira, Victor de Freitas, Nuno Mateus, and André Melo. On the contribution of intramolecular kinetics properties of an important rotamer of vinylpyranoanthocyanin-phenol pigment (portisin). *International Journal of Quantum Chemistry*, 111 (7–8):1355–1360, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Conradie:2010:BTC

[Con10] Jeanet Conradie. Bonding in titanocenyl complexes containing O,O′-cyclic ligands. *International Journal of Quantum Chemistry*, 110(5):1100–1107, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cooper:2012:CSC

[Coo12] W. Grant Cooper. Coherent states as consequences of keto-amino $\rightarrow$ enol-imine hydrogen bond arrangements driven by quantum uncertainty limits on amino DNA protons. *International Journal of Quantum Chemistry*, 112(10):2301–2323, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cruz:2016:LEC

[COP16] S. A. Cruz and H. Olivares-Pilón. Letters to the Editor: Comment on "The effect of confinement on the electronic energy and polarizability of a hydrogen molecular ion" by Josimar Fernando da Silva, Fabricio Ramos Silva and Elso Drigo Filho, Int. J. Quantum Chem. 2016, **116**, 497–503. *International Journal of Quantum Chemistry*, 116(24):1891–1893, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [dSSF16b, dSSF16a].

Corongiu:2016:UPN

[Cor16] Giorgina Corongiu. Unexpected properties of non-autoionizing doubly excited states of the H_2 molecule. *International Journal of Quantum Chemistry*, 116(16):1214–1223, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbonniere:2010:TIT

[CP10] Philippe Carbonniere and Claude Pouchan. Time-independent and time-dependent methods for the calculation of the vibrational spectra: H_2 CN as example. *International Journal of Quantum Chemistry*, 110(3):578–585, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Clavero:2011:DMQ

[CP11] Esteban Clavero and Juliana Palma. Direct mixed-quantum/classical computations of $k(T)$. An analysis of the use of different coordinate systems. *International Journal of Quantum Chemistry*, 111(7–8):1773–1783, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cooper:2013:BFD

[CP13] David L. Cooper and Robert Ponec. Bond formation in diatomic transition metal hydrides: Insights from the analysis of domain-averaged Fermi holes. *International Journal of Quantum Chemistry*, 113(2):102–111, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Coe:2016:OSS

[CP16] J. P. Coe and M. J. Paterson. Open-shell systems investigated with Monte Carlo configuration interaction. *International Journal of Quantum Chemistry*, 116(23):1772–1782, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Crespo:2011:TSS

[CPAT11] R. Crespo, M.-C. Piqueras, J. M. Aulló, and O. Tapia. A theoretical study of semiclassic models: Toward a quantum mechanical representation of chemical processes. *International Journal of Quantum Chemistry*, 111(2):263–271, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cacheiro:2011:CMC

[CPF+11] Javier López Cacheiro, Thomas Bondo Pedersen, Berta Fernández, Alfredo Sánchez De Merás, and Henrik Koch. The CCSD(T) model with Cholesky decomposition of orbital energy denominators. *International Journal of Quantum Chemistry*, 111(2):349–355, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caramori:2012:ISB

[CPF12] Giovanni F. Caramori, Renato L. T. Parreira, and Ana Maria Da Costa Ferreira. Isatin–Schiff base copper(II) complexes — a DFT study of the metal-ligand bonding situation. *International Journal of Quantum Chemistry*, 112 (2):625–646, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caputo:2015:TPO

[CPL15] Maria C. Caputo, Stefano Pelloni, and Paolo Lazzeretti. Theoretical prediction of the optical rotation of chiral

molecules in ordered media: a computational study of (R_a)-1,3-dimethylallene, (2R)-2-methyloxirane, and (2R)-*N*-methyloxaziridine. *International Journal of Quantum Chemistry*, 115(14):900–906, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2018:IPD

[CR18] Lili Cao and Ulf Ryde. Influence of the protein and DFT method on the broken-symmetry and spin states in nitrogenase. *International Journal of Quantum Chemistry*, 118(15):e25627:1–e25627:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caetano:2011:UNN

[CRA+11] C. Caetano, J. L. Reis, Jr., J. Amorim, M. Ruv Lemes, and A. Dal Pino, Jr. Using neural networks to solve nonlinear differential equations in atomic and molecular physics. *International Journal of Quantum Chemistry*, 111(12):2732–2740, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Caetano:2012:UIP

[CRB+12] Melissa S. Caetano, Teodorico C. Ramalho, Douglas F. Botrel, Elaine F. F. da Cunha, and Walclee Carvalho de Mello. Understanding the inactivation process of organophosphorus herbicides: a DFT study of glyphosate metallic complexes with Zn^{2+}, Ca^{2+}, Mg^{2+}, Cu^{2+}, Co^{3+}, Fe^{3+}, Cr^{3+}, and Al^{3+}. *International Journal of Quantum Chemistry*, 112(15):2752–2762, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cerqueira:2011:VIV

[CRFR11] N. M. F. S. A. Cerqueira, J. Ribeiro, P. A. Fernandes, and M. J. Ramos. vsLab — an implementation for virtual high-throughput screening using AutoDock and VMD. *International Journal of Quantum Chemistry*, 111(6):1208–1212, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chashchikhin:2012:DMB

[CRSB12] Vladimir Chashchikhin, Elena Rykova, Andrei Scherbinin, and Alexander Bagaturyants. DFT modeling of band

shifts and widths in the absorption spectrum of a 9-(diphenylamino)acridine/silica receptor center upon its interaction with gas-phase NH_3, C_2H_5OH, and $(CH_3)_2CO$ molecules. *International Journal of Quantum Chemistry*, 112(18):3110–3118, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2013:ISH

[CS13] Cheng Cheng and Li Sheng. Ab-initio study of helium–small carbon cage systems. *International Journal of Quantum Chemistry*, 113(1):35–38, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chiou:2017:CTS

[CS17] Mong-Feng Chiou and Wen-Shyan Sheu. Charge-transfer-to-solvent absorption spectra of I^- $(H_2$ $O)_{3--5}$ at a finite temperature via simulation. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Czapla:2018:TPH

[CS18] Marcin Czapla and Piotr Skurski. Toward the preparation of the $HAuF_6$, HAu_2 F_{11}, and HAu_3 F_{16} superacids: Theoretical study. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2014:RAE

[CSG14] Lan Cheng, Stella Stopkowicz, and Jürgen Gauss. Review: Analytic energy derivatives in relativistic quantum chemistry. *International Journal of Quantum Chemistry*, 114 (17):1108–1127, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2012:CSD

[CSK12] Jiangchao Chen, Andrew Schmitz, and Dmitri S. Kilin. Computational simulation of the *p*-*n* doped silicon quantum dot. *International Journal of Quantum Chemistry*, 112(24):3879–3888, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chuvylkin:2010:GPN

[CSMZ10] Nikolai D. Chuvylkin, Evgenii A. Smolenskii, Marina S. Molchanova, and Nikolai S. Zefirov. Geometrical properties of nodal surfaces of many-electron wave functions. *International Journal of Quantum Chemistry*, 110(10):1809–1819, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Contreras:2010:NSS

[CSP+10] R. H. Contreras, R. Suardíaz, C. Pérez, R. Crespo-Otero, J. San Fabián, and J. M. García de la Vega. NMR spin–spin coupling constants and hyperconjugative interactions. *International Journal of Quantum Chemistry*, 110(3):532–539, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chang:2016:RME

[CSS16] Bo Y. Chang, Ignacio R. Sola, and Seokmin Shin. Reviews: Molecular events in the light of strong fields: a light-induced potential scenario. *International Journal of Quantum Chemistry*, 116(8):608–621, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cordova-Sintjago:2012:MDL

[CSSK+12] Tania Córdova-Sintjago, Rajeev Sakhuja, Krishnakanth Kondabolu, Clinton E. Canal, and Raymond G. Booth. Molecular determinants for ligand binding at serotonin 5-HT_{2A} and 5-HT_{2C} GPCRs: Experimental affinity results analyzed by molecular modeling and ligand docking studies. *International Journal of Quantum Chemistry*, 112(24):3807–3814, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cuevas-Saavedra:2016:AOZ

[CSTA16] Rogelio Cuevas-Saavedra, David C. Thompson, and Paul W. Ayers. Alternative Ornstein–Zernike models from the homogeneous electron liquid for density functional theory calculations. *International Journal of Quantum Chemistry*, 116(11):852–861, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cordova-Sintjago:2012:HSH

[CSVCB12] Tania Córdova-Sintjago, Nancy Villa, Clinton Canal, and Raymond Booth. Human serotonin 5-HT_{2C}G protein-coupled receptor homology model from the β_2 adrenoceptor structure: Ligand docking and mutagenesis studies. *International Journal of Quantum Chemistry*, 112(1):140–149, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ciftcioglu:2014:CET

[ÇT14] Gökçen A. Çiftcioğlu and Carl Trindle. Computational estimates of thermochemistry and pK_a values of cyclopropenyl imine superbases. *International Journal of Quantum Chemistry*, 114(6):392–399, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cruz-Torres:2010:HSI

[CTDOLA10] A. Cruz-Torres, F. De L. Castillo-Alvarado, J. Ortíz-López, and J. S. Arellano. Hydrogen storage inside a toroidal carbon nanostructure C_{120}: Density functional theory computer simulation. *International Journal of Quantum Chemistry*, 110(13):2495–2508, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Carbonniere:2012:VAB

[CTVA12] Philippe Carbonniere, Sandrine Thicoipe, Thibault Very, and Xavier Assfeld. Vibrational analysis beyond the harmonicity from Ab initio molecular dynamics: Case of cytosine in its anhydrous and aqueous forms. *International Journal of Quantum Chemistry*, 112(9):2221–2230, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2012:TSA

[CTW12] Ya Kun Chen, Wei Quan Tian, and Yan Alexander Wang. Theoretical studies of Au_m and $PtAu_n$ clusters and their N_2 and O_2 adsorption complexes. *International Journal of Quantum Chemistry*, 112(1):65–77, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2011:AAD

[CW11] Chia-Chun Chou and Robert E. Wyatt. Applications of automatic differentiation to the time-dependent Schrödinger equation. *International Journal of Quantum Chemistry*, 111(15):4072–4079, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Certik:2013:CST

[ČW13a] Ondřej Čertík and Peter Winkler. Computation of screened two-electron matrix elements. *International Journal of Quantum Chemistry*, 113(16):2012–2018, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2013:TDS

[CW13b] Chia-Chun Chou and Robert E. Wyatt. Time-dependent Schrödinger equation with Markovian outgoing wave boundary conditions: Applications to quantum tunneling dynamics and photoionization. *International Journal of Quantum Chemistry*, 113(1):39–44, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chatterjee:2016:HDP

[CW16] Subhojyoti Chatterjee and Feng Wang. How different is pyrimidine as a core component of DNA base from its diazine isomers: a DFT study? *International Journal of Quantum Chemistry*, 116(24):1836–1845, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2013:TSS

[CWB+13] Jie Chen, Jian Wang, Fu-Quan Bai, Qing-Jiang Pan, and Hong-Xing Zhang. Theoretical studies on structural and spectroscopic properties of photoelectrochemical cell ruthenium sensitizers, derivatives of AR20. *International Journal of Quantum Chemistry*, 113(7):891–901, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2011:OMM

[CwCW+11] Chao Cao, Yun wen Chen, Yuning Wu, Erik Deumens, and Hai-Ping Cheng. OPAL: a multiscale multicenter simulation package based on MPI-2 protocol. *International Journal of Quantum Chemistry*, 111(15):4020–4029, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Campos:2011:TEI

[CWF11] Renan Borsoi Campos, Fernando Wypych, and Harley Paiva Martins Filho. Theoretical estimates of the IR spectrum of formamide intercalated into kaolinite. *International Journal of Quantum Chemistry*, 111(9):2137–2148, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2013:SEP

[CWL+13] Yang Cao, Dawei Wang, Bin Liu, Guijun Yao, Yutuo Fu, Xiaojun Li, and Zhenggang Bi. The structure and electronic property of the smallest C_{20}-glycine and Gd-encapsulated C_{20}-glycine derivatives with potentially biological activity. *International Journal of Quantum Chemistry*, 113(10):1440–1446, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2015:TSD

[CWS15] Li Ping Cheng, Jing Li Wang, and Ying Xin Sun. Theoretical study of the decomposition mechanism of a series of group III triazides $X(N_3)_3$ (X = B, Al, Ga). *International Journal of Quantum Chemistry*, 115(2):68–76, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cui:2013:GSI

[CWSZ13] Wenwen Cui, Cheng Wang, Jingling Shao, and Xiaolei Zhu. Geometry, stability, and isomerization of B_nN_2 (n = 1–6) isomers. *International Journal of Quantum Chemistry*, 113 (20):2251–2260, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cancio:2012:LBM

[CWW12] A. C. Cancio, Chris E. Wagner, and Shaun A. Wood. Laplacian-based models for the exchange energy. *International Journal of Quantum Chemistry*, 112(24):3796–3806, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2016:SEM

[CWW+16] Guo-Xiang Chen, Dou-Dou Wang, Jun-Qing Wen, A-Ping Yang, and Jian-Min Zhang. Structural, electronic, and magnetic properties of 3*d* transition metal doped GaN nanosheet: a first-principles study. *International Journal of Quantum Chemistry*, 116(13):1000–1005, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2010:TMS

[CWZ+10] Dezhan Chen, Qingli Wang, Honghong Zhang, Shizhen Mi, Juliang Wang, Qiang Zeng, and Guiqiu Zhang. Theoretical mechanisms of the superoxide radical anion catalyzed by the copper-zinc superoxide dismutase. *International Journal of Quantum Chemistry*, 110(7):1394–1401, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cybulski:2011:VCG

[Cyb11] Sławomir M. Cybulski. Vibrational corrections to geometry and nuclear shielding constants of cytosine. *International Journal of Quantum Chemistry*, 111(4):873–879, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2015:SNU

[CYC+15] Zhenhua Chen, Fuming Ying, Xun Chen, Jinshuai Song, Peifeng Su, Lingchun Song, Yirong Mo, Qianer Zhang, and Wei Wu. Software news & updates: XMVB 2.0: a new version of Xiamen valence bond program. *International Journal of Quantum Chemistry*, 115(11):731–737, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chou:2017:VIS

[CYK17] Chia-Chun Chou, Jie Yao, and Donald J. Kouri. Volterra inverse scattering series method for one-dimensional quantum barrier scattering. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2018:SSO

[CYL+18] Chang-Yuan Chen, Yuan You, Fa-Lin Lu, Dong-Sheng Sun, and Shi-Hai Dong. Study of spin-orbit interaction for the Makarov potential. *International Journal of Quantum Chemistry*, 118(23):e25774:1–e25774:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2019:PHM

[CYL+19] Jiatian Chen, Le Yang, Ying Li, Qinghua Hou, Lanlan Li, and Peng Jin. Pentapnictogen heterocyclic monoanions: Structure, stability, and aromaticity. *International Journal of Quantum Chemistry*, 119(16):e25961:1–e25961:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2011:MTS

[CYLL11] Shu-Feng Chen, Ling Yue, Ya-Jun Liu, and Roland Lindh. Multireference theoretical studies on the solvent effect of firefly multicolor bioluminescence. *International Journal of Quantum Chemistry*, 111(13):3371–3377, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cysewski:2011:NNN

[Cys11] Piotr Cysewski. Nonadditive nature of nucleobases interactions in model d(GpG) dinucleotide steps. *International Journal of Quantum Chemistry*, 111(3):616–623, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Czapla:2018:SAA

[Cza18] Marcin Czapla. Silicon amino acids. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cheng:2019:SCP

[CZCW19] Junxia Cheng, Hong Zhang, Xinlu Cheng, and Shenjiang Wu. Selective control of photoassociation of alkaline earth dimers: a theoretical study. *International Journal of Quantum Chemistry*, 119(24):e26027:1–e26027:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Cao:2012:RBM

[CZJZ12] Jun Cao, Lijiao Zhao, Shubin Jin, and Rugang Zhong. Relationship between the molecular structure and the anticancer activity of N-(2-chloroethyl)-N'-cyclohexyl-N-nitrosoureas: a theoretical investigation. *International Journal of Quantum Chemistry*, 112(3):747–758, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Chen:2017:EOP

[CZLD17] Juan Chen, Xingfeng Zhu, Chenglin Luo, and Yafei Dai. Electronic and optical properties of pyrrole and thiophene oligomers: a density functional theory study. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAndrade:2012:PCP

[dA12] Paulo Cesar Peres de Andrade. Probability current in protein electron transfer: Löwdin population analysis. *International Journal of Quantum Chemistry*, 112(20):3325–3332, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DelGaldo:2016:SCB

[DAA16] Sara Del Galdo, Massimiliano Aschi, and Andrea Amadei. In silico characterization of bimolecular electron transfer reactions: the ferrocene–ferrocenium reaction as a test case. *International Journal of Quantum Chemistry*, 116 (22):1723–1730, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deArmino:2017:QFF

[dAB17] Diego J. Alonso de Armiño and Carlos M. Bustamante. A quartic force field coordinate substitution scheme using hyperbolic sine coordinates. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:2011:SPD

[DAC11] Sumita Datta, S. A. Alexander, and R. L. Coldwell. Sigma, pi, and delta wavefunction forms for the hydrogen molecule. *International Journal of Quantum Chemistry*, 111(15): 4106–4112, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Datta:2012:LOR

[DAC12] Sumita Datta, S. A. Alexander, and R. L. Coldwell. The lowest order relativistic corrections for the hydrogen molecule. *International Journal of Quantum Chemistry*, 112(3):731–739, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dhouib:2012:DIC

[DAE+12] A. Dhouib, M. Abderrabba, K. Essalah, V. Brites, and M. Hochlaf. DFT and Ab Initio calculations of spectroscopic properties of tetramethyltin and of its cation. *International Journal of Quantum Chemistry*, 112(9):2032–2042, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAndrade:2012:CMQ

[dAGNJT12] Deyse Valverde Gomes de Andrade, Aristóteles Góes-Neto, Moacyr Comar Junior, and Alex Gutterres Taranto. Comparative modeling and QM/MM studies of cysteine protease mutant of Theobroma cacao. *International Journal of Quantum Chemistry*, 112(19):3164–3168, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeOliveira-Filho:2011:CMS

[DAR+11] Antonio G. S. De Oliveira-Filho, Tiago V. Alves, Vladir W. Ribas, Luiz F. A. Ferrão, Orlando Roberto-Neto, Francisco B. C. Machado, and Fernando R. Ornellas. A CASSCF/

MRCI study of the low-lying electronic states of the BeS molecule. *International Journal of Quantum Chemistry*, 111(7–8):1694–1700, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAlmeida:2012:TIV

[dARAV12] K. J. de Almeida, T. C. Ramalho, M. C. Alves, and O. Vahtras. Theoretical insights into the visible near-infrared absorption spectra of Bis(hexafluoroacetylacetonate) copper(II) in pyridine. *International Journal of Quantum Chemistry*, 112(13):2571–2577, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daud:2016:FDQ

[Dau16] Mohammad Noh Daud. Full-dimensional quantum molecular dynamics calculations of the rovibrationally mediated X $1A\prime$ 2 $1A''$ transition of nitrous oxide. *International Journal of Quantum Chemistry*, 116(6):452–468, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deAndrade:2017:SET

[dAVdM17] Railton B. de Andrade, Elizete Ventura, and Silmar A. do Monte. Solvent effect on the tautomers' stabilities of protonated N, N-dimethylnitrosamine: the role of hydrogen bonds network. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dhatt:2011:PTE

[DB11] S. Dhatt and K. Bhattacharyya. A perturbation theory without energy corrections. *International Journal of Quantum Chemistry*, 111(9):1950–1960, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dhatt:2012:SNP

[DB12] Sharmistha Dhatt and Kamal Bhattacharyya. Surprises in nonlinear perturbations: Case of a multiple well potential problem. *International Journal of Quantum Chemistry*, 112(1):171–177, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dhatt:2013:ESR

[DB13a] Sharmistha Dhatt and Kamal Bhattacharyya. Embedding scaling relations in Padé approximants: Detours to tame divergent perturbation series. *International Journal of Quantum Chemistry*, 113(7):916–924, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunne:2013:SRE

[DB13b] Lawrence J. Dunne and Erkki J. Brändas. Superconductivity from repulsive electronic correlations on alternant cuprate and iron-based lattices. *International Journal of Quantum Chemistry*, 113(17):2053–2059, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dutta:2015:DSH

[DB15] Biswa Jyoti Dutta and Pradip Kr. Bhattacharyya. DFT studies on hydrogen-bonding, stacking, and X H$\cdots\pi$-bonded systems in presence of external electric field. *International Journal of Quantum Chemistry*, 115(20):1459–1466, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delgado-Barrio:2011:P

[DBMPB11] Gerardo Delgado-Barrio, Jean Maruani, Piotr Piecuch, and Erkki Brändas. Preface. *International Journal of Quantum Chemistry*, 111(2):203–204, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehesa:2019:SEH

[DBTA19] Jesús S. Dehesa, Elena D. Belega, Irene V. Toranzo, and Alexander I. Aptekarev. The Shannon entropy of high-dimensional hydrogenic and harmonic systems. *International Journal of Quantum Chemistry*, 119(18):e25977:1–e25977:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Degreve:2010:PPX

[DC10] Léo Degréve and Sylvio Canuto. Preface: Proceedings of the XV Brazilian Symposium of Theoretical Chemistry. *International Journal of Quantum Chemistry*, 110

(11):2005, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duarte:2012:PBS

[DC12] Hélio Duarte and Sylvio Canuto. Proceedings of the 16th Brazilian symposium of theoretical chemistry. *International Journal of Quantum Chemistry*, 112(19):3131, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2014:GHI

[DC14a] Ranjita Das and Pratim Kumar Chattaraj. Guest–host interaction in an aza crown analog. *International Journal of Quantum Chemistry*, 114(11):708–719, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duca:2014:RQM

[DC14b] José S. Duca and Jason B. Cross. Review: Quantum mechanical approaches to structurally informed design. *International Journal of Quantum Chemistry*, 114(5):305–313, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dai:2011:DFTb

[DCBB11] Yafei Dai, Sugata Chowdhury, and Estela Blaisten-Barojas. Density functional theory study of the structure and energetics of negatively charged oligopyrroles. *International Journal of Quantum Chemistry*, 111(10):2295–2305, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Debnath:2011:BMF

[DCD11] P. K. Debnath, Barnali Chakrabarti, and Tapan Kumar Das. Beyond mean-field effects in attractive Bose–Einstein condensate. *International Journal of Quantum Chemistry*, 111(7–8):1333–1338, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deCourcy:2011:IWA

[dCDC+11] Benoît de Courcy, Jean-Pierre Dognon, Carine Clavaguéra, Nohad Gresh, and Jean-Philip Piquemal. Interactions

within the alcohol dehydrogenase Zn(II)-metalloenzyme active site: Interplay between subvalence, electron correlation/dispersion, and charge transfer/induction effects. *International Journal of Quantum Chemistry*, 111(6):1213–1221, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Demichelis:2010:PDF

[DCDD10] Raffaella Demichelis, Bartolomeo Civalleri, Philippe D'Arco, and Roberto Dovesi. Performance of 12 DFT functionals in the study of crystal systems: Al_2 SiO_5 orthosilicates and Al hydroxides as a case study. *International Journal of Quantum Chemistry*, 110(12):2260–2273, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Domingo:2010:SCF

[DCdG10] Alex Domingo, Maria Àngels Carvajal, and Coen de Graaf. Spin crossover in Fe(II) complexes: an ab initio study of ligand σ-donation. *International Journal of Quantum Chemistry*, 110(2):331–337, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Demichelis:2010:PED

[DCFD10] Raffaella Demichelis, Bartolomeo Civalleri, Matteo Ferrabone, and Roberto Dovesi. On the performance of eleven DFT functionals in the description of the vibrational properties of aluminosilicates. *International Journal of Quantum Chemistry*, 110(2):406–415, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

delCampo:2012:RDG

[dCGAMV12] Jorge M. del Campo, José L. Gázquez, Rodrigo J. Alvarez-Mendez, and Alberto Vela. The reduced density gradient in atoms. *International Journal of Quantum Chemistry*, 112(22):3594–3598, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2011:LPO

[DCHC11] Hua Dong, Bo-Zhen Chen, Ming-Bao Huang, and Hai-Bo Chang. O-loss photodissociation of the OCS^+ ion in the low-lying electronic states studied using multiconfiguration second-order perturbation theory. *International Journal*

of Quantum Chemistry, 111(14):3578–3587, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dzib:2019:EPC

[DCOC+19] Eugenia Dzib, José Luis Cabellos, Filiberto Ortíz-Chi, Sudip Pan, Annia Galano, and Gabriel Merino. Eyringpy: a program for computing rate constants in the gas phase and in solution. *International Journal of Quantum Chemistry*, 119(2):e25686:1–e25686:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ducati:2010:EGM

[DCR10] Lucas Colucci Ducati, Rogério Custodio, and Roberto Rittner. Exploring the G3 method in the study of rotational barrier of some simple molecules. *International Journal of Quantum Chemistry*, 110(11):2006–2014, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daCosta:2013:DFT

[dCSDdMC13] Leonardo M. da Costa, Stanislav R. Stoyanov, Raimundo N. Damasceno, and José Walkimar de M. Carneiro. Density functional theory investigation of the binding interactions between phosphoryl, carbonyl, imino, and thiocarbonyl ligands and the pentaaqua nickel(II) complex: Coordination affinity and associated parameters. *International Journal of Quantum Chemistry*, 113(24):2621–2628, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Drazic:2017:TTD

[DCZ17] Miloš S. Dražić, Viktor Cerovski, and Radomir Zikic. Theory of time-dependent nonequilibrium transport through a single molecule in a nonorthogonal basis set. *International Journal of Quantum Chemistry*, 117(1):57–73, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dickerson:2017:GPE

[DD17] Shelby D. Dickerson and Nathan J. DeYonker. Gas phase electronic structure of the 3*d* metal monoacetylides

(MCCH, M = Sc ... Zn). *International Journal of Quantum Chemistry*, 117(2):104–128, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Demir:2012:ETI

[DDÇY12] Sibel Demir, Muharrem Dinçer, Alaaddin Çukurovali, and Ibrahim Yilmaz. Experimental and theoretical investigation of the molecular and electronic structure of N'-benzylidene-N-[4-(3-methyl-3-phenyl-cyclobutyl)-thiazol-2-yl]-chloro-acetic acid hydrazide. *International Journal of Quantum Chemistry*, 112(4):1016–1028, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DosSantosGrasel:2012:AAN

[DDF+12] Fábio Dos Santos Grasel, Tiago Charão De Oliveira, Luiz Antonio Mazzini Fontoura, Italo José Da Cruz Rigotti, and Paulo Augusto Netz. N-arylamides and N-arylcarbamates N — CO internal rotation barrier study by molecular modeling. *International Journal of Quantum Chemistry*, 112 (6):1678–1687, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DosSantosRodrigues:2011:DSV

[DdG+11] Guilherme Dos Santos Rodrigues, Ivan da Silva Cunha, Guilherme Gomes Silva, Antonio Luiz Oliveira de Noronha, Heitor Avelino de Abreu, and Hélio Anderson Duarte. DFT study of vanadyl (IV) complexes with low molecular mass ligands: Picolinate, oxalate, malonate, and maltolate. *International Journal of Quantum Chemistry*, 111 (7–8):1395–1402, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garrido:2010:IOV

[dDGNB10] Juan de Dios Garrido, Marco Antonio Chaer Nascimento, and Maikel Yusat Ballester. Influence of oxygen vibrational excitation on HS + O_2 reactive collisions. *International Journal of Quantum Chemistry*, 110(3):549–557, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dhillon:2018:CPS

[DE18] Shamneet Dhillon and Allan L. L. East. Challenges in predicting Δ_{rxn}G in solution: Hydronium, hydroxide, and water autoionization. *International Journal of Quantum Chemistry*, 118(19):e25703:1–e25703:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Denis:2013:TCH

[Den13] Pablo A. Denis. Theoretical characterization of hydrogen pentoxide, H_2O_5. *International Journal of Quantum Chemistry*, 113(19):2206–2212, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Denis:2019:ESS

[Den19] Pablo A. Denis. On the estimation of the strength of supramolecular complexes of fullerenes. *International Journal of Quantum Chemistry*, 119(2):e25670:1–e25670:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Defranceschi:2011:O

[DEPP11] Mireille Defranceschi, Yves Ellinger, Olivier Parisel, and Françoise Pauzat. Obituary. *International Journal of Quantum Chemistry*, 111(2):213–214, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dziedzic:2013:LSD

[DFF+13] Jacek Dziedzic, Stephen J. Fox, Thomas Fox, Christofer S. Tautermann, and Chris-Kriton Skylaris. Large-scale DFT calculations in implicit solvent — a case study on the T4 lysozyme L99A/M102Q protein. *International Journal of Quantum Chemistry*, 113(6):771–785, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diniakhmetova:2016:QCM

[DFK16] Diana Radikovna Diniakhmetova, Anna Konstantinovna Friesen, and Sergey Viktorovich Kolesov. Quantum chemical modeling of the addition reactions of 1-*n*-phenylpropyl

radicals to C_{60} fullerene. *International Journal of Quantum Chemistry*, 116(7):489–496, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilvadosSantos:2015:LER

[dFR15a] Carlos da Silva dos Santos, Elso D. Filho, and Regina M. Ricotta. Letter to the Editor: Reply to the comment on: "Quantum Confinement in Hydrogen Bond" by Carlos da Silva dos Santos, Elso Drigo Filho, and Regina Maria Ricotta, Int. J. Quantum Chem. 2015, **115**, 765–770. *International Journal of Quantum Chemistry*, 115(20):1512–1513, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [HS15].

daSilvadosSantos:2015:QCH

[dFR15b] Carlos da Silva dos Santos, Elso Drigo Filho, and Regina Maria Ricotta. Quantum confinement in hydrogen bond. *International Journal of Quantum Chemistry*, 115(12):765–770, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [HS15] and reply [dFR15a].

DosSantos:2012:PCP

[DFV+12] Hélio F. Dos Santos, Mauro L. Franco, Mateus F. Venâncio, Dalva E. C. Ferreira, Cleber P. A. Anconi, Willian R. Rocha, and Wagner B. De Almeida. Prediction of conformational population of large cycloalkanes using ab initio correlated methods: Cycloundecane, cyclododecane, and cyclotridecane. *International Journal of Quantum Chemistry*, 112(19):3188–3197, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dmitriev:2019:IDF

[DG19] Alexey A. Dmitriev and Nina P. Gritsan. Ab initio and density functional theory study of the electronic structure of rhenium complexes with noninnocent dioxolene ligands: Localized vs delocalized valence states. *International Journal of Quantum Chemistry*, 119(23):e26018:1–e26018:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Doemer:2013:APC

[DGA+13] Manuel Doemer, Matteo Guglielmi, Prashanth Athri, Natalia S. Nagornova, Thomas R. Rizzo, Oleg V. Boyarkin, Ivano Tavernelli, and Ursula Rothlisberger. Assessing the performance of computational methods for the prediction of the ground state structure of a cyclic decapeptide. *International Journal of Quantum Chemistry*, 113(6):808–814, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deGraaf:2014:RMD

[dGR14] Coen de Graaf and Mar Reguero. Review: Methods for describing open-shell systems: Following the trail of Rosa Caballol's research. *International Journal of Quantum Chemistry*, 114(8):481–492, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2016:MDS

[DGR+16] Xiong Ding, Rui-Jun Gou, Fu-De Ren, Fa Liu, Shu-Hai Zhang, and Hong-Fei Gao. Molecular dynamics simulation and density functional theory insight into the cocrystal explosive of hexaazaisowurtzitane/nitroguanidine. *International Journal of Quantum Chemistry*, 116(2):88–96, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daHora:2012:CSR

[dHLdS12] Gabriel Costa A. da Hora, Ricardo L. Longo, and João Bosco P. da Silva. Calculations of structures and reaction energy profiles of As_2O_3 and As_4O_6 species by quantum chemical methods. *International Journal of Quantum Chemistry*, 112(20):3320–3324, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2019:RSE

[DHYC19] Caixia Dong, Limin Han, Jucai Yang, and Lin Cheng. Revisiting the structural and electronic properties of neutral, mono- and di-anionic titanium-doped silicon clusters $TiSi_n^{0/-/2-}$ (n = 6–16). *International Journal of Quantum Chemistry*, 119(18):e25978:1–e25978:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dou:2011:PEC

[DHZS11] Xiaotong Dou, Huixian Han, Gaohong Zhai, and Bingbing Suo. Potential energy curves and interpretation of electronic spectrum of the yttrium nitride. *International Journal of Quantum Chemistry*, 111(13):3378–3384, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Denis:2010:DCA

[DI10] Pablo A. Denis and Federico Iribarne. The 1,3 dipolar cycloaddition of azomethine ylides to graphene, single wall carbon nanotubes, and C60. *International Journal of Quantum Chemistry*, 110(9):1764–1771, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Denis:2011:ASR

[DI11] Pablo A. Denis and Federico Iribarne. Addition of sulfur radicals to fullerenes. *International Journal of Quantum Chemistry*, 111(15):4266–4275, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Denis:2015:BPV

[DI15] Pablo A. Denis and Federico Iribarne. Buckycatcher polymer versus fullerene-buckycatcher complex: Which is stronger? *International Journal of Quantum Chemistry*, 115(23):1668–1672, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Denis:2018:APA

[DI18] Pablo A. Denis and Federico Iribarne. Adsorption of polycyclic aromatic hydrocarbons and inversion barriers of curved conjugated systems inside the molecular cage ExCage^{6+}. *International Journal of Quantum Chemistry*, 118(11):e25539:1–e25539:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dillen:2013:CMW

[Dil13] Jan Dillen. Congested molecules. Where is the steric repulsion? An analysis of the electron density by the method of interacting quantum atoms. *International Journal of Quantum Chemistry*, 113(18):2143–2153, September 15,

2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dardouri:2012:TSE

[DIOG12] Riadh Dardouri, Khaled Issa, Brahim Oujia, and Florent Xavier Gadéa. Theoretical study of the electronic structure of LiX and NaX (X = Rb, Cs) molecules. *International Journal of Quantum Chemistry*, 112(15):2724–2734, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dahl:1995:DKP

[DJ95] Jens Peder Dahl and Thomas Jøorgensen. On the Dirac–Kepler problem: The Johnson–Lippmann operator, supersymmetry, and normal-mode representations. *International Journal of Quantum Chemistry*, 53(2):161–181, January 15, 1995. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [DJ12].

Dahl:2012:EDK

[DJ12] Jens Peder Dahl and Thomas Jørgensen. Erratum: On the Dirac–Kepler problem. The Johnson–Lippmann operator, supersymmetry, and normal-mode representations. *International Journal of Quantum Chemistry*, 112(14):2690, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [DJ95].

Driver:2018:EAM

[DJ18] Nicholas Driver and Purusottam Jena. Electron affinity of modified benzene. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeLeon:2010:AAI

[DJB10] Ained De Leon, Abraham F. Jalbout, and Vladimir A. Basiuk. [80]fullerene–amino acid interactions: Theoretical insights. *International Journal of Quantum Chemistry*, 110 (4):953–959, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehestani:2013:CVE

[DK13] M. Dehestani and Z. Kalantari. The calculation of vibrational energy levels of polyatomic molecules including an-

harmonic effect using contact transformation perturbation method. *International Journal of Quantum Chemistry*, 113 (8):1180–1191, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dekhtyar:2010:DMM

[DKR10] Marina L. Dekhtyar, Taisiya Ye. Korochkova, and Viktor M. Rozenbaum. Directed mechanical motion in nonequilibrium nanosystems: Occurrence conditions and kinematic controllability. *International Journal of Quantum Chemistry*, 110(1):67–76, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deepa:2011:SPE

[DKS11] P. Deepa, P. Kolandaivel, and K. Senthilkumar. Structural properties and the effect of 2,6-diaminoanthraquinone on *G*-tetrad, non-*G*-tetrads, and mixed tetrads — a density functional theory study. *International Journal of Quantum Chemistry*, 111(12):3239–3250, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DYachkov:2010:QCM

[DKZ+10] Pavel N. D'Yachkov, Nina V. Kharchevnikova, Zoya I. Zholdakova, Nathalia Fjodorova, Mariana Novich, and Marian Vrachko. Quantum chemical metabolism-based simulation of carcinogenic potency of benzene derivatives. *International Journal of Quantum Chemistry*, 110(7):1402–1411, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Daud:2015:QCE

[DLCB15] Mohammad Noh Daud, Huizhong Lu, Szczepan Chelkowski, and Andre D. Bandrauk. Quantum control of electron-proton symmetry breaking in dissociative ionization of H_2 by intense laser pulses. *International Journal of Quantum Chemistry*, 115(6):369–380, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deLima:2012:SHA

[dLdOdAD12] Guilherme Ferreira de Lima, Cláudio de Oliveira, Heitor Avelino de Abreu, and Hélio Anderson Duarte. Sulfuric and hydrochloric acid adsorption on the reconstructed sulfur terminated (001) chalcopyrite surface. *International Jour-*

nal of Quantum Chemistry, 112(19):3216–3222, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2012:DCF

[DLG12] Yan-Li Ding, En-Bo Li, and Li-Dong Gong. Dynamic changing features of the molecular face for interaction of a rare gas atom with a hydrogen molecule. *International Journal of Quantum Chemistry*, 112(12):2515–2524, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deng:2014:SCE

[DLJT14] Xiao-Yan Deng, Guang-Hua Liu, Xi-Ping Jing, and Guang-Shan Tian. On-site correlation of p-electron in d^{10} semiconductor zinc oxide. *International Journal of Quantum Chemistry*, 114(7):468–472, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dumont:2010:EER

[DLLA10] Élise Dumont, Pierre-François Loos, Adèle D. Laurent, and Xavier Assfeld. Electronic effects and ring strain influences on the electron uptake by selenium-containing bonds. *International Journal of Quantum Chemistry*, 110(3):513–523, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

delaLuz:2012:TDE

[dlLIAI$^+$12] Alexander Pérez de la Luz, Cristina Iuga, Juan Raúl Alvarez-Idaboy, Elba Ortíz, and Annik Vivier-Bunge. Tropospheric degradation of ethylene glycol monovinyl and divinyl ethers: a mechanistic and kinetic study. *International Journal of Quantum Chemistry*, 112(21):3525–3534, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2011:QCM

[DLM$^+$11] S. P. Dolin, A. A. Levin, T. Yu. Mikhailova, M. V. Solin, and N. V. Zinova. Quantum-chemical modeling of squaric acid ferroelectric behavior. *International Journal of Quantum Chemistry*, 111(11):2671–2676, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2012:NAC

[DLM12] S. P. Dolin, A. A. Levin, and T. Yu. Mikhailova. A novel approach to coupled proton–phonon macroscopic system in H-bonded solids with strong low-barrier hydrogen bonds on the examples of KH_2PO_4 and KD_2PO_4. *International Journal of Quantum Chemistry*, 112(17):2976–2979, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2016:CLI

[DLO16] Wenhui Ding, Xueling Lei, and Chuying Ouyang. Coordination of lithium ion with ethylene carbonate electrolyte solvent: a computational study. *International Journal of Quantum Chemistry*, 116(2):97–102, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Domagala:2017:HBV

[DLP17] Małgorzata Domagała, Aneta Lutyńska, and Marcin Palusiak. Halogen bond versus hydrogen bond: the many-body interactions approach. *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehesa:2010:ITD

[DLRMFY10] J. S. Dehesa, S. López-Rosa, A. Martínez-Finkelshtein, and R. J. Yáñez. Information theory of D-dimensional hydrogenic systems: Application to circular and Rydberg states. *International Journal of Quantum Chemistry*, 110(8):1529–1548, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deLima:2011:HBB

[dLRR11] NatháLia B. de Lima, Victor H. Rusu, and Mozart N. Ramos. Hydrogen bonds between phthalimide and hydrogen fluoride: a theoretical study. *International Journal of Quantum Chemistry*, 111(7–8):1387–1394, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Duan:2011:MDS

[DLZ11] Xiao-Hui Duan, Jian-Feng Li, and Wen-Jun Zhu. Molecular dynamics simulation of ionic transport on molten Li–KCl interface. *International Journal of Quantum Chemistry*, 111(14):3873–3880, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2012:ADTb

[DM12] Anita Das and Debasis Mukhopadhyay. The adiabatic-to-diabatic transformation angle and topological phases for strongly interacting states: Solution with four states. *International Journal of Quantum Chemistry*, 112(16):2767–2774, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deMarothy:2013:ADC

[dM13] Sven A. de Marothy. Autocatalytic decomposition of carbonic acid. *International Journal of Quantum Chemistry*, 113(20):2306–2311, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dyachkov:2016:ISD

[DM16] Pavel D'yachkov and Dmitry Makaev. Ab initio spin-dependent band structures of carbon nanotubes. *International Journal of Quantum Chemistry*, 116(4):316–324, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2012:ADTa

[DMAB12] Anita Das, Debasis Mukhopadhyay, Satrajit Adhikari, and Michael Baer. The adiabatic-to-diabatic transformation angle and the Berry phase for coupled Jahn–Teller/ Renner–Teller systems: The F + H_2 as a case study. *International Journal of Quantum Chemistry*, 112(13):2561–2570, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Determan:2015:SPT

[DMBJ15] John J. Determan, Salvador Moncho, Edward N. Brothers, and Benjamin G. Janesko. Simulating periodic trends in the structure and catalytic activity of coinage metal

nanoribbons. *International Journal of Quantum Chemistry*, 115(24):1718–1725, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2016:RPQ

[DMBL16] S. P. Dolin, T. Yu. Mikhailova, N. N. Breslavskaya, and A. A. Levin. Reviews: On the possibility of quantum-chemical cluster approach to the description of structural phase transition in H-bonded materials on the example of KDP. *International Journal of Quantum Chemistry*, 116 (3):202–210, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dogaru:2010:RMF

[DMG10] Daniela Dogaru, Stefan Motiu, and Valentin Gogonea. Residue mutations in [Fe Fe]-hydrogenase impedes O_2 binding: A QM/MM investigation. *International Journal of Quantum Chemistry*, 110(9):1784–1792, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oliveira:2012:IVC

[dMOB12] Rodrigo C. de M. Oliveira and Glauco F. Bauerfeldt. Implementation of a variational code for the calculation of rate constants and application to barrierless dissociation and radical recombination reactions: $CH_3OH = CH_3 + OH$. *International Journal of Quantum Chemistry*, 112 (19):3132–3140, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolin:2010:TDH

[DMS+10] S. P. Dolin, T. Yu. Mikhailova, M. V. Solin, N. N. Breslavskaya, and A. A. Levin. Three-dimensional H-bonding and ferroelectric transition in KDP. Quantum-chemical study. *International Journal of Quantum Chemistry*, 110(1):77–82, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2011:IMR

[DMWY11] Yan-Li Ding, Ji-Rong Mu, Chun-Hui Wang, and Zhong-Zhi Yang. Insight into Markovnikov regioselectivity rule via molecular face and ABEEM-$\sigma\pi$ theory. *International*

Journal of Quantum Chemistry, 111(12):2778–2787, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Durand-Niconoff:2012:RBL

[DNCKCS+12] José S. Durand-Niconoff, Luis Cruz-Kuri, Jesús S. Cruz-Sánchez, Myrna H. Matus, and Fernando R. Ramos-Morales. Relationship between local reactivity indices and the Hammett constant for isatoic anhydride and its derivatives. *International Journal of Quantum Chemistry*, 112 (22):3570–3577, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dobson:2014:PBP

[Dob14] John F. Dobson. Perspectives: Beyond pairwise additivity in London dispersion interactions. *International Journal of Quantum Chemistry*, 114(18):1157–1161, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deOliveira:2011:TAT

[dOdCMUdALR11] Boaz Galdino de Oliveira, Regiane de Cássia Maritan Ugulino de Araújo, Elisa Soares Leite, and Mozart Neves Ramos. A theoretical analysis of topography and molecular parameters of the $CFCl_3 \cdots O_3$ complex: Linear and bifurcate halogen-oxygen bonding interactions. *International Journal of Quantum Chemistry*, 111(1):111–116, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deOliveira:2012:TSD

[dOdONM12] Daniel Augusto Barra de Oliveira, Marçal de Oliveira Neto, and João B. L. Martins. Theoretical study of disubstituted pyrrolopyrimidines as focal adhesion kinase inhibitors. *International Journal of Quantum Chemistry*, 112(10):2324–2329, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dovesi:2014:SNU

[DOE+14] Roberto Dovesi, Roberto Orlando, Alessandro Erba, Claudio M. Zicovich-Wilson, Bartolomeo Civalleri, Silvia Casassa, Lorenzo Maschio, Matteo Ferrabone, Marco De La Pierre, Philippe D'Arco, Yves Noël, Mauro Causà, Michel

Rérat, and Bernard Kirtman. Software news & updates: CRYSTAL14: a program for the ab initio investigation of crystalline solids. *International Journal of Quantum Chemistry*, 114(19):1287–1317, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

delOlmo:2013:EMS

[dOLdlV13] Lourdes del Olmo, Rafael López, and José M. García de la Vega. Effect of the molecular structure in the prediction of thermodynamic properties for 1-butyl-3-methylimidazolium chloride ionic liquid. *International Journal of Quantum Chemistry*, 113(6):852–858, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deOliveira:2010:DBB

[dOR10] Boaz Galdino de Oliveira and Mozart Neves Ramos. Dihydrogen bonds and blue-shifting hydrogen bonds: a theoretical study of $AH\cdots HCF_3$ and $TH_2\cdots HCF_3$ model systems with A = Li or Na and T = Be or Mg. *International Journal of Quantum Chemistry*, 110(2):307–316, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Durand:2011:TUF

[DP11] Philippe Durand and Ivana Paidarová. Towards a unified formulation of dynamics and thermodynamics. I. From microscopic to macroscopic time scales. *International Journal of Quantum Chemistry*, 111(2):225–236, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deuri:2012:SMU

[DP12] Sanjib Deuri and Prodeep Phukan. A stepwise mechanism for the uncatalyzed Michael addition of acetylacetone to methyl vinyl ketone. *International Journal of Quantum Chemistry*, 112(3):801–808, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dimic:2016:CPC

[DP16] Dušan Dimić and Milena Petković. Control of a photoswitching chelator by metal ions: DFT, NBO, and QTAIM analysis. *International Journal of Quantum Chemistry*, 116

(1):27–34, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dias:2011:DSL

[DPDR11] Roberta P. Dias, Mauro S. L. Prates Jr., Wagner B. De Almeida, and Willian R. Rocha. DFT study of the ligand effects on the regioselectivity of the insertion reaction of olefins in the complexes $[HRh(CO)_2(PR_3)(L)]$ (R = H, F, Et, Ph, OEt, OPh, and L = propene, styrene). *International Journal of Quantum Chemistry*, 111(7–8):1280–1292, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deepa:2018:DPW

[DPK18] Palanisamy Deepa, B. Vijaya Pandiyan, and Ponmalai Kolandaivel. Does the presence of water clusters induce the binding affinity of CK2 halogen ligands?: a quantum chemical perspective study. *International Journal of Quantum Chemistry*, 118(16):e25644:1–e25644:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Devipriya:2012:CDD

[DPRK12] Balu Devipriya, Azhagesan Renuga Parameswari, Gnanasekaran Rajalakshmi, and Poomani Kumaradhas. Charge density distribution and electrostatic moments of *N*-(4-chloro-3-trifluromethyl-phenyl)-2-ethoxy-benzamide molecule at the active site of p300 enzyme: a quantum chemical and theoretical charge density study. *International Journal of Quantum Chemistry*, 112(4):1185–1197, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2012:DFT

[DQZF12] Dongmei Du, Mei Qin, Zhengyu Zhou, and Aiping Fu. Density functional theoretical study of p K_a of RCOOH (R H, CH_3, and C_2H_5) using the combination of the extended clusters-continuum model. *International Journal of Quantum Chemistry*, 112(2):351–358, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Demissie:2018:DRC

[DR18] Taye B. Demissie and Kenneth Ruud. Darmstadtium, roentgenium, and copernicium form strong bonds with cyanide. *International Journal of Quantum Chemistry*, 118 (1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeGraaf:2011:RML

[DS11] Coen De Graaf and Carmen Sousa. On the role of the metal-to-ligand charge transfer states in the light-induced spin crossover in Fe^{II} $(bpy)_3$. *International Journal of Quantum Chemistry*, 111(13):3385–3393, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehestani:2012:MRS

[DS12] Maryam Dehestani and Fahimeh Shojaie. Multichannel RRKM study on the mechanism and kinetics of the CH_3Cl + OH reaction. *International Journal of Quantum Chemistry*, 112(5):1307–1315, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeCastroFaria:2011:NIT

[DSC+11] N. V. De Castro Faria, M. M. Sant'Anna, C. Carvalho, Ginette Jalbert, L. F. S. Coelho, B. F. Magnani, and F. Zappa. Negative ions and their behavior in collisions. *International Journal of Quantum Chemistry*, 111(7–8): 1836–1842, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2012:RLS

[dSCC12] Arnaldo Machado da Silva, Sumana Chakraborty, and Puspitapallab Chaudhuri. Rayleigh light scattering from hydrogen-bonded dimers of small astrophysical molecules. *International Journal of Quantum Chemistry*, 112(16): 2822–2827, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeLaVega:2013:TDK

[DSCO+13] J. M. García De La Vega, J. San Fabián, R. Crespo-Otero, R. Suardíaz, and C. Pérez. Theoretical DFT Karplus

equations: Amino acid side-chain torsion angle χ_1. *International Journal of Quantum Chemistry*, 113(5):656–660, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeSouza:2018:DSM

[DSD18] Leonardo A. De Souza, Malucia M. Soeiro, and Wagner B. De Almeida. A DFT study of molecular structure and^1 H NMR, IR, and UV-Vis spectrum of Zn(II)-kaempferol complexes: a metal-flavonoid complex showing enhanced anticancer activity. *International Journal of Quantum Chemistry*, 118(23):e25773:1–e25773:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2013:APD

[dSdS13a] Luís Pinto da Silva and Joaquim C. G. Esteves da Silva. Analysis of the performance of DFT functionals in the study of light emission by oxyluciferin analogs. *International Journal of Quantum Chemistry*, 113(1):45–51, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2013:CDS

[dSdS13b] Luís Pinto da Silva and Joaquim C. G. Esteves da Silva. Chemiluminescence of 1,2-dioxetanone studied by a closed-shell DFT approach. *International Journal of Quantum Chemistry*, 113(12):1709–1716, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2011:TST

[dSdSPG11] Larissa Tunes da Silva, José Roberto dos Santos Politi, and Ricardo Gargano. Theoretical study of tetrahydrofuran: Comparative investigation of spectroscopic and structural properties between gas and liquid phases. *International Journal of Quantum Chemistry*, 111(12):2914–2921, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dudek:2017:CSC

[DSFT17] John B. Dudek, Thomas Salomon, Sven Fanghänel, and Sven Thorwirth. Carbon–sulfur chains: a high-resolution infrared and quantum-chemical study of C_3 S and SC_7S.

International Journal of Quantum Chemistry, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2013:TSE

[DSH+13] Ranran Du, Bingbing Suo, Huixian Han, Yibo Lei, and Gaohong Zhai. Theoretical study of electronic structure of rhodium mononitride and interpretation of experimental spectra. *International Journal of Quantum Chemistry*, 113(22):2464–2470, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Deglmann:2015:RAQ

[DSL15] Peter Deglmann, Ansgar Schäfer, and Christian Lennartz. Review: Application of quantum calculations in the chemical industry — an overview. *International Journal of Quantum Chemistry*, 115(3):107–136, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2019:MIE

[dSM19a] Luís Pinto da Silva and Carla M. Magalhães. Mechanistic insights into the efficient intramolecular chemiexcitation of dioxetanones from TD-DFT and multireference calculations. *International Journal of Quantum Chemistry*, 119 (9):e25881:1–e25881:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DiRemigio:2019:POS

[DSM+19b] Roberto Di Remigio, Arnfinn Hykkerud Steindal, Krzysztof Mozgawa, Ville Weijo, Hui Cao, and Luca Frediani. PCMSolver: an open-source library for solvation modeling. *International Journal of Quantum Chemistry*, 119(1): e25685:1–e25685:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinheiro:2018:MZO

[dSMPRSF18] Pedro de Sena Murteira Pinheiro, Daniel Alencar Rodrigues, Carlos Mauricio R. Sant'Anna, and Carlos Alberto Manssour Fraga. Modeling zinc-oxygen coordination in histone deacetylase: a comparison of semiempirical methods performance. *International Journal of Quantum Chemistry*, 118(21):e25720:1–e25720:??, November 5,

2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deSantiago:2018:QCE

[dSMT+18] Francisco de Santiago, Álvaro Miranda, Alejandro Trejo, Fernando Salazar, Eliel Carvajal, Miguel Cruz-Irisson, and Luis A. Pérez. Quantum confinement effects on the harmful-gas-sensing properties of silicon nanowires. *International Journal of Quantum Chemistry*, 118(20): e25713:1–e25713:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

dosSantos:2008:SEO

[dSNBG08] Daniel J. V. A. dos Santos, Ana S. Newton, Raul Bernardino, and Rita C. Guedes. Substituent effects on O — H and S — H bond dissociation enthalpies of disubstituted phenols and thiophenols. *International Journal of Quantum Chemistry*, 108(4):754–761, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Derrar:2012:TSS

[DSRGD12] S. N. Derrar, M. Sekkal-Rahal, K. Guemra, and P. Dereumaux. Theoretical study on a series of push–pull molecules grafted on methacrylate copolymers serving for nonlinear optics. *International Journal of Quantum Chemistry*, 112(15):2735–2742, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

dosSantos:2012:MMB

[dSSdSGA12] Luísa Silva Nangi dos Santos, Milton Taidi Sonoda, Roseli Aparecida da Silva Gomes, and Odonírio Abrahão, Jr. Molecular modeling of bioactive neuropeptides: Substrates of angiotensin I-converting enzyme. *International Journal of Quantum Chemistry*, 112(20):3414–3420, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2016:LER

[dSSF16a] J. Fernando da Silva, F. Ramos Silva, and E. Drigo Filho. Letters to the Editor: Response to: "Comment on 'The effect of confinement on the electronic energy and polarizability of a hydrogen molecular ion'". *International Journal of Quantum Chemistry*, 116(24):1894–1897, December

15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [dSSF16b, COP16].

daSilva:2016:ECE

[dSSF16b] Josimar Fernando da Silva, Fabrício Ramos Silva, and Elso Drigo Filho. The effect of confinement on the electronic energy and polarizability of a hydrogen molecular ion. *International Journal of Quantum Chemistry*, 116(7): 497–503, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [COP16, dSSF16a].

Dutta:2018:RVM

[DSSM18] Sayantan Dutta, Amar N. Sil, Jayanta K. Saha, and Tapan K. Mukherjee. Ritz variational method for the high-lying nonautoionizing doubly excited $^{1,3}F^e$ states of two-electron atoms. *International Journal of Quantum Chemistry*, 118(14):e25577:1–e25577:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dutta:2019:EIM

[DSSM19] Sayantan Dutta, Amar N. Sil, Jayanta K. Saha, and Tapan K. Mukherjee. Extensive investigations for metastable-bound and resonance $^3F^e$ states of He atom. *International Journal of Quantum Chemistry*, 119(18): e25981:1–e25981:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

daSilva:2017:QTA

[dSTH17] Natieli Alves da Silva, Luiz Alberto Terrabuio, and Roberto Luiz Andrade Haiduke. A quantum theory atoms in molecules investigation of Lewis base protonation. *International Journal of Quantum Chemistry*, 117(3):197–207, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dutta:2015:EAD

[DSVP15] Achintya Kumar Dutta, Turbasu Sengupta, Nayana Vaval, and Sourav Pal. Electron attachment to DNA and RNA nucleobases: an EOMCC investigation. *International Journal of Quantum Chemistry*, 115(12):753–764, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2011:TSC

[DSWL11] Lihua Dong, Junyou Shi, Jinhu Wang, and Yongjun Liu. Theoretical studies on the conformational change of adenosine kinase induced by inhibitors. *International Journal of Quantum Chemistry*, 111(14):3980–3990, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dong:2018:DFT

[DSZB18] Shaonan Dong, Wenjing Shi, Jing Zhang, and Shuping Bi. Density functional theory studies on the external OH^--induced barrierless proton dissociation mechanism for the forced hydrolysis reaction of Al^{3+} (aq). *International Journal of Quantum Chemistry*, 118(19):e25682:1–e25682:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Diaz-Torrejon:2011:CTS

[DTEMK11] C. C. Díaz-Torrejón, F. Espinosa-Magaña, and Ilya G. Kaplan. Comparative theoretical study of the electron affinities of the alkaline-earth clusters: Be_n, Mg_n, and Ca_n ($n = 2, 3$). *International Journal of Quantum Chemistry*, 111(1):103–110, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delfino:2011:DCT

[DTF+11] A. Delfino, V. S. Timóteo, T. Frederico, Lauro Tomio, and C. E. Cordeiro. Dimensional compactification and two-particle binding. *International Journal of Quantum Chemistry*, 111(7–8):1458–1465, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dang:2015:DCP

[DTFK15] Adamou Koko Dang, Conrad Bertrand Tabi, Henri Paul Ekobena Fouda, and Timoleon Crepin Kofané. Discrete charge patterns in a Holstein–SSH DNA lattice. *International Journal of Quantum Chemistry*, 115(1):34–41, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dehesa:2017:EMR

[DTPC17] Jesús S. Dehesa, Irene V. Toranzo, and David Puertas-Centeno. Entropic measures of Rydberg-like harmonic states. *International Journal of Quantum Chemistry*, 117 (1):48–56, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Delgado-Tellez:2012:HIP

[DTVP+12] Laura Delgado-Tellez, Alvaro Valdés, Rita Prosmiti, Pablo Villarreal, and Gerardo Delgado-Barrio. HeI_2 interaction potential based on an interpolation scheme. *International Journal of Quantum Chemistry*, 112(17):2971–2975, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2012:WIT

[Du12] Zhibin Du. Wiener indices of trees and monocyclic graphs with given bipartition. *International Journal of Quantum Chemistry*, 112(6):1598–1605, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dumont:2012:OEA

[Dum12] Élise Dumont. One-electron addition on short-loop selenylsulfide and diselenide-linked biomolecules: From diethyldichalcogens to Grx3-like selenopeptides. *International Journal of Quantum Chemistry*, 112(8):2018–2029, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dunne:2015:RHT

[Dun15] Lawrence J. Dunne. Review: High-temperature superconductivity and long-range order in strongly correlated electronic systems. *International Journal of Quantum Chemistry*, 115(20):1443–1458, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Das:2014:RCR

[DVC14] Ranjita Das, Jean-Louis Vigneresse, and Pratim Kumar Chattaraj. Review: Chemical reactivity through structure-stability landscape. *International Journal of Quantum Chemistry*, 114(21):1421–1429, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

DeLaraCastells:2011:MDS

[DVDBM11] María Pilar De Lara Castells, Pablo Villarreal, Gerardo Delgado-Barrio, and Alexander O. Mitrushchenkov. Microscopic description of small doped ^{3}He clusters through the full-configuration-interaction nuclear orbital approach: The $(^3\mathrm{He})_N$-Br_2(X) case revisited. *International Journal of Quantum Chemistry*, 111(2):406–415, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luca:2019:DSE

[DVMC19] Giorgio De Luca, Marlon Basantes Valverde, Matilde Morrone, and Lorenzo S. Caputi. DFT study on electronic properties of single- and double-shell icosahedral fullerenes. *International Journal of Quantum Chemistry*, 119(10): e25890:1–e25890:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dutta:2018:LSA

[DVP18] Achintya Kumar Dutta, Nayana Vaval, and Sourav Pal. Lower scaling approximation to EOM–CCSD: a critical assessment of the ionization problem. *International Journal of Quantum Chemistry*, 118(15):e25594:1–e25594:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dharma-Wardana:2012:CMH

[DW12] M. W. C. Dharma-Wardana. The classical-map hypernetted-chain (CHNC) method and associated novel density-functional techniques for warm dense matter. *International Journal of Quantum Chemistry*, 112(1):53–64, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dharma-wardana:2013:ECE

[Dw13] M. W. C. Dharma-wardana. Exchange, correlation, and the effective mass m^* of electrons in two-dimensional layers calculated via a DFT-based classical map. *International Journal of Quantum Chemistry*, 113(6):873–879, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2012:TSA

[DWGX12] Hongchen Du, Guixiang Wang, Xuedong Gong, and Heming Xiao. Theoretical study on the adduct of chlorine trifluoride oxide and boron trifluoride—molecular and crystal structures, vibrational spectrum, and thermodynamic properties. *International Journal of Quantum Chemistry*, 112(5):1291–1298, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dai:2011:DFTa

[DWJZ11] Guo-Liang Dai, Chuan-Feng Wang, Yan-Xian Jin, and Ai-Guo Zhong. A density functional theory study on the reactions of Y atom and Y^+ cation with carbonyl sulfide. *International Journal of Quantum Chemistry*, 111(3):529–538, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

deWergifosse:2014:EMS

[dWLC14] Marc de Wergifosse, Vincent Liégeois, and Benoît Champagne. Evaluation of the molecular static and dynamic first hyperpolarizabilities. *International Journal of Quantum Chemistry*, 114(14):900–910, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dupont:2014:IMC

[DWPK14] Céline Dupont, Xiaowen Wan, Mikhail Petukhov, and Peter Krüger. Interaction of $Mo(CO)_6$ and its derivative fragments with the Cu(001) surface: Influence on the decomposition process. *International Journal of Quantum Chemistry*, 114(23):1630–1635, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2016:PEO

[DWX+16] Kaining Ding, Lili Wen, Lintao Xu, Huadeng Wu, Yiguang Ye, and Yongfan Zhang. Predicting the electronic and optical properties of IB metals doped monoclinic $BiVO_4$: First principle calculations. *International Journal of Quantum Chemistry*, 116(5):388–395, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2015:TAI

[DWZZ15] Shuangli Du, Bingqiang Wang, Jian Zhang, and Caiyun Zhang. Tuning anion-π interaction via halogen substituent effects in cyanuric acids and its derivatives. *International Journal of Quantum Chemistry*, 115(17):1147–1152, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dyachkov:2016:RLA

[D'y16] Pavel N. D'yachkov. Reviews: Linear augmented cylindrical wave method for nanotubes electronic structure. *International Journal of Quantum Chemistry*, 116(3):174–188, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ding:2011:GPR

[DZ11a] Ning Ding and Shi-Guo Zhang. Gas-phase reaction mechanism of Pd^+ with CH_3 CHO: a density functional theoretical study. *International Journal of Quantum Chemistry*, 111(10):2359–2365, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Du:2011:RIT

[DZ11b] Zhibin Du and Bo Zhou. On Randić indices of trees, unicyclic graphs, and bicyclic graphs. *International Journal of Quantum Chemistry*, 111(12):2760–2770, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2011:DDO

[DZO11] O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Delocalization of Dyson orbitals in $F^-(H_2O)$ and $Cl^-(H_2O)$. *International Journal of Quantum Chemistry*, 111(7–8): 1701–1708, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2012:IEP

[DZO12a] Olga Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Ab initio electron propagator calculations on electron detachment energies of nickel phthalocyanine tetrasulfonate tetraanions. *International Journal of Quantum Chemistry*,

112(1):184–194, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2012:ESB

[DZO12b] Olga Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Electronic structure of a beryllium half-sandwich complex, $Be(\eta^5 \cdots C_5H_5)$. *International Journal of Quantum Chemistry*, 112(18):2981–2985, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Dolgounitcheva:2012:EDE

[DZO12c] Olga Dolgounitcheva, Viatcheslav G. Zakrzewski, and Joseph Vincent Ortiz. Electron detachment energies of aqueous and cluster halide anions from electron propagator calculations with the polarizable continuum model. *International Journal of Quantum Chemistry*, 112(24):3840–3848, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2012:CII

[EA12] Mehdi D. Esrafili and Vahideh Alizadeh. Characterization of intermolecular interactions in crystalline aspirin: a computational NQR study. *International Journal of Quantum Chemistry*, 112(5):1392–1400, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Echeverria:2017:IIG

[EAA17] Jorge Echeverría, Gabriel Aullón, and Santiago Alvarez. Intermolecular interactions in group 14 hydrides: Beyond CH$\cdots$HC contacts. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elroby:2013:CPM

[EAH13] Shabaan A. K. Elroby, Ashour A. Ahmed, and Rifaat H. Hilal. Conformational preference and mechanism of decarboxylation of levodopa. A quantum dynamics/quantum mechanics study. *International Journal of Quantum Chemistry*, 113(16):1966–1974, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebenso:2010:TSS

[EAK+10a] Eno E. Ebenso, Taner Arslan, Fatma Kandemiırlı, Ian Love, Cemiıl Öğretır, Murat Saracoğlu, and Savıour A. Umoren. Theoretical studies of some sulphonamides as corrosion inhibitors for mild steel in acidic medium. *International Journal of Quantum Chemistry*, 110(14):2614–2636, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebenso:2010:QCS

[EAK+10b] Eno E. Ebenso, Taner Arslan, Fatma Kandemirli, Necmettin Caner, and Ian Love. Quantum chemical studies of some rhodanine azosulpha drugs as corrosion inhibitors for mild steel in acidic medium. *International Journal of Quantum Chemistry*, 110(5):1003–1018, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2016:ISE

[EAV16] Mehdi D. Esrafili, Soheila Asadollahi, and Mahshad Vakili. Investigation of substituent effects in aerogen-bonding interaction between ZO_3 (Z = Kr, Xe) and nitrogen bases. *International Journal of Quantum Chemistry*, 116(16):1254–1260, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2011:CSC

[EBH11] Mehdi D. Esrafili, Javad Beheshtian, and Nasser L. Hadipour. Computational study on the characteristics of the interaction in linear urea clusters. *International Journal of Quantum Chemistry*, 111(12):3184–3195, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ehinon:2011:PCN

[EBR11] Daniel Ehinon, Isabelle Baraille, and Michel Rérat. Polarizabilities of carbon nanotubes: Importance of the crystalline orbitals relaxation in presence of an electric field. *International Journal of Quantum Chemistry*, 111(4):797–806, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ellis:2016:DFA

[ED16] Matthew Ellis and Karen Downey. Density functional analysis of group 10 organometallic diphosphinito complexes for catalytic formation of C — P bonds. *International Journal of Quantum Chemistry*, 116(12):945–952, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2014:SEC

[EEMSS14] Mehdi D. Esrafili, Parvin Esmailpour, Fariba Mohammadian-Sabet, and Mohammad Solimannejad. Substituent effects on cooperativity between lithium bonds. *International Journal of Quantum Chemistry*, 114(4):295–301, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Erdogan:2011:ODSa

[EFO11] Rezan Erdogan, Mehmet Ferdi Fellah, and Isik Onal. An ONIOM and DFT study of water adsorption on rutile TiO_2 (110) cluster. *International Journal of Quantum Chemistry*, 111(1):174–181, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

El-Gogary:2010:IAD

[EG10] Tarek M. El-Gogary. Interaction of angelicin with DNA-bases (III) DFT and ab initio second-order Moeller–Plesset study. *International Journal of Quantum Chemistry*, 110 (8):1445–1454, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebrahimi:2011:SER

[EHKD11] A. Ebrahimi, S. M. Habibi-Khorassani, and M. Doosti. Substituent effects on S_N 2 reaction between substituted benzyl chloride and chloride ion in gas phase. *International Journal of Quantum Chemistry*, 111(5):1013–1024, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eddy:2011:ETS

[EI11] Nnabuk O. Eddy and Benedict I. Ita. Experimental and theoretical studies on the inhibition potentials of some derivatives of cyclopenta-1,3-diene for the corrosion of mild

steel in HCl solutions. *International Journal of Quantum Chemistry*, 111(14):3456–3474, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eilmes:2014:EMV

[Eil14] Andrzej Eilmes. Effect of molecular vibrations on the MD/QC-simulated absorption spectra. *International Journal of Quantum Chemistry*, 114(4):261–270, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebrahimi:2012:SER

[EKD12] A. Ebrahimi, M. Habibi Khorassani, and M. Doosti. Solvent effects on S_N2 reaction between substituted benzyl chloride and chloride ion. *International Journal of Quantum Chemistry*, 112(3):873–881, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebrahimi:2010:OHI

[EKN10] A. Ebrahimi, S. M. Habibi Khorasani, and R. S. Neyband. The O···H intramolecular hydrogen bond in 4-X-2-hydroxybenzaldehydes: The relationships between geometrical parameters, estimated binding energies, and NMR data. *International Journal of Quantum Chemistry*, 110 (10):1871–1879, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elroby:2008:SCD

[ELC08] Shabaan A. K. Elroby, Kyu Hwan Lee, and Seung Joo Cho. Significance of charge-dipolar moiety interaction: Computational study of cyanospherands. *International Journal of Quantum Chemistry*, 108(4):779–787, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elliott:2016:DMP

[EM16] Peter Elliott and Neepa T. Maitra. Density-matrix propagation driven by semiclassical correlation. *International Journal of Quantum Chemistry*, 116(10):772–783, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Enchev:2017:CIC

[EM17] Venelin Enchev and Aleksandar Y. Mehandzhiyski. Computational insight on the chalcone formation mechanism by the Claisen–Schmidt reaction. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2019:DSP

[EM19] Mehdi D. Esrafili and Parisasadat Mousavian. A DFT study on the possibility of using a single Cu atom incorporated nitrogen-doped graphene as a promising and highly active catalyst for oxidation of CO. *International Journal of Quantum Chemistry*, 119(7):e25857:1–e25857:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esquivel:2012:CPT

[EMED+12] Rodolfo O. Esquivel, Moyocoyani Molina-Espíritu, Jesús S. Dehesa, Juan Carlos Angulo, and Juan Antolín. Concurrent phenomena at the transition region of selected elementary chemical reactions: an information-theoretical complexity analysis. *International Journal of Quantum Chemistry*, 112(22):3578–3586, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esquivel:2015:QIS

[EMEPD15] Rodolfo O. Esquivel, Moyocoyani Molina-Espíritu, A. R. Plastino, and Jesus S. Dehesa. Quantum information from selected elementary chemical reactions: Maximum entangled transition state. *International Journal of Quantum Chemistry*, 115(19):1417–1430, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ebrahimi:2014:PNI

[EMK14] Ali Ebrahimi, Najmeh Mostafavi, and Pouya Karimi. Presentation of a new index for estimation of aromaticity in halo- and cyanobenzenes: the role of potential energy in aromaticity. *International Journal of Quantum Chemistry*, 114(2):154–161, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Elango:2011:QCD

[EML+11] Munusamy Elango, Glauciete S. Maciel, Andrea Lombardi, Simonetta Cavalli, and Vincenzo Aquilanti. Quantum chemical and dynamical approaches to intra and intermolecular kinetics: The $C_nH_{2n}O$ ($n = 1, 2, 3$) molecules. *International Journal of Quantum Chemistry*, 111(7–8): 1784–1791, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2016:HCC

[EMS16] Mehdi D. Esrafili and Fariba Mohammadian-Sabet. Homonuclear chalcogen-chalcogen bond interactions in complexes pairing YO_3 and YHX molecules (Y = S, Se; X = H, Cl, Br, CCH, NC, OH, OCH_3): Influence of substitution and cooperativity. *International Journal of Quantum Chemistry*, 116(7):529–536, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2015:DRH

[EMSB15] Mehdi D. Esrafili, Fariba Mohammadian-Sabet, and Mohammad Mehdi Baneshi. The dual role of halogen, chalcogen, and pnictogen atoms as Lewis acid and base: Triangular XBr:SHX:PH_2 X complexes (X = F, Cl, Br, CN, NC, OH, NH_2, and OCH_3). *International Journal of Quantum Chemistry*, 115(22):1580–1586, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Engel:2016:RSC

[Eng16] Eberhard Engel. Relevance of semi-core-valence interaction for exact exchange calculations for group IVA, IIIA–VA, and IIB–VIA semiconductors. *International Journal of Quantum Chemistry*, 116(11):867–879, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2015:ASD

[ENV15] Mehdi D. Esrafili, Roghaye Nurazar, and Esmail Vessally. Application of Si-doped graphene as a metal-free catalyst for decomposition of formic acid: a theoretical study. *International Journal of Quantum Chemistry*, 115(17):1153–1160, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Erdogan:2011:ODSb

[EO11] Rezan Erdogan and Isik Onal. An ONIOM and DFT study of water and ammonia adsorption on anatase TiO_2 (001) cluster. *International Journal of Quantum Chemistry*, 111 (9):2149–2159, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Eifler:2016:CDH

[EPS+16] Jay Eifler, Rudi Podgornik, Nicole F. Steinmetz, Roger H. French, V. Adrian Parsegian, and Wai-Yim Ching. Charge distribution and hydrogen bonding of a collagen α_2-chain in vacuum, hydrated, neutral, and charged structural models. *International Journal of Quantum Chemistry*, 116(9): 681–691, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2017:DSH

[ES17] Mehdi D. Esrafili and Nasibeh Saeidi. A DFT study on the healing of N-vacancy defects in boron nitride nanosheets and nanotubes by a methylene molecule. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Estrada-Salas:2012:ESR

[ESBVJY12] Rubén E. Estrada-Salas, Hector Barrón, Ariel A. Valladares, and Miguel José-Yacamán. Exploring the surface reactivity of Ag nanoparticles with antimicrobial activity: a DFT study. *International Journal of Quantum Chemistry*, 112(18):3033–3038, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

ElHoudaBensiradj:2016:TSS

[ESDO16] Nour El Houda Bensiradj, Amar Saal, Azeddine Dekhira, and Ourida Ouamerali. Theoretical study of selenium and tellurium impurities in $(ZnO)_6$ clusters using DFT and TDDFT. *International Journal of Quantum Chemistry*, 116(24):1862–1871, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Estevez:2019:CCM

[ESLM19] Laura Estévez, Marta Sánchez-Lozano, and Ricardo A. Mosquera. Complexation of common metal cations by cyanins: Binding affinity and molecular structure. *International Journal of Quantum Chemistry*, 119(6):e25834:1–e25834:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Esrafili:2018:SSA

[Esr18] Mehdi D. Esrafili. Single Si atom supported on defective boron nitride nanosheet as a promising metal-free catalyst for N_2 O reduction by CO or SO_2 molecule: a computational study. *International Journal of Quantum Chemistry*, 118(16):e25646:1–e25646:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Emelyanova:2013:DCR

[ESS13] Nina S. Emel'yanova, Alexander F. Shestakov, and Nataliya A. Sanina. DFT calculations of the redox potentials for the nitrosyl complexes [Fe_2 (μ-RS)$_2$ $(NO)_4$] with R = alkyl. *International Journal of Quantum Chemistry*, 113(5):740–744, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Espinosa-Torres:2019:TSE

[ETGLMJ+19] Néstor David Espinosa-Torres, Alfredo Guillén-López, Javier Martínez-Juárez, José Álvaro David Hernández de la Luz, Ángel Pedro Rodríguez-Victoria, and Jesús Muñiz. Theoretical study on the electronic structure nature of single and double walled carbon nanotubes and its role on the electron transport. *International Journal of Quantum Chemistry*, 119(17):e25974:1–e25974:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Exner:2011:CIP

[Exn11] Thomas E. Exner. Critical investigation on the pseudobond approach for QM/MM and fragment-based QM methods. *International Journal of Quantum Chemistry*, 111(5):1002–1012, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ezziane:2010:QCM

[Ezz10] Zoheir Ezziane. Quantum computing measurement and intelligence. *International Journal of Quantum Chemistry*, 110(5):981–992, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2017:EFP

[FA17] Kati Finzel and Paul W. Ayers. The exact Fermi potential yielding the Hartree–Fock electron density from orbital-free density functional theory. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2012:VAC

[FAFR12] F. M. Fernández, N. Aquino, and A. Flores-Riveros. Variational approach to the confined hydrogen atom with a moving nucleus. *International Journal of Quantum Chemistry*, 112(3):823–828, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frediani:2019:CSC

[FAK19] Luca Frediani, Oliviero Andreussi, and Heather J. Kulik. Coding solvation: challenges and opportunities. *International Journal of Quantum Chemistry*, 119(1):e25839:1–e25839:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2017:SMS

[FB17] Kati Finzel and Alexey I. Baranov. A simple model for the Slater exchange potential and its performance for solids. *International Journal of Quantum Chemistry*, 117(1):40–47, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frank:2013:SCH

[FBD+13] Andrea Frank, Andreas Berkefeld, Matthias Drexler, Heiko M. Möller, and Thomas E. Exner. Small changes — huge influences: NMR chemical shifts of Ni(II) complexes with polar substrates. *International Journal of Quantum Chemistry*, 113(13):1787–1793, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

FerreiraDaCunha:2010:TRC

[FBM+10] Wiliam Ferreira Da Cunha, Patricia R. P. Barreto, Geraldo Magela E. Silva, João B. L. Martins, and Ricardo Gargano. Thermal rate coefficients calculation for the H^+ + LiH reaction. *International Journal of Quantum Chemistry*, 110 (11):2024–2028, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fedoseeva:2011:ESC

[FBO+11] Yu. V. Fedoseeva, L. G. Bulusheva, A. V. Okotrub, I. P. Asanov, S. I. Troyanov, and D. V. Vyalikh. Electronic structure of the chlorinated fullerene C_{60} Cl_{30} studied by quantum chemical modeling of X-ray absorption spectra. *International Journal of Quantum Chemistry*, 111(11): 2688–2695, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fantuzzi:2012:PMI

[FBRBR12] F. Fantuzzi, L. Baptista, A. B. Rocha, and H. M. Boechat-Roberty. Positive molecular ions and ion-neutral complexes in the gas phase: Structure and stability of $C_2H_4O_2^{+\cdot}$ and $C_2H_4O_2^{2+}$ isomers. *International Journal of Quantum Chemistry*, 112(20):3303–3311, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freidzon:2011:ISS

[FBU+11] Alexandra Y. Freidzon, Alexander A. Bagatur'yants, Evgeny N. Ushakov, Sergey P. Gromov, and Michael V. Alfimov. Ab initio study of the structure, spectral, ionochromic, and fluorochromic properties of benzoazacrown-containing dyes as potential optical molecular sensors. *International Journal of Quantum Chemistry*, 111(11):2649–2662, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuster:2019:ACC

[FC19] Franck Fuster and Patrick Chaquin. Analysis of carbon-carbon bonding in small hydrocarbons and dicarbon using dynamic orbital forces: Bond energies and sigma/pi partition. Comparison with sila compounds. *International Journal of Quantum Chemistry*, 119(20):e25996:1–e25996:??,

October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Furtuna:2011:OMA

[FCC11] Renata Furtuna, Silvia Curteanu, and Maria Cazacu. Optimization methodology applied to feed-forward artificial neural network parameters. *International Journal of Quantum Chemistry*, 111(3):539–553, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fabiano:2013:ETB

[FCS13a] E. Fabiano, Lucian A. Constantin, and F. Della Sala. Erratum: Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. *International Journal of Quantum Chemistry*, 113(10):1600, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [FCS13b].

Fabiano:2013:TBA

[FCS13b] E. Fabiano, Lucian A. Constantin, and F. Della Sala. Testing the broad applicability of the PBEint GGA functional and its one-parameter hybrid form. *International Journal of Quantum Chemistry*, 113(5):673–682, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [FCS13a].

Finzel:2016:ESU

[FDA16] Kati Finzel, Joel Davidsson, and Igor A. Abrikosov. Energy-surfaces from the upper bound of the Pauli kinetic energy. *International Journal of Quantum Chemistry*, 116 (18):1337–1341, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Furtula:2018:CAS

[FDG18] Boris Furtula, Kinkar Ch. Das, and Ivan Gutman. Comparative analysis of symmetric division deg index as potentially useful molecular descriptor. *International Journal of Quantum Chemistry*, 118(17):e25659:1–e25659:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fileti:2011:GPA

[FDMR11] Eudes E. Fileti, Anselmo E. De Oliveira, Nelson H. Morgon, and José M. Riveros. Gas-phase acylium ion transfer reactions mediated by a proton shuttle mechanism. *International Journal of Quantum Chemistry*, 111(7–8):1596–1606, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferreira:2010:BSD

[FDNR10] Dalva E. C. Ferreira, Wagner B. De Almeida, Ademir Neves, and Willian R. Rocha. Broken symmetry density functional study of a mixed-valence unsymmetrical dinuclear iron complex. *International Journal of Quantum Chemistry*, 110(5):1048–1055, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

FerreiraDaSilva:2011:ICE

[Fer11] A. Ferreira Da Silva. Impurity cluster effects in high- and low-doping semiconductor materials. *International Journal of Quantum Chemistry*, 111(7–8):1466–1471, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2019:CCN

[Fer19] Francisco M. Fernández. Comment on "The consequences of neglecting permutation symmetry in the description of many-electrons systems". *International Journal of Quantum Chemistry*, 119(23):e26020:1–e26020:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Nas19].

Fartaria:2010:MAS

[FFF10] Rui P. S. Fartaria, Filomena F. M. Freitas, and Fernando M. S. Silva Fernandes. Models for the adsorption and self-assembly of ethanol and 1-decanethiol on Au(111) surfaces. A comparative study by computer simulation. *International Journal of Quantum Chemistry*, 110(2):293–306, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fazio:2016:RCE

[FFPD16] Gianluca Fazio, Lara Ferrighi, Daniele Perilli, and Cristiana Di Valentin. Reviews: Computational electrochemistry of doped graphene as electrocatalytic material in fuel cells. *International Journal of Quantum Chemistry*, 116 (22):1623–1640, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Franchini:2019:VBD

[FGD+19] Davide Franchini, Alessandro Genoni, Federico Dapiaggi, Stefano Pieraccini, and Maurizio Sironi. A valence bond description of the bromine halogen bond. *International Journal of Quantum Chemistry*, 119(15):e25946:1–e25946:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2014:ERD

[Fin14a] Kati Finzel. ELF and its relatives — a detailed study about the robustness of the atomic shell structure in real space. *International Journal of Quantum Chemistry*, 114 (22):1546–1558, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2014:HDA

[Fin14b] Kati Finzel. How does the ambiguity of the electronic stress tensor influence its ability to serve as bonding indicator. *International Journal of Quantum Chemistry*, 114 (9):568–576, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2015:SAP

[Fin15] Kati Finzel. A simple approximation for the Pauli potential yielding self-consistent electron densities exhibiting proper atomic shell structure. *International Journal of Quantum Chemistry*, 115(23):1629–1634, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2016:ADB

[Fin16a] Kati Finzel. About the difference between density functionals defined by energy criterion and density functionals defined by density criterion: Exchange functionals. *International Journal of Quantum Chemistry*, 116(15):1187–1189,

August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2016:APP

[Fin16b] Kati Finzel. Approximating the Pauli potential in bound Coulomb systems. *International Journal of Quantum Chemistry*, 116(16):1261–1266, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Finzel:2017:ACB

[Fin17] Kati Finzel. About the compatibility between ansatzes and constraints for a local formulation of orbital-free density functional theory. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frank:2018:TDM

[FK18] Irmgard Frank and Peter Kraus. The tardy dance of molecular orbitals. *International Journal of Quantum Chemistry*, 118(20):e25718:1–e25718:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferdjaoui:2019:CAA

[FKBG19] M. Ferdjaoui, A. Khodja, F. Benamira, and L. Guechi. Comment on "Approximate Analytical Versus Numerical Solutions of Schrödinger Equation Under Molecular Hua Potential". *International Journal of Quantum Chemistry*, 119(13):e25955:1–e25955:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [HYZS12] and reply [HYZS19].

Freindorf:2012:CAH

[FKC12] Marek Freindorf, Elfi Kraka, and Dieter Cremer. A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. *International Journal of Quantum Chemistry*, 112(19):3174–3187, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferrabone:2012:VCS

[FKL+12] Matteo Ferrabone, Bernard Kirtman, Valentina Lacivita, Michel Rérat, Roberto Orlando, and Roberto Dovesi. Vibrational contribution to static and dynamic (hyper)polarizabilities of zigzag BN nanotubes calculated by

the finite field nuclear relaxation method. *International Journal of Quantum Chemistry*, 112(9):2160–2170, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Faginas-Lago:2010:DCR

[FLCHL10] Noelia Faginas-Lago, Alessandro Costantini, and Fermín Huarte-Larrañaga. Direct calculation of the rate coefficients on the grid: Exact quantum versus semiclassical results for $N + N_2$. *International Journal of Quantum Chemistry*, 110(2):422–431, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Faber:2015:CSR

[FLvLA15] Felix Faber, Alexander Lindmaa, O. Anatole von Lilienfeld, and Rickard Armiento. Crystal structure representations for machine learning models of formation energies. *International Journal of Quantum Chemistry*, 115(16):1094–1101, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferdowsi:2016:TSM

[FM16] Parnian Ferdowsi and Javad Mokhtari. Theoretical study of metal-free organic dyes based on different configurations for efficient dye-sensitized solar cells. *International Journal of Quantum Chemistry*, 116(23):1796–1801, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferreira:2011:EEI

[FMCA11] Cristiane Ferreira, Hugo F. M. C. Martiniano, Benedito J. Costa Cabral, and Vincenzo Aquilanti. Electronic excitation and ionization of hydrogen peroxide–water clusters: Comparison with water clusters. *International Journal of Quantum Chemistry*, 111(7–8):1824–1835, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Figueredo:2014:QTP

[FMKJ14] Fernando A. Figueredo, Julio R. Maza, Steven R. Kirk, and Samantha Jenkins. Quantum topology phase diagrams for the cis- and trans-isomers of the cyclic contryphan-Sm peptide. *International Journal of Quantum Chemistry*, 114

(24):1697–1706, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Flores-Moreno:2010:TAN

[FMMD+10] R. Flores-Moreno, J. Melin, O. Dolgounitcheva, V. G. Zakrzewski, and J. V. Ortiz. Three approximations to the nonlocal and energy-dependent correlation potential in electron propagator theory. *International Journal of Quantum Chemistry*, 110(3):706–715, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2017:MSA

[FMP+17] Miguel Fernández, Reinaldo Marín, Fulgencio Proverbio, Delia I. Chiarello, and Fernando Ruette. Magnesium sulfate against oxidative damage of membrane lipids: a theoretical model. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Flores-Moreno:2014:SNU

[FMPM+14] Roberto Flores-Moreno, Edwin Posada, Félix Moncada, Jonathan Romero, Jorge Charry, Manuel Díaz-Tinoco, Sergio A. González, Néstor F. Aguirre, and Andrés Reyes. Software news & updates: LOWDIN: the any particle molecular orbital code. *International Journal of Quantum Chemistry*, 114(1):50–56, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Feng:2017:RHG

[FNBK17] Qingguo Feng, Raoul Noumbissi, Koushik Biswas, and Hideya Koizumi. The role of hydroxyl groups in interchain interactions in cellulose I_α and I_β. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fukuda:2016:CMR

[FNIT16] Masahiro Fukuda, Kento Naito, Kazuhide Ichikawa, and Akitomo Tachibana. Computational method for the retarded potential in the real-time simulation of quantum electrodynamics. *International Journal of Quantum Chemistry*, 116(12):932–938, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fellah:2010:DFS

[FO10] Mehmet Ferdi Fellah and Isik Onal. A density functional study of 1,1,5-tris(4-dimethylaminophenyl)-3-methyl-divinylene. *International Journal of Quantum Chemistry*, 110(5):1041–1047, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ford:2012:VSB

[For12] Thomas A. Ford. The vibrational spectra of the boron halides and their molecular complexes. Part 13. Ab initio studies of the complexes of boron trifluoride with formaldehyde and some of its analogs. *International Journal of Quantum Chemistry*, 112(2):478–488, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fortenberry:2017:ESI

[For17a] Ryan C. Fortenberry. Editorial: Special issue: Computational astrochemistry. *International Journal of Quantum Chemistry*, 117(2):80, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fortenberry:2017:RQA

[For17b] Ryan C. Fortenberry. Review: Quantum astrochemical spectroscopy. *International Journal of Quantum Chemistry*, 117(2):81–91, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Franco-Perez:2012:UVP

[FPRGMHGB12] Marco Franco-Pérez, Luis I. Reyes-García, Rosario Moya-Hernández, and Rodolfo Gómez-Balderas. UV–visible properties of oxicams in solution: a TD–DFT and experimental study. *International Journal of Quantum Chemistry*, 112(22):3637–3645, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frank:2017:SMR

[Fra17] Irmgard Frank. A single-molecule reaction cascade: First-principles molecular dynamics simulation. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Frapiccini:2010:GMO

[FRGC10] A. L. Frapiccini, J. M. Randazzo, G. Gasaneo, and F. D. Colavecchia. A general method to obtain Sturmian functions for continuum and bound state problems with Coulomb interactions. *International Journal of Quantum Chemistry*, 110(5):963–974, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fritzsche:2012:RMB

[Fri12] S. Fritzsche. Relativistic many-body theory: a new field-theoretical approach. *International Journal of Quantum Chemistry*, 112(14):2688–2689, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ferrao:2012:CHA

[FRNM12] Luiz Fernando Araujo Ferrão, Orlando Roberto-Neto, and Francisco Bolivar Correto Machado. $CH_3OH + 2H(^2S_g)$ hydrogen abstraction reactions occurring in the presence of a copper tetramer: a DFT study. *International Journal of Quantum Chemistry*, 112(19):3228–3233, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freire:2011:LCW

[FS11] Ricardo O. Freire and Alfredo M. Simas. The lanthanide contraction within the sparkle model. *International Journal of Quantum Chemistry*, 111(7–8):1734–1739, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fominykh:2016:CAD

[FSB16] Olga D. Fominykh, Anastasiya V. Sharipova, and Marina Yu. Balakina. The choice of appropriate density functional for the calculation of static first hyperpolarizability of azochromophores and stacking dimers. *International Journal of Quantum Chemistry*, 116(2):103–112, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Freidzon:2012:STI

[FSBA12] Alexandra Ya. Freidzon, Andrei A. Safonov, Alexander A. Bagaturyants, and Michael V. Alfimov. Solvatoflu-

orochromism and twisted intramolecular charge-transfer state of the Nile red dye. *International Journal of Quantum Chemistry*, 112(18):3059–3067, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fuks:2011:ICS

[FSK+11] David Fuks, Dina Shapiro, Arnold Kiv, Vyacheslav Golovanov, and Chung-Chiun Liu. Ab initio calculations of surface electronic states in indium oxide. *International Journal of Quantum Chemistry*, 111(9):1902–1906, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2011:DSS

[FSQ+11] Min Fan, Shi-Ling Sun, Yong-Qing Qiu, Xiao-Dong Liu, and Zhong-Min Su. DFT study on the second-order nonlinear optical property of 12-vertex close-carborane derivatives. *International Journal of Quantum Chemistry*, 111 (5):1039–1047, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fukuda:2016:LPQ

[FSST16] Masahiro Fukuda, Kota Soga, Masato Senami, and Akitomo Tachibana. Local physical quantities for spin based on the relativistic quantum field theory in molecular systems. *International Journal of Quantum Chemistry*, 116 (12):920–931, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fortenberry:2015:OCU

[FT15] Ryan C. Fortenberry and Russell Thackston. Optimal cloud use of quartic force fields: the first purely commercial cloud computing based study for rovibrational analysis of $SiCH^-$. *International Journal of Quantum Chemistry*, 115(23):1650–1657, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fernandez:2011:FPS

[FTB11] Eva M. Fernández, Maria B. Torres, and Luis C. Balbás. First principles study of CO adsorption–CO_2 desorption mechanisms on oxidized doped-gold cationic clusters

MAu_nO (M = Ti, Fe; $n = 1, 4--7$; $m = 1--2$). *International Journal of Quantum Chemistry*, 111(2):510–519, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fukushima:2012:MDA

[FUE+12] Kimichika Fukushima, Yukio Ugawa, Hiroshi Endo, Yoshihisa Shindo, Isao Tatewaki, Kazuo Haga, and Masaaki Inoue. Molecular dynamics approach to sodium-water reaction compensating macroscopic heat and mass flow dynamics for LMFBR safety. *International Journal of Quantum Chemistry*, 112(24):3829–3833, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fukushima:2012:CAU

[Fuk12] Kimichika Fukushima. $CaCuO_2$ antiferromagnetism using shallow well added solely to atomic potential for generating O^{2-} basis set of periodic molecular orbitals with consideration of Coulomb potential in solid in an LDA. *International Journal of Quantum Chemistry*, 112(1):44–52, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Felix:2011:DPH

[FV11] Martín Félix and Alexander A. Voityuk. DFT performance for the hole transfer parameters in DNA π stacks. *International Journal of Quantum Chemistry*, 111(1):191–201, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xin:2019:SUK

[fXxBhD19] Jing fan Xin, Xiao xu Bo, and Yi hong Ding. Structurally uneasy but kinetically stable nitrogens in 1,3-disubstituted cyclotetrazenes: Viable high-energy-density materials. *International Journal of Quantum Chemistry*, 119(18):e25976:1–e25976:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2011:CEB

[FYhC11] Hong-Yi Fan, Hong-Chun Yuan, and Jun hua Chen. Calculating electron binding energies for quadratic fermion Hamiltonian by virtue of the IEO method. *International*

Journal of Quantum Chemistry, 111(12):2910–2913, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Filatov:2014:RCR

[FZC14] Michael Filatov, Wenli Zou, and Dieter Cremer. Review: Calculation of response properties with the normalized elimination of the small component method. *International Journal of Quantum Chemistry*, 114(15):993–1005, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2018:DCM

[FZH+18] Wen-Jie Fan, Yan-Ling Zhao, Yu-Cai Hu, Hua Shi, Da-Zhi Tan, and Rui-Qin Zhang. Design of conjugated microporous polymer nanotubes for efficient benzene molecular adsorptions. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Fan:2018:DFT

[FZX18] Guohong Fan, Sheng Zhu, and Hong Xu. Density-functional theory study of the interaction mechanism and optical properties of flavonols on the boron nitride nanotubes. *International Journal of Quantum Chemistry*, 118 (7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghalavand:2019:OCU

[GA19] Ali Ghalavand and Ali R. Ashrafi. Ordering chemical unicyclic graphs by Wiener polarity index. *International Journal of Quantum Chemistry*, 119(17):e25973:1–e25973:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gagliardi:2011:SAC

[Gag11] Laura Gagliardi. The study of actinide chemistry with multiconfigurational quantum chemical methods. *International Journal of Quantum Chemistry*, 111(13):3302–3306, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Galano:2019:CSP

[GAI19] Annia Galano and Juan Raúl Alvarez-Idaboy. Computational strategies for predicting free radical scavengers' protection against oxidative stress: Where are we and what might follow? *International Journal of Quantum Chemistry*, 119(2):e25665:1–e25665:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goncalves:2010:ESB

[GAMM10] Rebeca D. Gonçalves, Sérgio Azevedo, Fernando Moraes, and M. Machado. Energetic stability of boron nitride nanostructures doped with one carbon atom. *International Journal of Quantum Chemistry*, 110(9):1778–1783, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ganesan:2014:IDO

[Gan14] Timothy Ganesan. Investigation of dephasing in an open quantum system under chaotic influence via a fractional Kohn–Sham scheme. *International Journal of Quantum Chemistry*, 114(24):1660–1669, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2011:MWF

[Gao11] Shan Gao. Meaning of the wave function. *International Journal of Quantum Chemistry*, 111(15):4124–4138, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2012:TSC

[Gao12] Hong-Ze Gao. Theoretical study on charge transport of quinacridone polymorphs. *International Journal of Quantum Chemistry*, 112(3):740–746, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gam:2019:SHC

[GAPK+19a] Franck Gam, Ramiro Arratia-Pérez, Samia Kahlal, Jean-Yves Saillard, and Alvaro Muñoz-Castro. Stabilizing heteroatom-centered 16-vertex group 11 tetrahedral architectures: Bonding and structural considerations to-

ward versatile endohedral species. *International Journal of Quantum Chemistry*, 119(24):e26038:1–e26038:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gam:2019:SLC

[GAPK+19b] Franck Gam, Ramiro Arratia-Perez, Samia Kahlal, Jean-Yves Saillard, and Alvaro Muñoz-Castro. Symmetry lowering by cage doping in spherical superatoms: Evaluation of electronic and optical properties of 18-electron $W@Au_{12}$ Pt_n ($n = 0$–4) superatomic clusters from relativistic DFT calculations. *International Journal of Quantum Chemistry*, 119(6):e25827:1–e25827:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garai:2008:MFD

[Gar08] Jozsef Garai. Mathematical formulas describing the sequences of the periodic table. *International Journal of Quantum Chemistry*, 108(4):667–670, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2010:LSD

[GB10] S. Ghosh and S. P. Bhattacharyya. Localization in some discontinuously and randomly driven quantum systems. *International Journal of Quantum Chemistry*, 110(14):2637–2644, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gomez:2013:ESE

[GB13] Vivian B. Gomez and Kyle A. Beran. Energetic stability and electronic properties of exohedral derivatives of C_{20}: $C_{20}X_n$ (X = H, F, Cl; $n = 1$–4). *International Journal of Quantum Chemistry*, 113(7):925–933, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gormley:2018:BMS

[GB18] Eoghan L. Gormley and Robert F. Berger. Binding maps for the study and prediction of bimetallic catalyst surface reactions: the case of methanol oxidation. *International Journal of Quantum Chemistry*, 118(15):e25606:1–e25606:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gall:2018:GBB

[GBK18] Marián Gall, Lukás Bucinský, and Stanislav Komorovsky. General build up of K_+ basis and K_+^2 matrix in the diagonalization approach. Determination of Kramers configuration state functions. *International Journal of Quantum Chemistry*, 118(16):e25638:1–e25638:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Galvez:2017:CEE

[GBS17] Francisco J. Gálvez, Enrique Buendía, and Antonio Sarsa. Confinement effects on the electronic structure of M-shell atoms: a study with explicitly correlated wave functions. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gil-bernal:2010:QCA

[GbZA10] Hernan Gil-bernal, Martha L. Zambrano, and Julio C. Arce. Quantum-chemical-aided design of copolymers with tailored bandgaps and effective masses: The role of composition. *International Journal of Quantum Chemistry*, 110(13):2522–2531, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghara:2018:FNO

[GC18] Manas Ghara and Pratim K. Chattaraj. Fixation of nitrous oxide (N_2 O) by 1, 4, 2, 5-diazadiborinine: a DFT study. *International Journal of Quantum Chemistry*, 118 (15):e25593:1–e25593:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guido:2019:DEP

[GC19] Ciro A. Guido and Stefano Caprasecca. On the description of the environment polarization response to electronic transitions. *International Journal of Quantum Chemistry*, 119(1):e25711:1–e25711:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2013:SEI

[GCD13] Chen Guo, Zhong-Hua Cui, and Yi-Hong Ding. Structures, energetics, and isomerism of [Be, C, O, S]: Stability

of triply bonded sulfur. *International Journal of Quantum Chemistry*, 113(19):2213–2219, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghalami-Choobar:2012:TCP

[GCDNGS12] Bahram Ghalami-Choobar, Hamid Dezhampanah, Paria Nikparsa, and Ali Ghiami-Shomami. Theoretical calculation of the pK_a values of some drugs in aqueous solution. *International Journal of Quantum Chemistry*, 112 (10):2275–2280, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Genova:2017:EOS

[GCK+17] Alessandro Genova, Davide Ceresoli, Alisa Krishtal, Oliviero Andreussi, Robert A. DiStasio, Jr., and Michele Pavanello. eQE: an open-source density functional embedding theory code for the condensed phase. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2014:DFT

[GCZ+14] Xiaokang Guo, Lihui Chen, Yanyan Zhu, Anqi Zhang, Donghui Wei, and Mingsheng Tang. A density functional theory study on Lewis acid-catalyzed transesterification of β-oxodithioesters. *International Journal of Quantum Chemistry*, 114(13):862–868, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Granja:2011:DFS

[GD11] Faustino Aguilera Granja and Reinaldo Pis Diez. A density functional study of the interaction of dihydrogen with Mo_N clusters ($N = 28$). Adsorption and dissociation of H_2 and cluster reconstruction after desorption. *International Journal of Quantum Chemistry*, 111(12):3201–3211, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grether:2012:GBP

[GdLT12] M. Grether, M. de Llano, and V. V. Tolmachev. A generalized BEC picture of superconductors. *International Journal of Quantum Chemistry*, 112(18):3018–3024, September

15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Giro:2010:TAA

[GDM+10] Ronaldo Giro, Liliana Y. A. Davila, Angelita M. Machado, Marilia J. Caldas, and Leni Akcelrud. Theoretical analysis of aggregation in block-copolymer films: The optical signature. *International Journal of Quantum Chemistry*, 110(4):885–892, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gruner:2012:CBO

[GE12a] Markus E. Gruner and Peter Entel. Competition between ordering, twinning, and segregation in binary magnetic 3d–5d nanoparticles: a supercomputing perspective. *International Journal of Quantum Chemistry*, 112(1):277–288, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2012:UNG

[GE12b] I. I. Guseinov and M. Ertürk. Use of noninteger n-generalized exponential type orbitals with hyperbolic cosine in atomic calculations. *International Journal of Quantum Chemistry*, 112(6):1559–1565, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goings:2018:PCD

[GEL18] Joshua J. Goings, Franco Egidi, and Xiaosong Li. Perspective: Current development of noncollinear electronic structure theory. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia-Fernandez:2012:PJT

[GFB12a] Pablo Garcia-Fernandez and Isaac B. Bersuker. Pseudo Jahn–Teller origin of bending distortions in Renner–Teller molecules and its spectroscopic implications. *International Journal of Quantum Chemistry*, 112(18):3025–3032, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghanmi:2012:TSL

[GFB12b] C. Ghanmi, M. Farjallah, and H. Berriche. Theoretical study of low-lying electronic states of the $LiRb^+$ molecular ion: Structure, spectroscopy and transition dipole moments. *International Journal of Quantum Chemistry*, 112 (11):2403–2410, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gazquez:2019:TDA

[GFPAV19] José L. Gázquez, Marco Franco-Pérez, Paul W. Ayers, and Alberto Vela. Temperature-dependent approach to chemical reactivity concepts in density functional theory. *International Journal of Quantum Chemistry*, 119(2):e25797:1–e25797:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Greco:2011:FGB

[GFRdG11] Claudio Greco, Piercarlo Fantucci, Ulf Ryde, and Luca de Gioia. Fast generation of broken-symmetry states in a large system including multiple iron–sulfur assemblies: Investigation of QM/MM energies, clusters charges, and spin populations. *International Journal of Quantum Chemistry*, 111(14):3949–3960, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2011:NWN

[GfWlZ11] Ying Guo, Yan fang Wang, and Sheng li Zhang. A novel way to numerically characterize DNA sequences and its application. *International Journal of Quantum Chemistry*, 111(14):3971–3979, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goel:2012:DFS

[GGD12] Neetu Goel, Seema Gautam, and Keya Dharamvir. Density functional studies of Li_N and Li_N^+ ($N = 2$–30) clusters: Structure, binding and charge distribution. *International Journal of Quantum Chemistry*, 112(2):575–586, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2013:MCC

[GGJD13] Si-Meng Gao, Wen-Ping Guo, Lin Jin, and Yi-Hong Ding. Maximum carbonyl-coordination number of scandium: Computational study of $Sc(CO)_n$ (n = 1–7), $Sc(CO)_7^-$ and $Sc(CO)_6^{3-}$. *International Journal of Quantum Chemistry*, 113(8):1192–1199, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guha:2013:RRD

[GGP13] Ankur Kanti Guha, Ujjal Gogoi, and Ashwini K. Phukan. Revisiting the reactivity of different carbon bases: a theoretical study. *International Journal of Quantum Chemistry*, 113(22):2471–2477, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Golubeva:2016:RQC

[GGZZ16] Elena N. Golubeva, Oleg I. Gromov, Georgy M. Zhidomirov, and Ekaterina M. Zubanova. Reviews: Quantum chemistry of organocuprates as intermediates of catalytic and photochemical reactions. *International Journal of Quantum Chemistry*, 116(4):295–300, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghoshal:2011:PHM

[GH11] Arijit Ghoshal and Y. K. Ho. Properties of hydrogen molecular ion with static screened Coulomb and exponential cosine screened Coulomb potentials. *International Journal of Quantum Chemistry*, 111(15):4288–4295, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez:2017:GDC

[GHCMCMQ17] Marco Martínez González, David Hernández-Castillo, Luis A. Montero-Cabrera, and Ramón Alain Miranda-Quintana. Geometrical distortions and charge transfer in munchnöne regio-selectivity: a conceptual density functional study. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2012:CCC

[GHGF12] Manuel Garcia, David Alejandro Hernández, Patricia Guadarrama, and Serguei Fomine. Complexes of C60 with cyclic oligoisothianaphthenes. a theoretical study. *International Journal of Quantum Chemistry*, 112(17):2868–2874, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gottlieb:2011:NMS

[GHP11] Alex D. Gottlieb, John D. Head, and Dennis Perusse. Natural molecular shells as open subsystems of small molecules. *International Journal of Quantum Chemistry*, 111(15): 4158–4173, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gross:2012:CCH

[GHS12] Kevin C. Gross, Christopher M. Hadad, and Paul G. Seybold. Charge competition in halogenated hydrocarbons. *International Journal of Quantum Chemistry*, 112(1):219–229, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2010:SEG

[GI10] Dulal C. Ghosh and Nazmul Islam. Semiempirical evaluation of the global hardness of the atoms of 103 elements of the periodic table using the most probable radii as their size descriptors. *International Journal of Quantum Chemistry*, 110(6):1206–1213, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2011:CTA

[GI11a] Dulal C. Ghosh and Nazmul Islam. Charge transfer associated with the physical process of hardness equalization and the chemical event of the molecule formation and the dipole moments. *International Journal of Quantum Chemistry*, 111(12):2811–2819, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2011:DSDa

[GI11b] Dulal C. Ghosh and Nazmul Islam. Determination of some descriptors of the real world working on the fundamental

identity of the basic concept and the origin of the electronegativity and the global hardness of atoms, part 1: Evaluation of internuclear bond distance of some heteronuclear diatomics. *International Journal of Quantum Chemistry*, 111(9):1942–1949, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2011:DSDb

[GI11c] Dulal C. Ghosh and Nazmul Islam. Determination of some descriptors of the real world working on the fundamental identity of the basic concept and the origin of the electronegativity and the global hardness of atoms. Part 2: Computation of the dipole moments of some heteronuclear diatomics. *International Journal of Quantum Chemistry*, 111(12):2802–2810, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2011:QAE

[GI11d] Dulal C. Ghosh and Nazmul Islam. A quest for the algorithm for evaluating the molecular hardness. *International Journal of Quantum Chemistry*, 111(9):1931–1941, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2011:WEH

[GI11e] Dulal C. Ghosh and Nazmul Islam. Whether electronegativity and hardness are manifest two different descriptors of the one and the same fundamental property of atoms — a quest. *International Journal of Quantum Chemistry*, 111 (1):40–51, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2011:WTH

[GI11f] Dulal C. Ghosh and Nazmul Islam. Whether there is a hardness equalization principle analogous to the electronegativity equalization principle — a quest. *International Journal of Quantum Chemistry*, 111(9):1961–1969, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gaszowski:2014:NBA

[GI14] Dawid Gaszowski and Marek Ilczyszyn. Nature of Brønsted acid–noble atom contacts: a reevaluation of hydrogen

bonding criteria. *International Journal of Quantum Chemistry*, 114(7):473–480, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gineityte:2010:TRR

[Gin10] Viktorija Gineityte. Terms representing the reorganization of bonding within charge-bond order matrices of reacting molecules. *International Journal of Quantum Chemistry*, 110(7):1327–1343, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghalla:2012:TSP

[GIO12] Houcine Ghalla, Noureddine Issaoui, and Brahim Oujia. Theoretical study of the polarized infrared spectra of the hydrogen bond in 2-furoic acid crystal dimer. *International Journal of Quantum Chemistry*, 112(5):1373–1383, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goli:2018:HIN

[GJ18] Mohammad Goli and Seifollah Jalili. How intrinsic nuclear nonadiabaticity affects molecular structure, electronic density, and conformational stability: Insights from the multicomponent DFT calculations of Mu/H isotopologues. *International Journal of Quantum Chemistry*, 118(22): e25758:1–e25758:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garifzianova:2012:TSF

[GK12] Guzel G. Garifzianova and Grigorii M. Khrapkovskii. Theoretical study of the fragmentation and isomerization of ethyltoluene radical cations. *International Journal of Quantum Chemistry*, 112(8):1984–1989, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gordeychuk:2018:SBV

[GKGM18] Mark V. Gordeychuk, Konstantin P. Katin, Konstantin S. Grishakov, and Mikhail M. Maslov. Silicon buckyballs versus prismanes: Influence of spatial confinement on the structural properties and optical spectra of the Si_{18} H_{12} and Si_{19} H_{12} clusters. *International Journal of Quantum Chemistry*, 118(15):e25609:1–e25609:??, August 5, 2018. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gaididei:2010:MVD

[GKS10] Yuri Gaididei, Volodymyr P. Kravchuk, and Denis D. Sheka. Magnetic vortex dynamics induced by an electrical current. *International Journal of Quantum Chemistry*, 110(1):83–97, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gogtas:2012:RWP

[GKT+12] Fahrettin Gogtas, Ezman Karabulut, Tomokazu Tanaka, Toshiyuki Takayanagi, and Rukiye Tutuk. Real wave packet and flux analysis studies of the H + F_2 → HF + F reaction. *International Journal of Quantum Chemistry*, 112(11):2348–2354, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2012:TSD

[GLF+12] Aimei Gao, Guoliang Li, David Finlow, Hongyu Chen, and Qian-Shu Li. A theoretical study of the dependence of the $AS_xSi_{6-}x$ cluster structures and properties on composition. *International Journal of Quantum Chemistry*, 112(5):1499–1506, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez-Luque:2011:RTS

[GLOGM+11] Remedios González-Luque, Gloria Olaso-González, Manuela Merchán, Pedro B. Coto, Luis Serrano-Andrés, and Marco Garavelli. On the role of the triplet state in the *cis /trans* isomerization of rhodopsin: A CASPT2//CASSCF study of a model chromophore. *International Journal of Quantum Chemistry*, 111(13):3431–3437, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guizado:2010:SAW

[GLPA10] Teobaldo R. Cuya Guizado, Sonia R. W. Louro, Pedro G. Pascutti, and Celia Anteneodo. Solvation of anionic water-soluble porphyrins: a computational study. *International Journal of Quantum Chemistry*, 110(11):2094–2100, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2013:CSP

[GLT13] Min Gao, Andrey Lyalin, and Tetsuya Taketsugu. Computations of structures, properties and functions of complex systems: Oxygen activation and dissociation on h-BN supported Au atoms. *International Journal of Quantum Chemistry*, 113(4):443–452, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Glushkov:2013:ECI

[Glu13] V. N. Glushkov. Excited and core-ionized state calculations with a local potential expressed in terms of the external potential. *International Journal of Quantum Chemistry*, 113(5):637–642, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ge:2018:CSS

[GLXL18] Yang Ge, Yunxiang Lu, Zhijian Xu, and Honglai Liu. Controlling the spin state of diphenylcarbene via halogen bonding: a theoretical study. *International Journal of Quantum Chemistry*, 118(15):e25616:1–e25616:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goel:2011:DCB

[GM11] Satyender Goel and Artëm E. Masunov. Dissociation curves and binding energies of diatomic transition metal carbides from density functional theory. *International Journal of Quantum Chemistry*, 111(15):4276–4287, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Giovannini:2019:SVE

[GMA+19] Tommaso Giovannini, Marina Macchiagodena, Matteo Ambrosetti, Alessandra Puglisi, Piero Lafiosca, Giulia Lo Gerfo, Franco Egidi, and Chiara Cappelli. Simulating vertical excitation energies of solvated dyes: From continuum to polarizable discrete modeling. *International Journal of Quantum Chemistry*, 119(1):e25684:1–e25684:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia-Martinez:2012:ESS

[GMGRMP12] J. García-Martínez, J. García-Ravelo, J. Morales, and J. J. Peña. Exactly solvable Schrödinger equation for a class of multiparameter exponential-type potentials. *International Journal of Quantum Chemistry*, 112(1):195–200, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Graham:2018:DCT

[GMM+18] Christina Graham, Mónica Moral, Luca Muccioli, Yoann Olivier, Ángel J. Pérez-Jiménez, and Juan-Carlos Sancho-García. N-doped cycloparaphenylenes: Tuning electronic properties for applications in thermally activated delayed fluorescence. *International Journal of Quantum Chemistry*, 118(12):e25562:1–e25562:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gurgel:2011:BPP

[GMP+11] Maria F. C. Gurgel, Mário L. Moreira, Elaine C. Paris, José W. M. Espinosa, Paulo S. Pizani, José A. Varela, and Elson Longo. $BaZrO_3$ photoluminescence property: an ab initio analysis of structural deformation and symmetry changes. *International Journal of Quantum Chemistry*, 111(3):694–701, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosal:2018:DFE

[GMR18] Abhisek Ghosal, Tanmay Mandal, and Amlan K. Roy. Density functional electric response properties of molecules in Cartesian grid. *International Journal of Quantum Chemistry*, 118(20):e25708:1–e25708:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghigo:2016:TEP

[GMT16] Giovanni Ghigo, Andrea Maranzana, and Glauco Tonachini. Tuning of the electronic properties of H-passivated armchair graphene nanoribbons by mild border oxidation: Theoretical study on periodic models. *International Journal of Quantum Chemistry*, 116(17):1281–1284, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghigo:2018:MDG

[GMT18] Giovanni Ghigo, Andrea Maranzana, and Glauco Tonachini. Mechanistic dichotomy in the gas-phase addition of NO_3 to polycyclic aromatic hydrocarbons: Theoretical study. *International Journal of Quantum Chemistry*, 118(16):e25641:1–e25641:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghosh:2019:CAT

[GN19] Piu Ghosh and Debraj Nath. Complexity analysis of two families of orthogonal functions. *International Journal of Quantum Chemistry*, 119(17):e25964:1–e25964:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gerasov:2012:SWP

[GNM+12] Andrii O. Gerasov, Iffat H. Nayyar, Artëm E. Masunov, Olga V. Przhonska, Olexiy D. Kachkovsky, Dmytro O. Melnyk, Olexiy B. Ryabitsky, and Olexander O. Viniychuk. Solitonic waves in polyene dications and principles of charge carrier localization in π-conjugated organic materials. *International Journal of Quantum Chemistry*, 112(14):2659–2667, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gomez:2019:PPH

[GORW19] Sara Gómez, Yan Oueis, Albeiro Restrepo, and Adam Wasserman. Partition potential for hydrogen bonding in formic acid dimers. *International Journal of Quantum Chemistry*, 119(4):e25814:1–e25814:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Galynska:2013:EPN

[GP13a] Marta Gałyńska and Petter Persson. Emerging polymorphism in nanostructured TiO_2: Quantum chemical comparison of anatase, rutile, and brookite clusters. *International Journal of Quantum Chemistry*, 113(24):2611–2620, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ghatee:2013:PAS

[GP13b] Mohammad Hadi Ghatee and Leila Pakdel. Pyridine adsorption on small Ni_n-cluster ($n = 2, 3, 4$): a study of geometry and electronic structure. *International Journal of Quantum Chemistry*, 113(10):1549–1555, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goswami:2015:UBP

[GPM+15] Tamal Goswami, Satadal Paul, Subhajit Mandal, Anirban Misra, Anakuthil Anoop, and Pratim K. Chattaraj. Unique bonding pattern and resulting bond stretch isomerism in Be_3^{2-}. *International Journal of Quantum Chemistry*, 115 (7):426–433, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gonzalez:2010:NQE

[GR10] Sergio A. González and Andrés Reyes. Nuclear quantum effects on the He_2 H^+ complex with the nuclear molecular orbital approach. *International Journal of Quantum Chemistry*, 110(3):689–696, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gaied:2011:MBE

[GR11] W. Gaied and M. Ben El Hadj Rhouma. Many-body effects on structures of small Ca^{2+} Ar_n clusters. *International Journal of Quantum Chemistry*, 111(3):652–660, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grassi:2008:RBA

[Gra08] A. Grassi. A relationship between atomic correlation energy and Tsallis entropy. *International Journal of Quantum Chemistry*, 108(4):774–778, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grassi:2011:RBA

[Gra11] A. Grassi. A relationship between atomic correlation energy of neutral atoms and generalized entropy. *International Journal of Quantum Chemistry*, 111(10):2390–2397, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gotz:2019:VWE

[GRCATG19] Andreas W. Götz, Juan I. Rodríguez, Fray L. Castillo-Alvarado, and Daniel E. Trujillo-González. Van der Waals effects on structure and optical properties in organic photovoltaics. *International Journal of Quantum Chemistry*, 119 (14):e25883:1–e25883:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia-Revilla:2019:LAC

[GRCGRRHT19] Marco A. García-Revilla, Fernando Cortés-Guzmán, Tomás Rocha-Rinza, and Jesús Hernández-Trujillo. Latin American contributions to quantum chemical topology. *International Journal of Quantum Chemistry*, 119(2): e25789:1–e25789:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gordon:2011:PRA

[GRD11] Mark S. Gordon, Luke Roskop, and Ajitha Devarajan. Perspective on "The restricted active space self-consistent-field method, implemented with a split-graph unitary group approach". *International Journal of Quantum Chemistry*, 111(13):3280–3283, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garzon-Ramirez:2018:BSD

[GRLA18] Antonio J. Garzón-Ramírez, José G. López, and Carlos A. Arango. Bond selective dissociation of the BrHBr transition state complex using linear chirp laser pulses. *International Journal of Quantum Chemistry*, 118(24):e25784:1–e25784:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Grunenberg:2017:IDC

[Gru17] Jörg Grunenberg. Ill-defined chemical concepts: the problem of quantification. *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guseinov:2010:EOE

[GS10] Israfil I. Guseinov and Ercan Sahin. Evaluation of one-electron molecular integrals over complete orthonormal sets

of Ψ^{α}-ETO using auxiliary functions. *International Journal of Quantum Chemistry*, 110(10):1803–1808, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goli:2011:QTA

[GS11] Mohammad Goli and Shant Shahbazian. The quantum theory of atoms in positronic molecules: a case study on diatomic species. *International Journal of Quantum Chemistry*, 111(9):1982–1998, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gamez:2011:TTS

[GSaY11] José A. Gámez, Luis Serrano-andrés, and Manuel Yáñez. Two- and three-state conical intersections in the electron capture dissociation of disulfides: The importance of multireference calculations. *International Journal of Quantum Chemistry*, 111(13):3316–3323, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Griffe:2010:TSC

[GSB10] Beulah Griffe, Anibal Sierraalta, and Joaquín L. Brito. Theoretical study of the CO catalytic oxidation on Au/SAPO-11 zeolite. *International Journal of Quantum Chemistry*, 110(13):2573–2582, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goncalves:2019:NRR

[GSPR19] Mateus A. Gonçalves, Lizandro S. Santos, Fernando C. Peixoto, and Teodorico C. Ramalho. NMR relaxation and relaxivity parameters of MRI probes revealed by optimal wavelet signal compression of molecular dynamics simulations. *International Journal of Quantum Chemistry*, 119 (10):e25896:1–e25896:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Genheden:2012:TCD

[GSR12] Samuel Genheden, Pär Söderhjelm, and Ulf Ryde. Transferability of conformational dependent charges from protein simulations. *International Journal of Quantum Chemistry*, 112(7):1768–1785, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gilka:2011:BHF

[GST11] Natalie Gilka, Jan Philip Solovej, and Peter R. Taylor. Behavior of the Hartree–Fock energy at short internuclear distances. *International Journal of Quantum Chemistry*, 111(13):3324–3328, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2010:EPW

[GSZ10] Yang Gao, Xiaohong Shen, and Haoping Zheng. Equivalent potential of water for electronic structure of asparagine. *International Journal of Quantum Chemistry*, 110(4):925–938, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gtari:2013:TSD

[GT13] Wiem Felah Gtari and Bahoueddine Tangour. A theoretical study of the dihydrogen molecule confined inside carbon nanotubes. *International Journal of Quantum Chemistry*, 113(21):2397–2404, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2011:GNU

[GTR11] Bin Gao, Andreas J. Thorvaldsen, and Kenneth Ruud. GEN1INT: a unified procedure for the evaluation of one-electron integrals over Gaussian basis functions and their geometric derivatives. *International Journal of Quantum Chemistry*, 111(4):858–872, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guerrero:2019:GRI

[GTSC+19] Tomás Guerrero, Adrián Torices-Saucedo, María Eugenia Castro, Sergio F. Juárez-Cerrillo, Francisco J. Meléndez, Myrna H. Matus, and J. Sergio Durand-Niconoff. Global reactivity indexes and nonparametric statistics in the study of the proapoptotic activity of coumarins. *International Journal of Quantum Chemistry*, 119(11):e25902:1–e25902:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guirao:2011:SRA

[GV11] Juan L. G. Guirao and Juan A. Vera. Stability of the Rydberg atom in the crossed magnetic and electric fields.

International Journal of Quantum Chemistry, 111(5):970–977, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia-Vela:2019:EDC

[GV19] A. García-Vela. Enhancement of the degree of control of photofragment distributions by laser phase modulation. *International Journal of Quantum Chemistry*, 119(4): e25813:1–e25813:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gamboa:2010:ITC

[GVPCK10] Gabriel U. Gamboa, José M. Vásquez-Pérez, Patrizia Calaminici, and Andreas M. Köster. Influence of thermostats on the calculations of heat capacities from Born–Oppenheimer molecular dynamics simulations. *International Journal of Quantum Chemistry*, 110(12):2172–2178, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gebremedhin:2013:CTR

[GW13] Daniel Gebremedhin and Charles Weatherford. Canonical two-range addition theorem for Slater-type orbitals. *International Journal of Quantum Chemistry*, 113(1):71–75, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2018:KEP

[GW18] Aihua Gao and Meishan Wang. The keto $\rightarrow$ enol photoisomerization of N-salicilydenemethylfurylamine: Nonadiabatic ab initio dynamics simulation. *International Journal of Quantum Chemistry*, 118(16):e25656:1–e25656:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2017:BWR

[GWHH17] Wei Gao, Bin-Bin Wang, Xue-Jin Hu, and Yong-Chang Han. The "bound wavefunction" on the repulsive excited $^2\Sigma_u^+(2p\sigma_u)$ state of the HD^+ molecule. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2012:RII

[GWJ12] Ling Guo, Hai-Shun Wu, and Zhi-Hao Jin. Retraction: Ab Initio investigation of structures and stability of Ga_nP_m (n = 1–3, m = 1–4) clusters. *International Journal of Quantum Chemistry*, 112(4):1233, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2011:SEE

[GWM11] Shulin Gao, Wei Wu, and Yirong Mo. Steric and electronic effects on the heterolytic H_2-splitting by phosphine-boranes R_3 B/PR'_3 (R = C_6F_5, Ph; R′ = $C_6H_2Me_3$, t Bu, Ph, C_6F_5, Me, H): a computational study. *International Journal of Quantum Chemistry*, 111(14):3761–3775, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Goss:2018:CDA

[GWME18] Jordan Goss, Tim Wilson, Amanda Morgenstern, and Mark Eberhart. Charge density analysis attending bond torsion: a bond bundle case study. *International Journal of Quantum Chemistry*, 118(24):e25783:1–e25783:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2014:DPH

[GWZ+14a] Shoubao Gao, Wei Wei, Bin Zheng, Yuzhi Song, and Qingtian Meng. Dynamical properties of S(^{3}P) + HD reaction on $1^3A''$ state and their quantum wavepacket calculation. *International Journal of Quantum Chemistry*, 114 (11):748–754, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2014:EBN

[GWZ+14b] Ying Gao, Heng-Qing Wu, Rong-Lin Zhong, Hong-Liang Xu, Shi-Ling Sun, Liang Zhao, and Zhong-Min Su. The effect of boron nitride nanotubes size on the HArF interaction by NBO and AIM analysis. *International Journal of Quantum Chemistry*, 114(24):1692–1696, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2014:PRB

[GXZ+14] Ying Gao, Hong-Liang Xu, Rong-Lin Zhong, Shi-Ling Sun, and Zhong-Min Su. Probing the relationship between spin contamination and first hyperpolarizability: Open-shell Möbius anion. *International Journal of Quantum Chemistry*, 114(11):720–724, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2014:HSP

[GZ14] Teng-Fei Gao and Hong Zhang. Hydrogen storage in porous structures of adamantane-based nitrogen-heterocyclic ring with diamond-like structure. *International Journal of Quantum Chemistry*, 114(21):1438–1444, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guan:2018:RCS

[GZBH18] Jia Guan, Snezana D. Zarić, Edward N. Brothers, and Michael B. Hall. Recent computational studies on transition-metal carbon-hydrogen bond activation of alkanes. *International Journal of Quantum Chemistry*, 118(9): e25605:1–e25605:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2013:ECE

[GZF13] Victor García, David Zorrilla, and Manuel Fernández. Electronic confinement effects on the reaction field type calculations of solvent effects. *International Journal of Quantum Chemistry*, 113(18):2172–2179, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2014:SBO

[GZF14] Victor García, David Zorrilla, and Manuel Fernández. Simplified box orbitals: a spatially restricted alternative to the Slater-type orbitals. *International Journal of Quantum Chemistry*, 114(23):1581–1593, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Guo:2011:EIC

[GZMC11] Jing-Hua Guo, Hong Zhang, Yoshiyuki Miyamoto, and Xin-Lu Cheng. The effect of ionization and CH_3 ligand for

hydrogen storage in Co- and Ni-based organometallic compounds. *International Journal of Quantum Chemistry*, 111 (15):4443–4451, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Garcia:2016:SBO

[GZSMFN16] Victor García, David Zorrilla, Jesús Sánchez-Márquez, and Manuel Fernández-Núñez. Simplified Box Orbitals (SBO) for H to Ar atoms: Exact expressions, SBO-3G approximations, and relations with the ZDO approximation. *International Journal of Quantum Chemistry*, 116(17):1303–1312, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Gao:2016:TSM

[GZW16] Xu Gao, Li-Juan Zhao, and Dong-Lai Wang. Theoretical study on monometallic cyanide cluster fullerenes YCN@C_{72}. *International Journal of Quantum Chemistry*, 116(6):438–443, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hajigeorgiou:2018:EHH

[Haj18] Photos G. Hajigeorgiou. The extended Hulburt–Hirschfelder-long-range oscillator model for direct-potential-fit analysis. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Han:2019:CBA

[Han19] Yong-Chang Han. Comparison between the analysis of the asymptotic wavepacket and the associated flux for the calculation of kinetic-energy-releases function. *International Journal of Quantum Chemistry*, 119(7):e25858:1–e25858:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hatanaka:2013:EOA

[Hat13] Masashi Hatanaka. Evaluation of optical activities by modern semi-empirical methods. *International Journal of Quantum Chemistry*, 113(22):2447–2456, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2018:VBR

[HAX+18] Wei Jie Huang, Alireza Azizi, Tianlv Xu, Steven R. Kirk, and Samantha Jenkins. A vector-based representation of the chemical bond for the normal modes of benzene. *International Journal of Quantum Chemistry*, 118(19): e25698:1–e25698:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoggan:2014:QMC

[HB14] Philip E. Hoggan and Ahmed Bouferguène. Quantum Monte Carlo for activated reactions at solid surfaces: Time well spent on stretched bonds. *International Journal of Quantum Chemistry*, 114(17):1150–1156, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoffmann:2018:P

[HB18] Mark Hoffmann and Erkki Brändas. Preface. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2011:KEMb

[HBMM11] Lulu Huang, Hugo J. Bohorquez, Chérif F. Matta, and Lou Massa. The Kernel energy method: Application to graphene and extended aromatics. *International Journal of Quantum Chemistry*, 111(15):4150–4157, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ha:2018:IQM

[HCH+18] Nguyen Ngoc Ha, Le Minh Cam, Nguyen Thi Thu Ha, Zhong-Tao Jiang, Mohanad El-Harbawi, and Chun-Yang Yin. Integrated QMMM and Monte Carlo methods for analysis of adsorptive interactions between goethite cluster, carbon nanotubes, and arsenate. *International Journal of Quantum Chemistry*, 118(17):e25653:1–e25653:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2013:CIA

[HCL13] Wen-Fei Huang, Hsin-Tsung Chen, and M. C. Lin. Computational investigation of the adsorption and reactions of SiH_x ($x = 0$–4) on TiO_2 anatase (101) and rutile (110) surfaces. *International Journal of Quantum Chemistry*, 113 (12):1696–1708, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Han:2011:TSR

[HDC+11] De-Man Han, Guo-Liang Dai, Hao Chen, Yong Wang, Ai-Guo Zhong, Cai-Ping Lin, and Dan Chen. Theoretical study on the reactions of Nb and Nb^+ with CO_2 in gas phase. *International Journal of Quantum Chemistry*, 111 (12):2898–2909, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hall:2012:WPD

[HDÖS12] Benjamin Hall, Erik Deumens, Yngve Öhrn, and John R. Sabin. Wave packet dynamics on multiply-valued potential surfaces: Report on work in progress. *International Journal of Quantum Chemistry*, 112(1):247–252, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Han:2013:TIG

[HDQ+13] Guangzhan Han, Yanli Ding, Ping Qian, Chao Zhang, and Wei Song. Theoretical investigation of gas phase ethanol–$(water)_n$ ($n = 1$–5) clusters and comparison with gas phase pure water clusters $(water)_n$ ($n = 2$–6). *International Journal of Quantum Chemistry*, 113(10):1511–1521, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hernandez-Esparza:2019:GBA

[HEVMSA+19] Raymundo Hernández-Esparza, Álvaro Vázquez-Mayagoitia, Luis-Antonio Soriano-Agueda, Rubicelia Vargas, and Jorge Garza. GPUs as boosters to analyze scalar and vector fields in quantum chemistry. *International Journal of Quantum Chemistry*, 119(2):e25671:1–e25671:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hadad:2019:MSC

[HFA+19] Cacier Hadad, Elizabeth Florez, Nancy Acelas, Gabriel Merino, and Albeiro Restrepo. Microsolvation of small cations and anions. *International Journal of Quantum Chemistry*, 119(2):e25766:1–e25766:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hyers:2019:RWR

[HFBC19] Matthew J. Hyers, Alex M. Fodor, Dominic K. Bierwisch, and Emanuele Curotto. Re-weighted random series path integral simulations of molecular clusters: Applications to lithium solvated by a mixed Stockmayer cluster. *International Journal of Quantum Chemistry*, 119(13):e25915:1–e25915:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

HerreriasdeOliveira:2011:IMS

[HFD11] Marcos Herrerias de Oliveira, Harley Paiva Martins Filho, and Joaquim Delphino Da Motta Neto. Ab initio multireference singles and doubles configuration interaction study of the low-energy states of iron mononitride. *International Journal of Quantum Chemistry*, 111(7–8):1453–1457, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Himmetoglu:2014:RHC

[HFdGC14] Burak Himmetoglu, Andrea Floris, Stefano de Gironcoli, and Matteo Cococcioni. Review: Hubbard-corrected DFT energy functionals: The $LDA+U$ description of correlated systems. *International Journal of Quantum Chemistry*, 114 (1):14–49, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2017:CSI

[HFL+17] Jiayao Huang, Aiping Fu, Hongliang Li, Hao Li, Tianshu Chu, and Zonghua Wang. A computational study of ion speciation in mixtures of protic ionic liquids with various molecular solvents: Insight into the solvent polarity and anion basicity. *International Journal of Quantum Chemistry*, 117(3):170–179, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang-Fu:2012:ESM

[HFZ12] Guo-Qing Huang-Fu and Min-Cang Zhang. Exact solution of the modified Pöschl–Teller potential in the tridiagonal representation. *International Journal of Quantum Chemistry*, 112(12):2482–2485, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hazra:2008:QAS

[HGB08] Ram Kuntal Hazra, Manas Ghosh, and S. P. Bhattacharyya. Quantum adiabatic switching route to the impurity modulated states of 2-D quantum dots with different switching functions. *International Journal of Quantum Chemistry*, 108(4):719–730, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hanson-Heine:2018:UCP

[HH18] Magnus W. D. Hanson-Heine. Uncontracted core Pople basis sets in vibrational frequency calculations. *International Journal of Quantum Chemistry*, 118(22):e25761:1–e25761:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hammoutene:2010:ESP

[HHCA10] D. Hammoutène, M. Hochlaf, I. Ciofini, and C. Adamo. Electronic spectrum of 2-pyridone$^+$: Ab initio and time-dependent density functional calculations. *International Journal of Quantum Chemistry*, 110(3):498–504, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huo:2017:MES

[HhGqZZ17] Rui-Ping Huo, Li hui Guo, Fu qiang Zhang, and Xiang Zhang. Multiple electronic state mechanism for carboryne reaction with benzene: a DFT study. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ho:2012:TSA

[HHL12a] Minhhuy Hô and Ramón Hernández-Lamoneda. Theoretical study of the agostic bond in Me_2 Al(tBu_2 pz)$_2$Li(THF). *International Journal of Quantum Chemistry*, 112(22):

3630–3636, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [HHL14].

Huo:2012:DID

[HHL+12b] Rui-Ping Huo, Xu-Ri Huang, Ji-Lai Li, Xiang Zhang, Na Li, and Chia-Chung Sun. Direct ab initio dynamics study of the reaction of C_2 ($A^3\ \Pi_u$) with CH_4. *International Journal of Quantum Chemistry*, 112(4):1078–1085, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ho:2014:CTS

[HHL14] Minhhuy Hô and Ramón Hernández-Lamoneda. Corrigendum: Theoretical study of the agostic bond in Me_2 $Al(tBu_2\ pz)_2$ Li(THF). *International Journal of Quantum Chemistry*, 114(3):239, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [HHL12a].

Hernandez-Hernandez:2018:TEE

[HHYC+18] Luis Alberto Hernández-Hernández, Ruiqin Yi, Henderson James Cleaves II, Miguel Fuentes-Cabrera, Bobby G. Sumpter, Arturo Hernández-Hernández, Eduardo Rangel, and Emmanuel Vallejo. Theoretical and experimental evidence of conformational transformation in stereoisomers of nucleoside analogues. *International Journal of Quantum Chemistry*, 118(20):e25714:1–e25714:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hill:2013:GBS

[Hil13] J. Grant Hill. Gaussian basis sets for molecular applications. *International Journal of Quantum Chemistry*, 113 (1):21–34, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hayat:2019:CBE

[HIL19] Sakander Hayat, Muhammad Imran, and Jia-Bao Liu. Correlation between the Estrada index and π-electronic energies for benzenoid hydrocarbons with applications to boron nanotubes. *International Journal of Quantum Chemistry*, 119(23):e26016:1–e26016:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hashimoto:2016:AEV

[HITU16] Marina Hashimoto, Takayoshi Ishimoto, Masanori Tachikawa, and Taro Udagawa. Analysis of exponent values of Gaussian-type functions on quantum protons and deuterons in charged or polarized systems. *International Journal of Quantum Chemistry*, 116(12):961–970, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Heiles:2013:RGO

[HJ13] Sven Heiles and Roy L. Johnston. Review: Global optimization of clusters using electronic structure methods. *International Journal of Quantum Chemistry*, 113(18):2091–2109, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hedegaard:2014:PPE

[HJK14] Erik D. Hedegård, Hans Jørgen Aa. Jensen, and Jacob Kongsted. Perspectives: Polarizable embedding based on multiconfigurational methods: Current developments and the road ahead. *International Journal of Quantum Chemistry*, 114(17):1102–1107, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hermoso:2013:ENS

[HJRO13] Willian Hermoso, Naziah B. Jaufeerally, Ponnadurai Ramasami, and Fernando R. Ornellas. Exploring new species on the [H, S, Se, Cl] potential energy surface. *International Journal of Quantum Chemistry*, 113(2):112–118, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamdan:2011:TSV

[HK11] A. Hamdan and M. Korek. Theoretical study with vibration–rotation and dipole moment calculations of quartet states of the CrCl molecule. *International Journal of Quantum Chemistry*, 111(12):2960–2965, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Higuchi:2013:CDF

[HKIH13] Katsuhiko Higuchi, Kazuki Koide, Tatsuya Imanishi, and Masahiko Higuchi. Current-density functional theory for a superconductor. *International Journal of Quantum Chemistry*, 113(5):709–714, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2013:FDF

[HKLW13] Chunping Hu, Ryo Komakura, Zhengcao Li, and Kazuyuki Watanabe. Frontiers in density functional theory: TDDFT study on quantization behaviors of nonadiabatic couplings in polyatomic systems. *International Journal of Quantum Chemistry*, 113(3):263–271, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Han:2015:RTD

[HKZZ15] Lu Han, Yaling Ke, Xinxin Zhong, and Yi Zhao. Reviews: Time-dependent wavepacket diffusion method and its applications in organic semiconductors. *International Journal of Quantum Chemistry*, 115(9):578–588, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hill:2019:NPC

[HL19] J. Grant Hill and Anthony C. Legon. Nonbonding pairs in cyclic thioethers: Electrostatic modeling and ab initio calculations for complexes of 2,5-dihydrothiophene, thietane, and thiirane with hydrogen fluoride. *International Journal of Quantum Chemistry*, 119(10):e25885:1–e25885:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Haynes:2019:IMS

[HLB19] Caleb A. Haynes, Serafin Lopez, and Kyle A. Beran. Investigation into the molecular structure and energetic stability of endohedral and exohedral metallofullerene derivatives of C_{24}. *International Journal of Quantum Chemistry*, 119(19):e25992:1–e25992:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

He:2011:TSM

[HLJZ11] Jianyong He, Zhengwen Long, Jian Jing, and Jin-Sheng Zhang. Theoretical study on the mechanisms of the nucleophilic substitution reactions of hydrosulfide ion and halomethanes. *International Journal of Quantum Chemistry*, 111(14):3643–3653, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hao:2011:TAS

[HLMO11] Hua Hao, Han-Xing Liu, Xin-Min Min, and Shi-Xi Ouyang. Theoretical analysis on the structure of Nb-doped $SrBi_4$ Ti_4 O_{15}. *International Journal of Quantum Chemistry*, 111(3): 669–674, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hernandez-Laguna:2014:P

[HLSD14] Alfonso Hernández-Laguna and Claro Ignacio Sainz-Díaz. Preface. *International Journal of Quantum Chemistry*, 114 (19):1237–1238, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

He:2014:DFT

[HLZ+14] Xiaobo He, Jinghui Lyu, Hu Zhou, Guilin Zhuang, Xing Zhong, Jian-Guo Wang, and Xiaonian Li. Density functional theory study of *p*-chloroaniline adsorption on Pd surfaces and clusters. *International Journal of Quantum Chemistry*, 114(14):895–899, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2010:TSS

[HM10a] H. Z. Hu and S. Y. Ma. Theoretical study on the structures and aromaticity of N-confused porphyrazine isomers. *International Journal of Quantum Chemistry*, 110(9):1682–1690, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2010:KEM

[HM10b] Lulu Huang and Lou Massa. Kernel energy method: Drug–target interaction energies for drug design. *International Journal of Quantum Chemistry*, 110(15):2886–2893, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2011:KEMa

[HM11] Lulu Huang and Lou Massa. Kernel energy method applied to an energetic nitrate ester. *International Journal of Quantum Chemistry*, 111(10):2180–2186, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hongo:2012:BQM

[HM12] Kenta Hongo and Ryo Maezono. A benchmark quantum Monte Carlo study of the ground state chromium dimer. *International Journal of Quantum Chemistry*, 112(5):1243–1255, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2018:NGQ

[HMA+18] Wei Jie Huang, Roya Momen, Alireza Azizi, Tianlv Xu, Steven R. Kirk, Michael Filatov, and Samantha Jenkins. Next-generation quantum theory of atoms in molecules for the ground and excited states of fulvene. *International Journal of Quantum Chemistry*, 118(22):e25768:1–e25768:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hajji:2019:CFP

[HMA+19] Melek Hajji, Hasan Mtiraoui, Nesrine Amiri, Moncef Msaddek, and Taha Guerfel. Crystallographic and first-principles density functional theory study on the structure, noncovalent interactions, and chemical reactivity of 1,5-benzodiazepin-2-ones derivatives. *International Journal of Quantum Chemistry*, 119(21):e26000:1–e26000:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Higuchi:2010:CVV

[HMH10a] Katsuhiko Higuchi, Mitiyasu Miyasita, and Masahiko Higuchi. Checking the validity of the vorticity expansion approximation of the current-density functional theory. *International Journal of Quantum Chemistry*, 110(12):2286–2289, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Higuchi:2010:RCA

[HMH10b] M. Higuchi, M. Miyasita, and K. Higuchi. A restrictive condition on approximate forms of the kinetic energy functional of the pair density functional theory. *International Journal of Quantum Chemistry*, 110(12):2283–2285, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hatakeyama:2013:TAC

[HMH+13] Makoto Hatakeyama, Takako Mashiko, Hisanao Hazama, Kunio Awazu, and Masanori Tachikawa. Theoretical analysis of correlation between ionization threshold fluence in IR-MALDI and IR absorption spectrum of matrix molecules. *International Journal of Quantum Chemistry*, 113(2):125–129, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Habli:2015:ICE

[HMI+15] Héla Habli, Leila Mejrissi, Noureddine Issaoui, Saud Jamil Yaghmour, Brahim Oujia, and Florent Xavier Gadéa. Ab initio calculation of the electronic structure of the strontium hydride ion (SrH^+). *International Journal of Quantum Chemistry*, 115(3):172–186, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hernando:2011:LAA

[HMP+11] Alberto Hernando, Ricardo Mayol, Martí Pi, Manuel Barranco, Ioannis S. K. Kerkines, and Aristides Mavridis. Li atoms attached to helium nanodroplets. *International Journal of Quantum Chemistry*, 111(2):400–405, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hornyak:2012:IPS

[HN12] I. Hornyák and Á. Nagy. Inequalities for phase-space Rényi entropies. *International Journal of Quantum Chemistry*, 112(5):1285–1290, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hizhnyi:2015:CSB

[HNBG15] Yuriy Hizhnyi, Sergii G. Nedilko, Viktor Borysiuk, and Viktor A. Gubanov. Computational studies of boron- and

nitrogen-doped single-walled carbon nanotubes as potential sensor materials of hydrogen halide molecules HX (X = F, Cl, Br). *International Journal of Quantum Chemistry*, 115 (20):1475–1482, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hizhnyi:2018:ROC

[HNBS18] Yuriy Hizhnyi, Sergii Nedilko, Viktor Borysiuk, and Andrii Shyichuk. Removal of oxoanions of M^{VI} (M^{VI} = Cr, Mo, W) metals by carbon nanostructures: Insights into mechanisms from DFT calculations. *International Journal of Quantum Chemistry*, 118(20):e25715:1–e25715:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hajiabadi:2012:CSO

[HNH+12] H. Hajiabadi, A. Nowroozi, M. Hasani, P. Mohammadzadeh Jahani, and H. Raissi. A comparative study of open-close and related rotamers methods to evaluate the intramolecular hydrogen bond energies in 3-imino-propen-1-ol and its derivatives. *International Journal of Quantum Chemistry*, 112(5):1384–1391, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoggan:2010:FCS

[Hog10] Philip E. Hoggan. Four-center Slater-type orbital molecular integrals without orbital translations. *International Journal of Quantum Chemistry*, 110(1):98–103, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hoggan:2013:CQC

[Hog13] Philip E. Hoggan. Computational quantum chemistry: Quantum Monte Carlo simulation of carbon monoxide reactivity when adsorbed at metal and oxide catalyst surfaces: Trial wave-functions with exponential type basis and quasi-exact three-body correlation. *International Journal of Quantum Chemistry*, 113(3):277–285, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hopmann:2015:RQC

[Hop15] Kathrin H. Hopmann. Reviews: Quantum chemical studies of asymmetric reactions: Historical aspects and recent examples. *International Journal of Quantum Chemistry*, 115 (18):1232–1249, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Horikoshi:2013:CFM

[Hor13] Atsushi Horikoshi. Concepts and fundamental methods in molecular simulations: External source method for Kubo-transformed quantum correlation functions. *International Journal of Quantum Chemistry*, 113(3):326–329, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamzavi:2012:EWS

[HR12] M. Hamzavi and A. A. Rajabi. Exact S-wave solution of the trigonometric Pöschl–Teller potential. *International Journal of Quantum Chemistry*, 112(6):1592–1597, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Haag:2013:RTQ

[HR13] Moritz P. Haag and Markus Reiher. Real-time quantum chemistry. *International Journal of Quantum Chemistry*, 113(1):8–20, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamid:2019:SES

[HR19] Aabid Hamid and Ram Kinkar Roy. Solvent effect on stabilization energy: an approach based on density functional reactivity theory. *International Journal of Quantum Chemistry*, 119(11):e25909:1–e25909:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamzavi:2012:RVS

[HRT12] M. Hamzavi, A. A. Rajabi, and K.-E. Thylwe. The rotation-vibration spectrum of diatomic molecules with the Tietz–Hua rotating oscillator. *International Journal of Quantum Chemistry*, 112(15):2701–2705, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [KBG17].

Hamada:2011:TDS

[HS11a] Shinji Hamada and Hideo Sekino. Time-dependent solution of molecular quantum systems using multiwavelet. *International Journal of Quantum Chemistry*, 111(7–8):1480–1492, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hasanein:2011:DCA

[HS11b] Ahmed A. Hasanein and Samir A. Senior. DFT calculations of amine-imine tautomerism in some pyrimidine derivatives and their 1:1 and 1:2 complexes with water. *International Journal of Quantum Chemistry*, 111(15):3993–4010, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Heidarzadeh:2011:QDB

[HS11c] Farnaz Heidarzadeh and Shant Shahbazian. The quantum divided basins: a new class of quantum subsystems. *International Journal of Quantum Chemistry*, 111(12):2788–2801, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Heger:2015:LEC

[HS15] Matthias Heger and Martin A. Suhm. Letter to the Editor: Comment on: "Quantum Confinement in Hydrogen Bond" by Carlos da Silva dos Santos, Elso Drigo Filho, and Regina Maria Ricotta, Int. J. Quantum Chem. 2015, **115**, 765–770. *International Journal of Quantum Chemistry*, 115 (20):1510–1511, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [dFR15b] and reply [dFR15a].

Hirate:2011:QEC

[HSN+11] Hiroshi Hirate, Yuki Saito, Ippei Nakaya, Hiroshi Sawai, Hiroshi Yukawa, Masahiko Morinaga, and Hiromi Nakai. Quantitative evaluation of catalytic effect of metal chlorides on the decomposition reaction of $NaAlH_4$. *International Journal of Quantum Chemistry*, 111(5):950–960, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hayami:2018:DER

[HSN18] Masao Hayami, Junji Seino, and Hiromi Nakai. Derivative of electron repulsion integral using accompanying coordinate expansion and transferred recurrence relation method for long contraction and high angular momentum. *International Journal of Quantum Chemistry*, 118(16):e25640:1–e25640:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hansson:2011:CFF

[HSS+11] Anders Hansson, Paulo C. T. Souza, Rodrigo L. Silveira, Leandro Martínez, and Munir S. Skaf. CHARMM force field parameterization of rosiglitazone. *International Journal of Quantum Chemistry*, 111(7–8):1346–1354, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2018:DZP

[HSS18] Zhubin Hu, Zhenrong Sun, and Haitao Sun. Design of zinc porphyrin–perylene diimide donor–bridge–acceptor chromophores for large second-order nonlinear optical response: a theoretical exploration. *International Journal of Quantum Chemistry*, 118(10):e25536:1–e25536:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hefferlin:2013:WDM

[HST13] Ray Hefferlin, Jonathan Sackett, and Jeremy Tatum. Why do molecules echo atomic periodicity? *International Journal of Quantum Chemistry*, 113(17):2078–2089, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hirate:2011:RHB

[HSYM11] H. Hirate, H. Sawai, H. Yukawa, and M. Morinaga. Role of O H bonding in catalytic activity of Nb_2 O_5 during the course of dehydrogenation of MgH_2. *International Journal of Quantum Chemistry*, 111(10):2251–2257, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hamade:2010:TES

[HTM10] Y. Hamade, F. Taher, and Y. Monteil. Theoretical electronic studies of aluminum monobromide and aluminum monoiodide. *International Journal of Quantum Chemistry*, 110(5):1030–1040, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Halasz:2011:NET

[HV11] G. J. Halász and Á. Vibók. Numerical evidence of two aligned conical intersections induced by the Renner effect in bent C_2 H cation. *International Journal of Quantum Chemistry*, 111(2):342–348, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Husch:2018:SMO

[HVR18] Tamara Husch, Alain C. Vaucher, and Markus Reiher. Semiempirical molecular orbital models based on the neglect of diatomic differential overlap approximation. *International Journal of Quantum Chemistry*, 118(24): e25799:1–e25799:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2012:NGR

[HW12] Yujuan Huang and Tianming Wang. New graphical representation of a DNA sequence based on the ordered dinucleotides and its application to sequence analysis. *International Journal of Quantum Chemistry*, 112(6):1746–1757, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2011:TIM

[HWHZ11] Mingqiang Huang, Zhenya Wang, Liqing Hao, and Weijun Zhang. Theoretical investigation on the mechanism and kinetics of OH radical with ethylbenzene. *International Journal of Quantum Chemistry*, 111(12):3125–3134, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hou:2016:TSS

[HWL16] Na Hou, Yuan-Yuan Wu, and Jia-Yuan Liu. Theoretical studies on structures and nonlinear optical properties of alkali doped electrides $B_{12}N_{12}$–M (M = Li, Na, K). *Interna-*

tional Journal of Quantum Chemistry, 116(17):1296–1302, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hou:2018:IES

[HWWW18] Na Hou, Yuan-Yuan Wu, Bing-Qiang Wang, and Hai-Shun Wu. Investigation on the electronic structures and nonlinear optical properties of alkali metal atom doped all- cis 1,2,3,4,5,6-hexafluorocyclohexane. *International Journal of Quantum Chemistry*, 118(15):e25619:1–e25619:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

He:2016:GCR

[HXDY16] Ping-An He, Suning Xu, Qi Dai, and Yuhua Yao. A generalization of CGR representation for analyzing and comparing protein sequences. *International Journal of Quantum Chemistry*, 116(6):476–482, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2015:RSS

[HXX15] Xixi Hu, Changjian Xie, and Daiqian Xie. Reviews: State-to-state reaction dynamics for the reactions of atom N with radicals. *International Journal of Quantum Chemistry*, 115 (10):596–606, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2011:DFT

[HYD11] Zhengguo Huang, Lei Yu, and Yumei Dai. Density functional theory and topological analysis on the hydrogen bonding interactions in cysteine-thymine complexes. *International Journal of Quantum Chemistry*, 111(14):3915–3927, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2010:TPA

[HYH$^+$10] Wen-Hui Hu, Kai-Jun Yuan, Yong-Chang Han, Chuan-Cun Shu, and Shu-Lin Cong. Three-peak Autler–Townes splitting in the photoelectron spectrum of Li_2 molecules caused by femtosecond laser pulses. *International Journal of Quantum Chemistry*, 110(6):1224–1234, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2013:ADM

[HYZ13] Shu-Xian Hu, Jian-Guo Yu, and Eddy Y. Zeng. Atmospheric degradation mechanisms of a simulant organophosphorus pesticide isopropyl methyl methylphosphonate: a theoretical consideration. *International Journal of Quantum Chemistry*, 113(8):1128–1136, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hassanabadi:2012:AAV

[HYZS12] H. Hassanabadi, B. H. Yazarloo, S. Zarrinkamar, and M. Solaimani. Approximate analytical versus numerical solutions of Schrödinger equation under molecular Hua potential. *International Journal of Quantum Chemistry*, 112 (23):3706–3710, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [FKBG19] reply [HYZS19].

Hassanabadi:2019:RCA

[HYZS19] Hassan Hassanabadi, Bentol Hoda Yazarloo, Saber Zarrinkamar, and Mehdi Solaimani. Reply to comment on "Approximate analytical versus numerical solutions of Schrödinger equation under molecular Hua potential". *International Journal of Quantum Chemistry*, 119(13): e25956:1–e25956:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [HYZS12, FKBG19].

He:2012:TTE

[HZG12] Xin He, Jiaheng Zhang, and Haixiang Gao. Theoretical thermochemistry: Enthalpies of formation of a set of nitrogen-containing compounds. *International Journal of Quantum Chemistry*, 112(6):1688–1700, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Hu:2014:BSO

[HZS14] Shi-Lin Hu, Zeng-Xiu Zhao, and Ting-Yun Shi. B-spline one-center method for molecular Hartree–Fock calculations. *International Journal of Quantum Chemistry*, 114 (7):441–448, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

He:2018:PPA

[HZW18] Ying He, Huali Zhao, and Wenji Wang. Photodissociation of phenol in the adiabatic representation: Tunneling, motions of phenyl ring, and kinetic isotope effects. *International Journal of Quantum Chemistry*, 118(24):e25786:1–e25786:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

He:2019:DFT

[HZZ+19] Nan He, Yanyan Zhu, Zhenhua Zhu, Yankai Yang, Wenjing Zhang, Donghui Wei, Lingbo Qu, Mingsheng Tang, and Hongsheng Chen. A density functional theory study on mechanisms of [4 + 2] annulation of enal with α-methylene cycloalkanone catalyzed by N-heterocyclic carbene. *International Journal of Quantum Chemistry*, 119 (24):e26039:1–e26039:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Huang:2011:SHD

[HZZW11] Huisheng Huang, Tonglai Zhang, Jianguo Zhang, and Liqiong Wang. A screened hybrid density functional study on energetic complexes: Metal carbohydrazide nitrates. *International Journal of Quantum Chemistry*, 111(10):2311–2316, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imamura:2013:CSP

[IA13] Akira Imamura and Yuriko Aoki. Computations of structures, properties and functions of complex systems: Electronic structures and molecular structures of polyynes. *International Journal of Quantum Chemistry*, 113(4):423–427, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iqbal:2015:PHN

[IAA15] Azmat Iqbal, Afaq Ahmad, and Raja J. Amjad. Photodetachment of hydrogen negative ion near inelastic surfaces: Arbitrary laser polarization direction. *International Journal of Quantum Chemistry*, 115(21):1526–1532, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ilatovskiy:2013:PQM

[IAK13] Andrey V. Ilatovskiy, Ruben Abagyan, and Irina Kufareva. Perspectives: Quantum mechanics approaches to drug research in the era of structural chemogenomics. *International Journal of Quantum Chemistry*, 113(12):1669–1675, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irgibaeva:2011:MPS

[IBA+11] Irina Smailovna Irgibaeva, Nikolay Barashkov, Anuar Aldongarov, Artur Mantel, and Irina Barashkova. Modeling of plastic scintillation composition of poly(methyl methacrylate)–naphthalene–POPOP. *International Journal of Quantum Chemistry*, 111(11):2540–2544, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ichikawa:2013:CFM

[IFT13] Kazuhide Ichikawa, Masahiro Fukuda, and Akitomo Tachibana. Concepts and fundamental methods in quantum chemistry: Study of simulation method of time evolution in rigged QED. *International Journal of Quantum Chemistry*, 113(3):190–202, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ichikawa:2014:SSM

[IFT14] Kazuhide Ichikawa, Masahiro Fukuda, and Akitomo Tachibana. Study of simulation method of time evolution of atomic and molecular systems by quantum electrodynamics. *International Journal of Quantum Chemistry*, 114(23): 1567–1580, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Islam:2011:NRD

[IG11] Nazmul Islam and Dulal C. Ghosh. A new radial dependent electrostatic algorithm for the evaluation of the electrophilicity indices of the atoms. *International Journal of Quantum Chemistry*, 111(14):3556–3564, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Inerbaev:2011:TSS

[IGMK11] Talgat M. Inerbaev, Feng Long Gu, Hiroshi Mizuseki, and Yoshiyuki Kawazoe. Theoretical study of solvent effect on the structure, first electronic excited state, and nonlinear optical properties of substituted stilbazolium cations. *International Journal of Quantum Chemistry*, 111(4):780–787, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ignatiev:2011:HSP

[Ign11] V. D. Ignatiev. How to solve the problem of dynamical correlation of electrons in the ground state helium atom? *International Journal of Quantum Chemistry*, 111(11):2568–2574, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Ign12].

Ignatiev:2012:EHS

[Ign12] V. D. Ignatiev. Erratum: How to solve the problem of dynamical correlation of electrons in the ground-state helium atom? *International Journal of Quantum Chemistry*, 112 (3):940, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Ign11].

Ipatov:2010:MES

[IHG10] Andrey Ipatov, Andreas Heßelmann, and Andreas Görling. Molecular excitation spectra by TDDFT with the nonadiabatic exact exchange kernel. *International Journal of Quantum Chemistry*, 110(12):2202–2220, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ikot:2016:SSM

[IIH16] Akpan N. Ikot, Eno J. Ibanga, and Hassan Hassanabadi. Scattering state of the multiparameter potential with an improved approximation for the centrifugal term in D-dimensions. *International Journal of Quantum Chemistry*, 116(2):81–87, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Irfan:2017:DDA

[IIS+17] Muhammad Irfan, Javed Iqbal, Sana Sadaf, Bertil Eliasson, Usman Ali Rana, Salah Ud din Khan, and Khur-

shid Ayub. Design of donor–acceptor–donor (D–A–D) type small molecule donor materials with efficient photovoltaic parameters. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ichikawa:2011:TSH

[IIW+11] Kazuhide Ichikawa, Yuji Ikeda, Ayumu Wagatsuma, Kouhei Watanabe, Paweł Szarek, and Akitomo Tachibana. Theoretical study of hydrogenated tetrahedral aluminum clusters. *International Journal of Quantum Chemistry*, 111(14):3548–3555, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Izadyar:2014:QCA

[IK14] Mohammad Izadyar and Mohammad Khavani. Quantum chemistry aspects of the solvent effects on the ene reaction of 1-Phenyl-1,3,4-triazolin-2,5-dione and 2-methyl-2-butene. *International Journal of Quantum Chemistry*, 114 (10):666–674, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishimoto:2018:CPW

[IK18] Takayoshi Ishimoto and Hiroyuki Kai. Combined plane wave and localized orbital electronic structure calculation: Adsorption energy of hydrogen on Pd(111). *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ingale:2018:OCG

[IKC18] Nilesh Ingale, Ravinder Konda, and Ajay Chaudhari. Organolithium complex as a gas sensing material for oxides from ab initio calculations and molecular dynamics simulations. *International Journal of Quantum Chemistry*, 118(15):e25623:1–e25623:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Imamura:2013:FDF

[IKN13] Yutaka Imamura, Rie Kobayashi, and Hiromi Nakai. Frontiers in density functional theory: Linearity condition for

orbital energies in density functional theory (IV): Determination of range-determining parameter. *International Journal of Quantum Chemistry*, 113(3):245–251, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isaev:2008:PPC

[IKS08] Alexander Isaev, Tapas Kar, and Steve Scheiner. Periodicity in proton conduction along a H-bonded chain. Application to biomolecules. *International Journal of Quantum Chemistry*, 108(3):607–616, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [IKS10].

Isaev:2010:EPP

[IKS10] Alexander Isaev, Tapas Kar, and Steve Scheiner. Erratum: Periodicity in proton conduction along a H-bonded chain. Application to biomolecules. *International Journal of Quantum Chemistry*, 110(5):1136, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [IKS08].

Ikuma:2017:TSR

[Iku17] Naohiko Ikuma. A theoretical study for the regioselective Diels–Alder reaction of 5,6-fulleroid with strained anti-Bredt olefins. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Improta:2010:TDT

[ILBS10] Roberto Improta, Alessandro Lami, Vincenzo Barone, and Fabrizio Santoro. Time-dependent and time-independent approaches for the computation of absorption spectra of Uracil derivatives in solution. *International Journal of Quantum Chemistry*, 110(3):624–636, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Islampour:2015:EST

[IM15] Reza Islampour and Mahsasadat Miralinaghi. An extensive study of transformation of the diatomics Hamiltonian operator from laboratory- to body-fixed frame. *International Journal of Quantum Chemistry*, 115(8):510–522, April 15,

2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ide:2013:CMN

[IMS+13] Julien Idé, Sébastien Mothy, Adrien Savoyant, Alain Fritsch, Philippe Aurel, Raphaël Méreau, Laurent Ducasse, Jérôme Cornil, David Beljonne, and Frédéric Castet. Computational meso- and nano-science: Interfacial dipole and band bending in model pentacene/C_{60} heterojunctions. *International Journal of Quantum Chemistry*, 113(4):580–584, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ikabata:2015:TRL

[IN15] Yasuhiro Ikabata and Hiromi Nakai. Tutorial review: Local response dispersion method: a density-dependent dispersion correction for density functional theory. *International Journal of Quantum Chemistry*, 115(5):309–324, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Isonguyo:2018:QIT

[IOO18] Cecilia N. Isonguyo, Kayode J. Oyewumi, and Opeyemi S. Oyun. Quantum information-theoretic measures for the static screened Coulomb potential. *International Journal of Quantum Chemistry*, 118(15):e25620:1–e25620:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ireta:2012:MES

[Ire12] Joel Ireta. Microsolvation effects on the stability of polyalanine in extended and polyproline II conformation. *International Journal of Quantum Chemistry*, 112(22):3612–3617, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Issaoui:2010:TIL

[IROW10] Noureddine Issaoui, Najeh Rekik, Brahim Oujia, and Marek J. Wójcik. Theoretical infrared line shapes of H-bonds within the strong anharmonic coupling theory and Fermi resonances effects. *International Journal of Quantum Chemistry*, 110(14):2583–2602, November 15, 2010.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ishii:2014:BMM

[Ish14] Keisaku Ishii. Best molecular multiple quantum bit for the diatomic molecular quantum computer using potassium nitride and calcium nitride through vibrational progression. *International Journal of Quantum Chemistry*, 114(21):1486–1494, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ikabata:2013:FDF

[ISN13] Yasuhiro Ikabata, Takeshi Sato, and Hiromi Nakai. Frontiers in density functional theory: Self-consistent field treatment and analytical energy gradient of local response dispersion method. *International Journal of Quantum Chemistry*, 113(3):257–262, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iyakutti:2012:WCQ

[ISRK12] Kombiah Iyakutti, Velappa Jayaraman Surya, Ratnavelu Rajeswarapalanichamy, and Yoshiyuki Kawazoe. Wigner crystallization of quadratically dispersing electrons in graphene. *International Journal of Quantum Chemistry*, 112(6):1725–1736, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Iuga:2010:SRA

[IUMVB10] Cristina Iuga, Simón Olguín Uribe, Luis D. Miranda, and Annik Vivier-Bunge. Selectivity in radical alkylation of substituted pyrroles. *International Journal of Quantum Chemistry*, 110(3):697–705, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2012:BSF

[JA12] Denis Jacquemin and Carlo Adamo. Basis set and functional effects on excited-state properties: Three bicyclic chromogens as working examples. *International Journal of Quantum Chemistry*, 112(9):2135–2141, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2012:TKA

[JAB12] Fei Jin, Rubik Asatryan, and Joseph W. Bozzelli. Thermodynamic and kinetic analysis on the reaction of dimethyl sulfide radical with oxygen. *International Journal of Quantum Chemistry*, 112(8):1945–1958, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2012:SPM

[Jac12] Denis Jacquemin. Spectroscopic properties of mono- and bis-azopyrroles. *International Journal of Quantum Chemistry*, 112(9):2043–2050, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2010:ESA

[Jal10] Abraham F. Jalbout. Endo[metallo] SWNT-amino acid interactions: a theoretical study. *International Journal of Quantum Chemistry*, 110(4):831–837, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jang:2010:DSM

[Jan10] Yun Hee Jang. A DFT study on molecular junction devices with cyclic disulfide anchors: Effect of anchor oxidation on electron transport. *International Journal of Quantum Chemistry*, 110(12):2290–2298, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Janesko:2013:PRD

[Jan13] Benjamin G. Janesko. Perspectives: Rung 3.5 density functionals: Another step on Jacob's ladder. *International Journal of Quantum Chemistry*, 113(2):83–88, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2011:DSR

[JB11] Ruifa Jin and Hongzheng Bao. A DFT study on the radical scavenging activity of hydroxyanthraquinone derivatives in rhubarb. *International Journal of Quantum Chemistry*, 111 (5):1064–1071, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jantschi:2018:CSC

[JB18] Lorentz Jäntschi and Sorana D. Bolboaca. Conformational study of C_{24} cyclic polyyne clusters. *International Journal of Quantum Chemistry*, 118(15):e25614:1–e25614:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jaramillo:2010:CDE

[JCC10] Paula Jaramillo, Kaline Coutinho, and Sylvio Canuto. Continuum, discrete, and explicit solvation models for describing the low-lying absorption spectrum of the pterin acid in aqueous environment. *International Journal of Quantum Chemistry*, 110(13):2371–2377, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2012:DMC

[JCCZ12] Xiaoxu Jiang, Xinlu Cheng, Guanyu Chen, and Hong Zhang. Diffusion Monte Carlo study of the hydrogen molecules adsorbed on C_4H_3Li. *International Journal of Quantum Chemistry*, 112(14):2627–2631, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jalbout:2008:CTS

[JdL08] Abraham F. Jalbout and Aned de Leon. Charge transfer stabilization of an excess electron on a molecular surface. *International Journal of Quantum Chemistry*, 108(4):808–813, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jorge:2016:CBO

[JdOS16] Francisco E. Jorge, Amanda Z. de Oliveira, and Thiago P. Silva. CAM–B3LYP optical rotations at different wavelengths: Comparison with CCSD results. *International Journal of Quantum Chemistry*, 116(1):21–26, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jones:2010:BBO

[JE10] Travis E. Jones and Mark E. Eberhart. The bond bundle in open systems. *International Journal of Quantum Chem-*

istry, 110(8):1500–1505, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jamshidi:2013:NCO

[JEA13] Zahra Jamshidi, Kiomars Eskandari, and S. Mohammad Azami. Nature of closed- and open-shell interactions between noble metals and rare gas atoms. *International Journal of Quantum Chemistry*, 113(16):1981–1991, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jenkins:2013:PQT

[Jen13] Samantha Jenkins. Perspective: Quantum topology phase diagrams for molecules, clusters, and solids. *International Journal of Quantum Chemistry*, 113(11):1603–1608, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeong:2018:NTP

[Jeo18] Keunhong Jeong. New theoretically predicted RDX- and β-HMX-based high-energy-density molecules. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Junqueira:2010:TSN

[JFDD10] G. M. A. Junqueira, M. S. Faria, A. M. Da Silva, Jr., and H. F. Dos Santos. Theoretical study of nonlinear optical properties of oxocarbon derivatives. *International Journal of Quantum Chemistry*, 110(3):489–497, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jamshidi:2013:GIA

[JFT13] Zahra Jamshidi, Hossien Farhangian, and Zahra Aliakbar Tehrani. Glucose interaction with Au, Ag, and Cu clusters: Theoretical investigation. *International Journal of Quantum Chemistry*, 113(8):1062–1070, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiao:2013:CSC

[JH13] Li Guang Jiao and Yew Kam Ho. Complex-scaling calculations for resonance states of He with screened Coulomb

potentials. *International Journal of Quantum Chemistry*, 113(24):2569–2579, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiao:2015:ALC

[JH15] Li Guang Jiao and Yew Kam Ho. Application of Löwdin's canonical orthogonalization method to the Slater-type orbital configuration-interaction basis set. *International Journal of Quantum Chemistry*, 115(7):434–441, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2018:FAN

[JHL+18] Hui-Hui Jiang, Hui-Min He, Ying Li, Di Wu, Jia-Yuan Liu, Hui Yang, Wei-Ming Sun, Rong-Lin Zhong, Zhong-Jun Zhou, Jian-Hua Hou, Jia-Jun Wang, and Zhi-Ru Li. Finding all-nonmetal transition-metal-like superatom and its magnetic building block. *International Journal of Quantum Chemistry*, 118(13):e25570:1–e25570:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jakowski:2018:TAN

[JHSG18] Jacek Jakowski, Jingsong Huang, Bobby G. Sumpter, and Sophya Garashchuk. Theoretical assessment of the nuclear quantum effects on polymer crystallinity via perturbation theory and dynamics. *International Journal of Quantum Chemistry*, 118(20):e25712:1–e25712:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2015:RFP

[Jia15] Hong Jiang. Reviews: First-principles approaches for strongly correlated materials: a theoretical chemistry perspective. *International Journal of Quantum Chemistry*, 115 (11):722–730, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:2012:ATF

[JK12] Stephanie Jensen and Dmitri Kilin. Anatase (100) thin film surface computational model for photoelectrochemical cell. *International Journal of Quantum Chemistry*, 112(24):

3874–3878, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ji:2012:SMP

[JL12a] Weixiao Ji and Chenglin Luo. Structures, magnetic properties, and electronic counting rule of metals-encapsulated cage-like M_2Si_{18} (M = Ti–Zn) clusters. *International Journal of Quantum Chemistry*, 112(12):2525–2531, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2012:DSC

[JL12b] Yan-Ke Jiang and Jian-Hui Liu. DFT studies of cobalt hydride intermediate on cobaloxime-catalyzed H_2 evolution pathways. *International Journal of Quantum Chemistry*, 112(13):2541–2546, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jing:2012:HBH

[JLG+12] Bo Jing, Qingzhong Li, Baoan Gong, Ran Li, Zhenbo Liu, Wenzuo Li, Jianbo Cheng, and Jiazhong Sun. Hydrogen bond and σ-hole interaction in $M_2C{=}S \cdots HCN$ (M = H, F, Cl, Br, HO, H_3C, H_2N) complex: Dual roles of C=S group and substitution effect. *International Journal of Quantum Chemistry*, 112(5):1491–1498, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jungsuttiwong:2011:CAB

[JLL11] Siriporn Jungsuttiwong, Jarun Lomratsiri, and Jumras Limtrakul. Characterization of acidity in [B], [Al], and [Ga] isomorphously substituted ZSM-5: Embedded DFT/UFF approach. *International Journal of Quantum Chemistry*, 111(10):2275–2282, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2018:TCC

[JLL+18] Peng Jin, Chang Liu, Ying Li, Lanlan Li, and Yujun Zhao. $Th@C_{76}$. Computational characterization of larger actinide endohedral fullerenes. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2013:IMB

[JLS13] Tao Jin, Xiaoyu Li, and Haiqing Sun. Interaction mechanisms between poly(amido-amine) and nano-silicon dioxide. *International Journal of Quantum Chemistry*, 113(8): 1213–1224, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiao:2017:TSI

[JLZ+17] Yinchun Jiao, Yi Liu, Wenjing Zhao, Zhaoxu Wang, Xunlei Ding, Hexiu Liu, and Tian Lu. Theoretical study on the interactions of halogen-bonds and pnicogen-bonds in phosphine derivatives with Br_2, BrCl, and BrF. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jesus:2019:EFS

[JMPP19] Wanderson S. Jesus, Jorge M. C. Marques, Frederico V. Prudente, and Francisco B. Pereira. Exploring the first-shell and second-shell structures arising in the microsolvation of Li^+ by rare gases. *International Journal of Quantum Chemistry*, 119(13):e25860:1–e25860:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jenkins:2015:BST

[JMX+15] Samantha Jenkins, Julio R. Maza, Tianlv Xu, Dong Jiajun, and Steven R. Kirk. Biphenyl: a stress tensor and vector-based perspective explored within the quantum theory of atoms in molecules. *International Journal of Quantum Chemistry*, 115(23):1678–1690, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jahani:2013:CAT

[JN13] Peyman Mohammadzadeh Jahani and Alireza Nowroozi. Conformational analysis, tautomeric preference, intramolecular hydrogen bonding, and solvent effect on dinitrosamine: a quantum chemical study. *International Journal of Quantum Chemistry*, 113(7):1026–1033, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Javadi:2017:RSN

[JNY17] Nabi Javadi, Mostafa Najafi, and Sirous Yourdkhani. On the role of substituent in noncovalent functionalization of graphene and organophosphor recognition: IQA and SAPT perspective. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jeszenszki:2014:PAB

[JNZ+14] Péter Jeszenszki, Péter R. Nagy, Tamás Zoboki, Ágnes Szabados, and Péter R. Surján. Perspectives of APSG-based multireference perturbation theories. *International Journal of Quantum Chemistry*, 114(16):1048–1052, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Johansson:2017:NLA

[Joh17] Adam Johannes Johansson. Noninnocence of the ligand atoms in iron-porphine: Chemical consequences of the delocalized electron spin. *International Journal of Quantum Chemistry*, 117(1):24–32, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jorgensen:2015:GCV

[Jør15] Flemming Jørgensen. Geometry of the canonical Van Vleck transformation. *International Journal of Quantum Chemistry*, 115(24):1691–1708, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jorgensen:2018:GCV

[Jør18] Flemming Jørgensen. Geometry of the canonical Van Vleck transformation part II: Further developments and numerical treatment. *International Journal of Quantum Chemistry*, 118(21):e25724:1–e25724:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Joubert:2013:SFP

[Jou13] Daniel P. Joubert. Some formal properties of ensemble density functionals. *International Journal of Quantum Chemistry*, 113(8):1076–1085, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2011:ASA

[JPP+11] Denis Jacquemin, Julien Preat, Eric A. Perpète, Daniel P. Vercauteren, Jean-Marie André, Ilaria Ciofini, and Carlo Adamo. Absorption spectra of azobenzenes simulated with time-dependent density functional theory. *International Journal of Quantum Chemistry*, 111(15):4224–4240, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacquemin:2010:ASR

[JPPA10] Denis Jacquemin, Julien Preat, Eric A. Perpète, and Carlo Adamo. Absorption spectra of recently synthesised organic dyes: A TD–DFT study. *International Journal of Quantum Chemistry*, 110(12):2121–2129, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jacob:2012:SDF

[JR12] Christoph R. Jacob and Markus Reiher. Spin in density-functional theory. *International Journal of Quantum Chemistry*, 112(23):3661–3684, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Joshi:2019:OCT

[JR19] Ankita Joshi and C. N. Ramachandran. Optoelectronic and charge transport properties of the complex of carbon nanotube with perylene bisimide. *International Journal of Quantum Chemistry*, 119(24):e26026:1–e26026:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jayasree:2017:DFE

[JS17] Elambalassery G. Jayasree and Soorya Sreedevi. Density functional evaluation and a feasibility study of intramolecular thione–thiol tautomerization. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jerbi:2018:RDD

[JS18] Jihène Jerbi and Michael Springborg. Reactivity descriptors for DNA bases and the methylation of cytosine. *International Journal of Quantum Chemistry*, 118

(11):e25538:1–e25538:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2014:TSM

[JSLH14] Haiyang Jiang, Yanwei Sun, Huiling Liu, and Xuri Huang. Theoretical study on mechanism of cinchona alkaloids catalyzed asymmetric conjugate addition of dimethyl malonate to β-nitrostyrene. *International Journal of Quantum Chemistry*, 114(10):642–651, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jensen:2018:TRN

[JW18] Daniel S. Jensen and Adam Wasserman. Tutorial reviews: Numerical methods for the inverse problem of density functional theory. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiang:2019:EEC

[JW19] Yue Jiang and Cuihong Wang. Endohedral and exohedral complexes of 1-benzene with carbon nanotubes and high-density assembly of multiple benzenes inside of a carbon nanotube. *International Journal of Quantum Chemistry*, 119(15):e25936:1–e25936:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jin:2012:TSP

[JWG+12] J. L. Jin, S. X. Wu, Y. Geng, S. Y. Yang, G. C. Yang, J. Wu, S. Muhammad, Y. Liao, Z. M. Su, and L. Z. Hao. Theoretical study on photophysical properties of novel bis(BF_2)-2,2′-bidipyrrins dyes: Effect of variation in monomer structure. *International Journal of Quantum Chemistry*, 112 (2):440–452, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ji:2012:TSR

[JWJ+12] Dafang Ji, Yongcheng Wang, Yanzi Jin, Lngling Lv, Cuilan Wang, and Jingyan Nian. A two-state reactivity rationale for the reaction of Ta atom with acetonitrile in the gas phase. *International Journal of Quantum Chemistry*, 112 (23):3685–3690, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jenkins:2015:QTR

[JXX+15] Samantha Jenkins, Chen-Xia Xiao, Tianlv Xu, Dulin Yin, Steven R. Kirk, and Gregory A. Chass. Quantum topological resolution of catalyst proficiency. *International Journal of Quantum Chemistry*, 115(14):875–883, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jia:2017:IPT

[JZP17] Chun-Sheng Jia, Lie-Hui Zhang, and Xiao-Long Peng. Improved Pöschl–Teller potential energy model for diatomic molecules. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Jiao:2017:BVS

[JZZH17] Li Guang Jiao, Li Rong Zan, Yong Zhi Zhang, and Yew Kam Ho. Benchmark values of Shannon entropy for spherically confined hydrogen atom. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koch:2011:SED

[KA11] Volker Koch and Dirk Andrae. Static electric dipole polarizabilities for isoelectronic sequences. *International Journal of Quantum Chemistry*, 111(4):891–903, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khan:2013:TSB

[KA13] Imad Khan and Iftikhar Ahmad. Theoretical studies of the band structure and optoelectronic properties of ZnO_xS_{1-x}. *International Journal of Quantum Chemistry*, 113(9):1285–1292, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kassaee:2008:NSN

[KAG08] M. Z. Kassaee, H. Arefrad, and M. Ghambarian. Novel silicon nanorings: Persilacyclacenes at DFT. *International Journal of Quantum Chemistry*, 108(4):696–707, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalemos:2018:NCB

[Kal18] Apostolos Kalemos. The nature of the chemical bond in borazine ($B_3N_3H_6$), boroxine ($B_3O_3H_3$), carborazine ($B_2N_2C_2H_6$), and related species. *International Journal of Quantum Chemistry*, 118(16):e25650:1–e25650:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2011:CSB

[Kan11] Lihua Kang. A comparison of the stereodynamics between C(^{1} D) H_2 and C(^{1} D) HD reactions. *International Journal of Quantum Chemistry*, 111(1):117–122, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2017:FPE

[Kan17] Sung Gu Kang. First-principles examination of low tolerance factor perovskites. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2018:CBM

[Kan18] Chol Jun Kang. Correlation of bond metallicity measures to electronegativity for binary oxides. *International Journal of Quantum Chemistry*, 118(11):e25548:1–e25548:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kosar:2011:TES

[KAOB11] Başak Koşar, Çiğdem Albayrak, Mustafa Odabaşoğlu, and Orhan Büyükgüngör. Theoretical and experimental studies on electronic structure, cocrystallization, and intramolecular proton transfer of two tautomers: (E)-2-[2-(hydroxymethyl)phenylimino]methyl-5-methoxyphenol and (Z)-6-[2-(hydroxymethyl)phenylamino] methylene-3-methoxy-cyclohexa-2, 4-dienone. *International Journal of Quantum Chemistry*, 111(14):3654–3663, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaplan:2012:ESD

[Kap12] Ilya G. Kaplan. Early stage of the development of quantum chemistry without spin and its recent applications. *International Journal of Quantum Chemistry*, 112(17):2858–2867, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:2009:IPQ

[Kar09] Jacek Karwowski. Inverse problems in quantum chemistry. *International Journal of Quantum Chemistry*, 109 (11):2456–2463, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Kar10].

Karwowski:2010:EIP

[Kar10] Jacek Karwowski. Erratum: Inverse problems in quantum chemistry. *International Journal of Quantum Chemistry*, 110(10):2004, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Kar09].

Kaliginedi:2012:KPR

[KAR12a] Veerabhadrarao Kaliginedi, Mohamad Akbar Ali, and B. Rajakumar. Kinetic parameters for the reaction of hydroxyl radical with CH_3OCH_2F(HFE-161) in the temperature range of 200–400K: Transition state theory and ab initio calculations. *International Journal of Quantum Chemistry*, 112(4):1066–1077, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karamanis:2012:IDM

[Kar12b] Panaghiotis Karamanis. The Importance of the DFT method on the computation of the second hyperpolarizability of semiconductor clusters of increasing size: a critical analysis on prolate aluminum phosphide clusters. *International Journal of Quantum Chemistry*, 112(9):2115–2125, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karlsson:2012:IHA

[Kar12c] Erik B. Karlsson. Interpretation of the hydrogen anomaly in neutron and electron Compton scattering. *International Journal of Quantum Chemistry*, 112(2):587–602, January

15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karwowski:2013:DFT

[Kar13] Jacek Karwowski. Density functional theory and multicomponent wave functions. *International Journal of Quantum Chemistry*, 113(5):667–672, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karlsson:2015:ECC

[Kar15] Erik B. Karlsson. Entanglement creation in Compton scattering of neutrons on protons and its possible energetic consequences. *International Journal of Quantum Chemistry*, 115(19):1412–1416, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawai:2015:PRC

[Kaw15] Shinnosuke Kawai. Perspectives: Reaction coordinates for elucidating reaction dynamics with anharmonic couplings. *International Journal of Quantum Chemistry*, 115(5):247–252, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2012:ESQ

[KB12] Susmita Kar and S. P. Bhattacharyya. Exploring sequential quantum adiabatic switching across supersymmetric partners for finding the eigenstates of a system. *International Journal of Quantum Chemistry*, 112(12):2463–2474, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kakkar:2013:TIA

[KB13] Rita Kakkar and Mamta Bhandari. Theoretical investigation of the alloxan–dialuric acid redox cycle. *International Journal of Quantum Chemistry*, 113(17):2060–2069, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krueger:2019:MEB

[KB19] Rachel A. Krueger and Guillaume Blanquart. Multireference exciplex binding energies: Basis set convergence and error. *International Journal of Quantum Chemistry*, 119

(5):e25819:1–e25819:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karanjit:2013:CSP

[KBF+13] Sangita Karanjit, Karan Bobuatong, Ryoichi Fukuda, Masahiro Ehara, and Hidehiro Sakurai. Computations of structures, properties and functions of complex systems: Mechanism of the aerobic oxidation of methanol to formic acid on Au_8^-: a DFT study. *International Journal of Quantum Chemistry*, 113(4):428–436, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khodja:2017:CRV

[KBG17] A. Khodja, F. Benamira, and L. Guechi. Comment on "The rotation–vibration spectrum of diatomic molecules with the Tietz–Hua rotating oscillator". *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [HRT12].

Kamal:2012:IPV

[KBGC12] C. Kamal, Arup Banerjee, Tapan K. Ghanty, and Aparna Chakrabarti. Interesting periodic variations in physical and chemical properties of homonuclear diatomic molecules. *International Journal of Quantum Chemistry*, 112(4):1097–1106, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kekisev:2017:CMS

[KBJ17] Ott Kekišev, Peeter Burk, and Jaak Järv. Computational modeling of strained alkenes: Choosing the right computational model. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kysel:2010:MDS

[KBMM10] Ondrej Kysel, Šimon Budzák, Pavel Mach, and Miroslav Medveď. MP2 and DFT study of IR spectra of TCNE-methylsubstituted benzene complexes: Is charge transfer important? *International Journal of Quantum Chemistry*, 110(9):1712–1728, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kanoun:2011:CSO

[KC11] Mohammed Benali Kanoun and Benoît Champagne. Calculating the second-order nonlinear optical susceptibilities of 3-methyl-4-nitropyridine N-oxide, 2-carboxylic acid-4-nitropyridine-1-oxide, 2-methyl-4-nitroaniline, and m-nitroaniline crystals. *International Journal of Quantum Chemistry*, 111(4):880–890, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2016:SCS

[KC16] Susmita Kar and Pratim Kumar Chattaraj. Solution of the "Classical" Schrödinger equation for a driven symmetric triple well: a comparison with its classical counterpart. *International Journal of Quantum Chemistry*, 116(16):1224–1243, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2018:TQL

[KC18] Susmita Kar and Pratim Kumar Chattaraj. Tunneling and quantum localization in chaos-driven symmetric triple well potential: an approach using quantum theory of motion. *International Journal of Quantum Chemistry*, 118 (10):e25531:1–e25531:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korona:2019:EPD

[KC19a] Tatiana Korona and Michał Chojecki. Exploring point defects in hexagonal boron-nitrogen monolayers. *International Journal of Quantum Chemistry*, 119(14):e25925:1–e25925:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kraka:2019:DCC

[KC19b] Elfi Kraka and Dieter Cremer. Dieter Cremer's contribution to the field of theoretical chemistry. *International Journal of Quantum Chemistry*, 119(6):e25849:1–e25849:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khatua:2013:RDD

[KCC13] Munmun Khatua, Debdutta Chakraborty, and Pratim Kumar Chattaraj. Reviews: Density dynamics in some quan-

tum systems. *International Journal of Quantum Chemistry*, 113(13):1747–1771, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2015:FAN

[KCDC15] Susmita Kar, Ramon Carbó-Dorca, and Pratim K. Chattaraj. Fermi accelerator: a new insight from quantum theory of motion. *International Journal of Quantum Chemistry*, 115(24):1733–1738, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2014:ICE

[KCK14] Yongseon Kim, Sujin Choi, and Subin Kim. Investigation of the change in the electronic properties of FeF_3 by the introduction of oxygen using a molecular orbital method. *International Journal of Quantum Chemistry*, 114(5):340–344, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kosinova:2011:HAA

[KDA+11] Pavlína Košinová, Florent Di Meo, El Hassane Anouar, Jean-Luc Duroux, and Patrick Trouillas. H-atom acceptor capacity of free radicals used in antioxidant measurements. *International Journal of Quantum Chemistry*, 111(6):1131–1142, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karakurt:2012:ISC

[KDÇ12] Tuncay Karakurt, Muharrem Dinçer, and Alaaddin Çukurovali. Ab initio and semiempirical computational studies on 1-(2E)-2-[(aminocarbonothioyl)hydrazono]-2-(3-mesityl-3-methylcyclobutyl)ethyl-pyrrolidine-2,5-dione. *International Journal of Quantum Chemistry*, 112(2):394–413, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kovacs:2017:BDF

[KDOR17] Attila Kovács, Jan Cz. Dobrowolski, Sławomir Ostrowski, and Joanna E. Rode. Benchmarking density functionals in conjunction with Grimme's dispersion correction for noble gas dimers (Ne_2, Ar_2, Kr_2, Xe_2, Rn_2). *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kasende:2016:HBS

[KdPNNS16] Okuma Emile Kasende, Vincent de Paul N. Nziko, and Steve Scheiner. H-bonding and stacking interactions between chloroquine and temozolomide. *International Journal of Quantum Chemistry*, 116(16):1196–1204, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korchowiec:2010:ECT

[KdSM+10] Jacek Korchowiec, Piotr de Silva, Marcin Makowski, Feng Long Gu, and Yuriko Aoki. Elongation cutoff technique at Kohn–Sham level of theory. *International Journal of Quantum Chemistry*, 110(12):2130–2139, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kraus:2017:DHA

[KF17] Peter Kraus and Irmgard Frank. On the dynamics of H_2 adsorption on the Pt(111) surface. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kraus:2019:VAC

[KF19] Peter Kraus and Irmgard Frank. Validating additive correction schemes against gradient-based extrapolations. *International Journal of Quantum Chemistry*, 119(16): e25953:1–e25953:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2018:AKS

[KFJ+18] Chandan Kumar, Heike Fliegl, Frank Jensen, Andrew M. Teale, Simen Reine, and Thomas Kjærgaard. Accelerating Kohn–Sham response theory using density fitting and the auxiliary-density-matrix method. *International Journal of Quantum Chemistry*, 118(16):e25639:1–e25639:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kroger:2013:CSH

[KFS13] Jessica L. Kroger, Joel R. Fried, and Adam A. Skelton. Computational simulations of hydrolysis of phosphazene oligomer utilizing atom-centered density matrix propagation. *International Journal of Quantum Chemistry*, 113(1): 63–70, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Komatsu:2012:CPN

[KFY+12] Yu Komatsu, Masaki Fukuda, Hironao Yamada, Shuhei Kawamoto, Takeshi Miyakawa, Ryota Morikawa, Masako Takasu, Satoshi Yokojima, Satoshi Akanuma, and Akihiko Yamagishi. Constructing protein nano-fiber and estimation of the electronic state around metal ions. *International Journal of Quantum Chemistry*, 112(24):3750–3755, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuganathan:2008:MTC

[KG08] Navaratnarajah Kuganathan and Jennifer C. Green. Mercury telluride crystals encapsulated within single walled carbon nanotubes: a density functional study. *International Journal of Quantum Chemistry*, 108(4):797–807, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khandy:2017:ISM

[KG17] Shakeel Ahmad Khandy and Dinesh C. Gupta. Investigation of structural, magneto-electronic, and thermoelectric response of ductile $SnAlO_3$ from high-throughput DFT calculations. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2013:CBB

[KGK13] Manoj Kumar, Wlodzimierz Galezowski, and Pawel M. Kozlowski. Computational biochemistry and biophysics: Computational modeling of standard reduction potentials of B_{12} cofactors. *International Journal of Quantum Chemistry*, 113(4):479–488, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kinzel:2011:RSP

[KGVG11] Daniel Kinzel, Jesús González-Vázquez, and Leticia González. The role of $\pi\sigma^*$ states in the photochemistry of the chiral fluoroethylene derivative (4-methylcyclohexylidene)fluoromethane. *International Journal of Quantum Chemistry*, 111(13):3394–3404, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2010:CDW

[KH10] Sabyasachi Kar and Y. K. Ho. Calculations of D-wave bound states and resonance states of the screened helium atom using correlated exponential wave functions. *International Journal of Quantum Chemistry*, 110(5):993–1002, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2012:DCL

[KH12] Sabyasachi Kar and Y. K. Ho. Dispersion coefficients for Li^+–H and Li^+–He systems with Coulomb and screened Coulomb potentials. *International Journal of Quantum Chemistry*, 112(15):2706–2709, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khan:2016:ESM

[Kha16] G. R. Khan. Exact solution of multidimensional hyperradial Schrödinger equation for many-electron quantum systems. *International Journal of Quantum Chemistry*, 116 (12):915–919, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korek:2010:TCL

[KHH10] M. Korek, S. Hammoud, and T. Harb. Theoretical calculation of the low laying electronic states of the molecular ion RbH^+. *International Journal of Quantum Chemistry*, 110(4):787–797, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2012:TSR

[KI12] Joonghan Kim and Hyotcherl Ihee. Theoretical study on the reaction of butadiynyl radical (C_4H) with ethylene (C_2H_4) to form C_6H_4 and H. *International Jour-*

nal of Quantum Chemistry, 112(8):1913–1925, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khavani:2015:CSS

[KI15] Mohammad Khavani and Mohammad Izadyar. A comprehensive study of the solvent effects on the cycloaddition reaction of diethyl azodicarboxylate and ethyl vinyl ether: Efficient implementation of QM and TD-DFT study. *International Journal of Quantum Chemistry*, 115(6):381–388, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2013:CST

[Kim13] Ki Chul Kim. Crystal structures and thermodynamic investigations of $NaSc(BH_4)_4$ from first-principles calculations. *International Journal of Quantum Chemistry*, 113(2):119–124, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2016:TUE

[Kim16] Dongwook Kim. A theoretical understanding of the energy difference between singlet and triplet states of oligoacene molecules. *International Journal of Quantum Chemistry*, 116(8):651–655, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2018:WAS

[Kim18] Yongseon Kim. Water adsorption on the surface of Ni- and Co-based layer-structured cathode materials for lithium-ion batteries. *International Journal of Quantum Chemistry*, 118(15):e25591:1–e25591:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2019:TIZ

[Kim19] Yongseon Kim. Thermochemical investigation of Zr doping in $LiNi_{8/12}\ Co_{2/12}\ Mn_{2/12}O_2$ based on phase equilibria simulation. *International Journal of Quantum Chemistry*, 119(24):e26028:1–e26028:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

King:2013:HPC

[Kin13] Frederick W. King. High-precision calculations of the hyperfine constants and some selected transition energies for the low-lying ^{4}S levels of the lithium atom. *International Journal of Quantum Chemistry*, 113(23):2534–2539, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitamura:2014:DMT

[Kit14] H. Kitamura. Density-matrix theory of quantum dynamics under a strong external field switched on nonadiabatically. *International Journal of Quantum Chemistry*, 114 (22):1518–1527, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitamura:2015:SHE

[Kit15] Hikaru Kitamura. Spherical-harmonics expansion method for density-matrix simulations of quantum electron dynamics in continuum states. *International Journal of Quantum Chemistry*, 115(22):1587–1596, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitamura:2017:DMA

[Kit17] Hikaru Kitamura. Density matrix approach to orbital relaxation dynamics in ionization. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krcha:2014:PCU

[KJ14] Matthew D. Krcha and Michael J. Janik. Perspectives: Challenges in the use of density functional theory to examine catalysis by M-doped ceria surfaces. *International Journal of Quantum Chemistry*, 114(1):8–13, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2015:PPE

[KJ15] Heejin Kim and Yousung Jung. Perspective: a perspective on the electronic structure calculations for properties of battery electrode materials. *International Journal*

of Quantum Chemistry, 115(17):1141–1146, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2016:CPD

[KJ16a] Jaehoon Kim and Yousung Jung. Corrigendum: A perspective on the density matrix purification for linear scaling electronic structure calculations. *International Journal of Quantum Chemistry*, 116(24):1898, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [KJ16b].

Kim:2016:PPD

[KJ16b] Jaehoon Kim and Yousung Jung. Perspectives: a perspective on the density matrix purification for linear scaling electronic structure calculations. *International Journal of Quantum Chemistry*, 116(8):563–568, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See corrigendum [KJ16a].

Kaur:2011:HBC

[KK11a] Damanjit Kaur and Ruchi Kohli. Hydrogen bond cooperativity in dimers of hydroxamic acids. *International Journal of Quantum Chemistry*, 111(12):2931–2943, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khamatgalimov:2011:ESS

[KK11b] Ayrat R. Khamatgalimov and Valeri I. Kovalenko. Electronic structure and stability of C_{86} fullerene Isolated-Pentagon-Rule isomers. *International Journal of Quantum Chemistry*, 111(12):2966–2971, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khokhriakov:2011:IHS

[KK11c] Nicolai Khokhriakov and Vladimir Kodolov. Influence of hydroxyfullerene on the structure of water. *International Journal of Quantum Chemistry*, 111(11):2620–2624, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2011:QCS

[KK11d] K. Senthil Kumar and R. Kumaresan. A quantum chemical study on the antioxidant properties of aureusidin and bracteatin. *International Journal of Quantum Chemistry*, 111(15):4483–4496, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khamatgalimov:2012:IIF

[KK12a] Ayrat R. Khamatgalimov and Valeri I. Kovalenko. 24 IPR isomers of fullerene C_{84}: Cage deformation as geometrical characteristic of local strains. *International Journal of Quantum Chemistry*, 112(4):1055–1065, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2012:GKC

[KK12b] Douglas J. Klein and Eugene S. Kryachko. I. G. Kaplan: Curriculum vitae. *International Journal of Quantum Chemistry*, 112(17):2857, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karafiloglou:2013:UES

[KK13] Padeleimon Karafiloglou and Katerina Kyriakidou. Unpaired electrons at the second-order reduced density matrix level: Covalent bonding, and Coulomb and Fermi correlations in closed shell systems. *International Journal of Quantum Chemistry*, 113(13):1775–1786, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karafiloglou:2014:UES

[KK14a] Padeleimon Karafiloglou and Katerina Kyriakidou. Unpaired electrons, spin polarization, and bond orders in radicals from the 2-RDM in orbital spaces: Basic notions and testing calculations. *International Journal of Quantum Chemistry*, 114(11):696–707, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2014:DFM

[KK14b] Joonghan Kim and Jeongho Kim. Density functional and multiconfigurational ab initio study of the ground and excited states of Os_2. *International Journal of Quantum*

Chemistry, 114(21):1466–1471, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaczmarek-Kedziera:2019:IPS

[KK19] Anna Kaczmarek-Kedziera. Influence of photodegradation and surface modification on the graphene–diclofenac physisorption process. *International Journal of Quantum Chemistry*, 119(24):e26030:1–e26030:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalescky:2014:CHD

[KKC14] Robert Kalescky, Elfi Kraka, and Dieter Cremer. Are carbon—halogen double and triple bonds possible? *International Journal of Quantum Chemistry*, 114(16):1060–1072, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kretschmer:2012:RHB

[KKG12] Robert Kretschmer, Daniel Kinzel, and Leticia González. The role of hydrogen bonds in protein–ligand interactions. DFT calculations in 1,3-dihydrobenzimidazole-2 thione derivatives with glycinamide as model HIV RT inhibitors. *International Journal of Quantum Chemistry*, 112(7):1786–1795, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koseki:2013:CCR

[KKH+13] Jun Koseki, Yukiumi Kita, Shuichi Hiraoka, Umpei Nagashima, and Masanori Tachikawa. Computations of chemical reactions and dynamics: Temperature dependence of self-assembled molecular capsules consisting of gear-shaped amphiphile molecules with molecular dynamics simulations. *International Journal of Quantum Chemistry*, 113 (4):397–400, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kanal:2018:SAS

[KKH18] Ilana Y. Kanal, John A. Keith, and Geoffrey R. Hutchison. A sobering assessment of small-molecule force field methods for low energy conformer predictions. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2012:I

[KKL+12] Douglas J. Klein, Eugene S. Kryachko, Jerzy Leszczynski, Octavio Novaro, and Jacques Soullard. Introduction. *International Journal of Quantum Chemistry*, 112(17):2849–2856, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2016:RRD

[KKL+16] Minho Kim, Won June Kim, Eok Kyun Lee, Sébastien Lebègue, and Hyungjun Kim. Reviews: Recent development of atom-pairwise van der Waals corrections for density functional theory: From molecules to solids. *International Journal of Quantum Chemistry*, 116(8):598–607, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khan:2012:RBA

[KKM+12] Ahmad Khalid Raza Khan, Suhail Ahmad Khan, Sunil Mishra, Tajuddin Khan, Mohiuddin Ansari, and Badshah Hasan Khan. Receptor binding affinity based comparative QSAR study of testosterone derivatives. *International Journal of Quantum Chemistry*, 112(11):2371–2377, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kostjukov:2011:CEC

[KKS+11] V. V. Kostjukov, N. M. Khomytova, A. A. Hernandez Santiago, R. Licona Ibarra, D. B. Davies, and M. P. Evstigneev. Calculation of the electrostatic charges and energies for intercalation of aromatic drug molecules with DNA. *International Journal of Quantum Chemistry*, 111 (3):711–721, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koyanagi:2013:CMS

[KKT13] Katsuhiko Koyanagi, Yukiumi Kita, and Masanori Tachikawa. Computations of molecular structure, properties and spectroscopies: Vibrational enhancement of positron affinities for nonpolar carbon dioxide and carbon disulfide molecules: Multi-component molecular orbital study for vibrational excited states. *International Journal of Quantum Chemistry*, 113(3):382–385, February 5, 2013. CODEN IJQCB2.

ISSN 0020-7608 (print), 1097-461X (electronic). See corrigendum [KKT14].

Koyanagi:2014:CVE

[KKT14] Katsuhiko Koyanagi, Yukiumi Kita, and Masanori Tachikawa. Corrigendum: Vibrational enhancement of positron affinities for nonpolar carbon dioxide and carbon disulfide molecules: Multi-component molecular orbital study for vibrational excited states. *International Journal of Quantum Chemistry*, 114(3):237–238, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [KKT13].

Kirtman:2011:CMT

[KL11] Bernard Kirtman and Josep M. Luis. On the contribution of mixed terms in response function treatment of vibrational nonlinear optical properties. *International Journal of Quantum Chemistry*, 111(4):839–847, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2011:SFQ

[Kle11] D. J. Klein. Spin-free quantum electronic structure: Its second quantization and para-Fermionics. *International Journal of Quantum Chemistry*, 111(1):76–95, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kupka:2019:PMD

[KLE+19] Teobald Kupka, Małgorzata Leszczyńska, Krzysztof Ejsmont, Adrianna Mnich, Małgorzata Broda, Karthick Thangavel, and Jakub Kaminský. Phosphorus mononitride: a difficult case for theory. *International Journal of Quantum Chemistry*, 119(24):e26032:1–e26032:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2013:IDM

[KLK13] Yongseon Kim, Jaehyuk Lim, and Shinhoo Kang. Investigation on the dissolution of Mn ions from $LiMn_2O_4$ cathode in the application of lithium ion batteries: First principle molecular orbital method. *International Journal of Quan-*

tum Chemistry, 113(2):148–154, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2015:EPM

[KLZQ15] Long-Juan Kong, Guang-Hua Liu, Yu Zhang, and Ling Qiang. Electronic properties and 1/3 magnetization plateau of the $S = 1/2$ magnetism Cu_3 $(P_2O_6OH)_2$. *International Journal of Quantum Chemistry*, 115(6):406–412, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kabanda:2012:CSD

[KM12a] Mwadham M. Kabanda and Liliana Mammino. A comparative study of the dimers of selected hydroxybenzenes. *International Journal of Quantum Chemistry*, 112(2):519–531, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kabanda:2012:CPA

[KM12b] Mwadham M. Kabanda and Liliana Mammino. The conformational preferences of acylphloroglucinols — a promising class of biologically active compounds. *International Journal of Quantum Chemistry*, 112(23):3691–3702, December 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2012:MCR

[KM12c] D. J. Klein and N. H. March. Molecular conductance in relation to inverse transport theory and to chemical bond order. *International Journal of Quantum Chemistry*, 112 (1):99–102, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2019:EEE

[KM19] Rahul Kumar and Dilip Kumar Maity. Effect of excess electron on structure, bonding, and spectral properties of sulfur/selenium based dichalcogen systems. *International Journal of Quantum Chemistry*, 119(7):e25855:1–e25855:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karu:2018:PSD

[KME+18] Karl Karu, Maksim Misin, Heigo Ers, Jianwei Sun, and Vladislav Ivanistsev. Performance of SCAN density functional for a set of ionic liquid ion pairs. *International Journal of Quantum Chemistry*, 118(13):e25582:1–e25582:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kiametis:2011:HDP

[KMF+11] Alessandra S. Kiametis, Thiago A. M. Matheus, A. L. A. Fonseca, Geraldo Magela E. Silva, and Ricardo Gargano. $H_2{}^+$ dynamical properties in the electronic states $7j\sigma$, $8j\sigma$, $8k\sigma$, $7i\pi$, and $8jp$. *International Journal of Quantum Chemistry*, 111(7–8):1316–1320, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khafizov:2016:QCC

[KMK+16] Nail R. Khafizov, Timur I. Madzhidov, Oleg N. Kadkin, Rui Tamura, and Igor S. Antipin. Quantum chemical calculation of exchange interactions in supramolecularly arranged N, N′-dioxy-2,6-diazaadamantane organic biradical. *International Journal of Quantum Chemistry*, 116(14): 1064–1070, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koval:2016:GES

[KMM16] Vitaliy V. Koval, Ruslan M. Minyaev, and Vladimir I. Minkin. Geometric and electronic structures of silicon fluorides $SiF_n^{(n-4)-}$ (n = 4–6) and potential energy surfaces for dissociation reactions SiF_5–SiF_4 + F^- and $SiF_6^{2-} \rightarrow SiF_5^- + F^-$. *International Journal of Quantum Chemistry*, 116(18):1358–1361, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khafizov:2018:ECS

[KMM+18] Nail R. Khafizov, Ravil Mukhametgaleev, Timur I. Madzhidov, Oleg N. Kadkin, and Igor S. Antipin. Effect of core substituents on the intramolecular exchange interaction in N, N'-dioxy-2,6-diazaadamantane biradical: DFT studies. *International Journal of Quantum Chemistry*, 118(13): e25568:1–e25568:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kasende:2017:IBT

[KMMS17] Okuma Emile Kasende, Aristote Matondo, Jules Tshishimbi Muya, and Steve Scheiner. Interactions between temozolomide and guanine and its S and Se-substituted analogues. *International Journal of Quantum Chemistry*, 117(3):157–169, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kopec:2019:VTA

[KMNSP19] Sabine Kopec, Emilio Martínez-Núñez, Juan Soto, and Daniel Peláez. vdW-TSSCDS — an automated and global procedure for the computation of stationary points on intermolecular potential energy surfaces. *International Journal of Quantum Chemistry*, 119(21):e26008:1–e26008:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kiametis:2013:AIM

[KMRG13] Alessandra S. Kiametis, João B. L. Martins, Luiz A. S. Romeiro, and Ricardo Gargano. Acetylcholinesterase inhibitors: Modeling potential candidates. *International Journal of Quantum Chemistry*, 113(10):1461–1466, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalaiselvan:2011:HRL

[KMS+11] Anbarasan Kalaiselvan, Kaliappan Muthukumar, Dhurairajan Senthilnathan, Pascale Maldivi, and Ponnambalam Venuvanalingam. Half rotations leading to retention of stereochemistry in epoxide ring opening by selenocyanate ion: Insights from DFT modeling. *International Journal of Quantum Chemistry*, 111(10):2317–2323, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawamoto:2012:CPP

[KMT+12] Shuhei Kawamoto, Takeshi Miyakawa, Masako Takasu, Ryota Morikawa, Tatsuki Oda, Hiroaki Saito, Shiroh Futaki, and Hidemi Nagao. Cell-penetrating peptide induces various deformations of lipid bilayer membrane: Inverted micelle, double bilayer, and transmembrane. *International Journal of Quantum Chemistry*, 112(1):178–183, January

2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kulatov:2013:MKO

[KMU+13] Erkin Kulatov, Maria Magnitskaya, Yurii Uspenskii, Svetlana Popova, Vadim Brazhkin, and Evgenii Maksimov. Magnetic, kinetic, and optical properties of new high-pressure phases in the system Cr–GaSb: Ab initio density functional theory study. *International Journal of Quantum Chemistry*, 113(6):820–829, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2015:VFF

[KN15] Eugene S. Kryachko and Tymofii Yu. Nikolaienko. Virtual Festschrift foreword: He_2 @C_{60}: Thoughts of the concept of a molecule and of the concept of a bond in quantum chemistry. *International Journal of Quantum Chemistry*, 115(14):859–867, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Klein:2010:CSM

[KO10] D. J. Klein and J. M. Oliva. Composite-system models. *International Journal of Quantum Chemistry*, 110(15):2784–2800, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kula:2012:TSE

[KO12] Mathias Kula and Lars Ojamäe. A theoretical study of the electronic structure of GaN nanorods. *International Journal of Quantum Chemistry*, 112(7):1796–1802, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karlicky:2014:PCT

[KO14] František Karlický and Michal Otyepka. Perspectives: Challenges in the theoretical description of nanoparticle reactivity: Nano zero-valent iron. *International Journal of Quantum Chemistry*, 114(15):987–992, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koch:2013:EIM

[Koc13a] Wolfhard H. G. Koch. Explicit and implicit multi-center integrations. *International Journal of Quantum Chemistry*, 113(10):1573–1583, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koch:2013:WHC

[Koc13b] Wolfhard H. G. Koch. On the "Wolfsberg–Helmholz Conjecture" of "Extended–Hückel Theory". *International Journal of Quantum Chemistry*, 113(10):1568–1572, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2010:OII

[Kon10] Liguo Kong. Orbital invariance issue in multireference methods. *International Journal of Quantum Chemistry*, 110(14):2603–2613, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2011:ECD

[Kon11] Liguo Kong. Extension of the cumulant definition for low particle number systems. *International Journal of Quantum Chemistry*, 111(14):3541–3547, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2010:ESH

[KP10] Rahul Kar and Sourav Pal. Effect of solvents having different dielectric constants on reactivity: a conceptual DFT approach. *International Journal of Quantum Chemistry*, 110(9):1642–1647, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Karamanis:2011:SDC

[KP11] Panaghiotis Karamanis and Claude Pouchan. On the shape dependence of cluster (hyper)polarizabilities. A combined ab initio and DFT study on large fullerene–like gallium arsenide semiconductor clusters. *International Journal of Quantum Chemistry*, 111(4):788–796, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Komarov:2012:III

[KP12] Platon Valerievich Komarov and Viktor Georgievich Plotnikov. Influence of intermolecular interactions on spectral-luminescent properties of a polyatomic molecule. *International Journal of Quantum Chemistry*, 112(18):3039–3045, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koufos:2013:ESF

[KP13] Alexander P. Koufos and Dimitrios A. Papaconstantopoulos. Electronic structure of francium. *International Journal of Quantum Chemistry*, 113(17):2070–2077, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kidd:2018:APB

[KPCV18] Daniel Kidd, Bailey Pearson, Cody Covington, and Kálmán Varga. Accelerated pseudospectral basis in density functional calculations. *International Journal of Quantum Chemistry*, 118(13):e25573:1–e25573:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kraus:2012:HCC

[KPH+12] Michal Kraus, Michal Pitoňák, Pavel Hobza, Miroslav Urban, and Pavel Neogrády. Highly correlated calculations using optimized virtual orbital space with controlled accuracy. Application to counterpoise corrected interaction energy calculations. *International Journal of Quantum Chemistry*, 112(4):948–959, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2017:IPE

[KPL+17] Ran Hee Kim, Jin Sun Park, Kwang-Sup Lee, Karin Zojer, and Jean-Luc Brédas. Impact of position of electron withdrawing cyano groups on nonlinear optical properties of centrosymmetric donor-π-acceptor system. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kang:2016:SNU

[KRC+16] Sungwoo Kang, Seongok Ryu, Sunghwan Choi, Jaewook Kim, Kwangwoo Hong, and Woo Youn Kim. Software news & updates: Update to ACE-molecule: Projector augmented wave method on Lagrange-sinc basis set. *International Journal of Quantum Chemistry*, 116(8):644–650, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kulkarni:2013:SDE

[KRG+13] Anant D. Kulkarni, Dhurba Rai, Shridhar P. Gejji, Libero J. Bartolotti, and Rajeev K. Pathak. Structuring and destructuring effects along a pathway toward formation of zwitterionic glycine$\cdots(H_2O)_2$ complex: many body analysis of clusters and molecular electrostatic potential investigations. *International Journal of Quantum Chemistry*, 113(9):1325–1332, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaiyawet:2013:CBB

[KRH13] Nopporn Kaiyawet, Thanyada Rungrotmongkol, and Supot Hannongbua. Computational biochemistry and biophysics: Probable polybasic residues inserted into the cleavage site of the highly pathogenic avian influenza A/H5N1 hemagglutinin: Speculation of the next outbreak in humans. *International Journal of Quantum Chemistry*, 113(4):569–573, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kristyan:2013:TVC

[Kri13] Sandor Kristyan. Theory of variational calculation with a scaling correct moment functional to solve the electronic Schrödinger equation directly for ground state one-electron density and electronic energy. *International Journal of Quantum Chemistry*, 113(10):1479–1492, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khungar:2017:PRP

[KRK+17] Bharti Khungar, Ankita Roy, Anand Kumar, Biswajit Sadhu, and Mahesh Sundararajan. Predicting the redox properties of uranyl complexes using electronic structure

calculations. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2010:TCM

[Kry10] Eugene S. Kryachko. Three computational mise-en-scènes of red- and blue-shifted hydrogen bonding motifs: Concept of negative intramolecular coupling — What else? *International Journal of Quantum Chemistry*, 110(1):104–119, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2011:BR

[Kry11a] Eugene S. Kryachko. Book Review. *International Journal of Quantum Chemistry*, 111(15):4501–4503, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2011:SPM

[Kry11b] Eugene S. Kryachko. Stability and protonation of multi-electron systems: The concept of proton affinity. I. Vague limits. *International Journal of Quantum Chemistry*, 111 (7–8):1792–1807, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2012:MMI

[Kry12a] Eugene S. Kryachko. Modeling molecular interactions by analytic potentials: Analytic perturbation treatment. *International Journal of Quantum Chemistry*, 112(18):2986–2997, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kryachko:2012:SPM

[Kry12b] Eugene S. Kryachko. On stability and protonation of multi-electron systems: The concept of proton affinity. II. Dissociative proton attachment and protonation—deprotonation mapping. *International Journal of Quantum Chemistry*, 112(2):382–393, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Krykunov:2012:IHT

[Kry12c] Mykhaylo Krykunov. Impurity Hamiltonian for transition metal complexes based on the exact exchange for correlated

electrons hybrid functional. *International Journal of Quantum Chemistry*, 112(15):2691–2700, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kakkar:2011:TSK

[KS11] Rita Kakkar and Chayannika Singh. Theoretical study of the kojic acid structure in gas phase and aqueous solution. *International Journal of Quantum Chemistry*, 111 (15):4318–4329, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kruse:2018:HAE

[KS18] Holger Kruse and Jirí Sponer. Highly accurate equilibrium structure of the C2h symmetric N1-to-O2 hydrogen-bonded uracil-dimer. *International Journal of Quantum Chemistry*, 118(15):e25624:1–e25624:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaur:2019:CBB

[KS19] Sarabjeet Kaur and Purshotam Sharma. Cyanoacetaldehyde as a building block for prebiotic formation of pyrimidines. *International Journal of Quantum Chemistry*, 119 (22):e25886:1–e25886:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kishida:2017:EIC

[KSAK17] Ryo Kishida, Adhitya Gandaryus Saputro, Ryan Lacdao Arevalo, and Hideaki Kasai. Effects of introduction of α-carboxylate, N-methyl, and N-formyl groups on intramolecular cyclization of o-quinone amines: Density functional theory-based study. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khatua:2015:RDC

[KSC15] Munmun Khatua, Utpal Sarkar, and Pratim Kumar Chattaraj. Reactivity dynamics of a confined molecule in presence of an external magnetic field. *International Journal of Quantum Chemistry*, 115(3):144–157, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kis:2010:ESB

[KSD10] Zoltán Kis and Radu Silaghi-Dumitrescu. The electronic structure of biologically relevant Fe(0) systems. *International Journal of Quantum Chemistry*, 110(10):1848–1856, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koitz:2012:SDM

[KSG+12] Ralph Koitz, Thomas M. Soini, Alexander Genest, S. B. Trickey, and Notker Rösch. Structure-dependence of the magnetic moment in small palladium clusters: Surprising results from the M06-L Meta-GGA functional. *International Journal of Quantum Chemistry*, 112(1):113–120, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitagawa:2010:DAS

[KSN+10] Y. Kitagawa, T. Saito, Y. Nakanishi, Y. Kataoka, T. Matsui, T. Kawakami, M. Okumura, and K. Yamaguchis. Development of approximately spin projected energy derivatives for biradical systems. *International Journal of Quantum Chemistry*, 110(15):3053–3060, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kumar:2019:NAP

[KSO19] Aditya Kumar, Ajeet Singh, and Animesh K. Ojha. A new approach to predict the formation of 3D hybrid organic-inorganic perovskites. *International Journal of Quantum Chemistry*, 119(22):e26012:1–e26012:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kido:2012:SAA

[KSS12] Kentaro Kido, Hirofumi Sato, and Shigeyoshi Sakaki. Systematic assessment on aqueous pK_a and pK_b of an amino acid base on RISM–SCF–SEDD method: Toward first principles calculations. *International Journal of Quantum Chemistry*, 112(1):103–112, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaur:2019:SDS

[KSS+19] Sandeep Kaur, Amrish Sharma, Hitesh Sharma, Shobhna Dhiman, and Isha Mudahar. Substitutional doping of symmetrical small fullerene dimers. *International Journal of Quantum Chemistry*, 119(23):e26019:1–e26019:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kim:2016:TIS

[KSSK16] Hong-Dal Kim, Hyun-Il Seo, Hui-Seong Song, and Seung-Joon Kim. Theoretical investigation of the structures and spectroscopic properties of $(H_2O_4)_n$ ($n = 1$–4) clusters. *International Journal of Quantum Chemistry*, 116(19):1427–1436, October 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koizumi:2012:IPI

[KSST12] Akihito Koizumi, Kimichi Suzuki, Motoyuki Shiga, and Masanori Tachikawa. Ab initio path integral simulation of $AgOH(H_2O)$. *International Journal of Quantum Chemistry*, 112(1):136–139, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koizumi:2011:TSE

[KSY+11] Kenichi Koizumi, Mitsuo Shoji, Kizashi Yamaguchi, Haruki Nakamura, and Yu Takano. Theoretical studies on electronic structure and magnetic properties of mixed-valence uteroferrin active site. *International Journal of Quantum Chemistry*, 111(3):702–710, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Katriel:2012:HRD

[KT12a] Jacob Katriel and Spyros I. Themelis. Hund's rule in the doubly excited states of the helium isoelectronic. *International Journal of Quantum Chemistry*, 112(17):2880–2893, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kozhushner:2012:CTC

[KT12b] Mortko Kozhushner and Leonid Trakhtenberg. Charge transfer in composites "dielectric + metal nanoparticles":

Effect of electric and magnetic fields. *International Journal of Quantum Chemistry*, 112(17):2904–2914, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawaguchi:2012:MDA

[KTI+12] Kazutomo Kawaguchi, Hiroyuki Takagi, Masashi Iwayama, Megumi Nishimura, Takeshi Miyakawa, Hiroaki Saito, Masako Takasu, and Hidemi Nagao. Molecular dynamics analyses of the dissociation process of ADP from Hsp90. *International Journal of Quantum Chemistry*, 112(24):3791–3795, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kubo:2012:GFO

[Kub12] Atsushi Kubo. Gauge function optimization 2: an accurately solvable model. *International Journal of Quantum Chemistry*, 112(6):1620–1641, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kohagen:2019:NIS

[KUS19] Miriam Kohagen, Frank Uhlig, and Jens Smiatek. On the nature of ion-stabilized cytosine pairs in DNA i-motifs: the importance of charge transfer processes. *International Journal of Quantum Chemistry*, 119(14):e25933:1–e25933:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kutzelnigg:2010:PTS

[Kut10] Werner Kutzelnigg. The periodic table. Its story and its significance. *International Journal of Quantum Chemistry*, 110(7):1443–1444, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kutzelnigg:2013:FWF

[Kut13] Werner Kutzelnigg. Frontiers in wave function theory: Expansion of a wave function in a Gaussian basis. I. Local versus global approximation. *International Journal of Quantum Chemistry*, 113(3):203–217, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Korzan:2010:QCS

[KUTS10] Rory Korzan, Brian Upton, Kenneth Turnbull, and Paul G. Seybold. Quantum chemical study of the energetics and directionality of acid-catalyzed aromatic epoxide ring openings. *International Journal of Quantum Chemistry*, 110 (15):2931–2937, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuvichkin:2010:LNA

[Kuv10] V. V. Kuvichkin. Lipid–nucleic acids interactions as base for organization and expression of cellular genome. *International Journal of Quantum Chemistry*, 110(1):120–126, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kunisada:2016:NII

[KUY16] Tomotaka Kunisada, Hiroshi Ushiyama, and Koichi Yamashita. A new implementation of ab initio Ehrenfest dynamics using electronic configuration basis: Exact formulation with molecular orbital connection and effective propagation scheme with locally quasi-diabatic representation. *International Journal of Quantum Chemistry*, 116 (16):1205–1213, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kuznetsov:2019:CHB

[Kuz19] Maxim L. Kuznetsov. Can halogen bond energy be reliably estimated from electron density properties at bond critical point? The case of the $(\mathrm{A})_n\mathrm{Z}\text{-}Y \cdots X^-$ (X, Y = F, Cl, Br) interactions. *International Journal of Quantum Chemistry*, 119(8):e25869:1–e25869:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kieninger:2011:CIR

[KV11] Martina Kieninger and Oscar N. Ventura. Calculations of the infrared and Raman spectra of simple thiols and thiol–water complexes. *International Journal of Quantum Chemistry*, 111(7–8):1843–1857, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Khordad:2019:MPT

[KV19] Reza Khordad and Behrooz Vaseghi. Magnetic properties in three electrons under Rashba spin-orbit interaction and magnetic field. *International Journal of Quantum Chemistry*, 119(20):e25994:1–e25994:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalamse:2010:QCS

[KWC10] Vijayanand Kalamse, Nitin Wadnerkar, and Ajay Chaudhari. Quantum chemical study of dissociation of H_2 on C_3 H_3 V organometallic compound. *International Journal of Quantum Chemistry*, 110(10):1947–1952, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kalamse:2011:TST

[KWC11] Vijayanand Kalamse, Nitin Wadnerkar, and Ajay Chaudhari. Theoretical study of third-row transition metal monofluorides. *International Journal of Quantum Chemistry*, 111(9):2014–2020, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2015:DPT

[KWLS15] Sabyasachi Kar, Yu-Shu Wang, Wei-Qi Li, and Xiu-Dong Sun. Dynamic polarizability of two-electron ions under Debye screening. *International Journal of Quantum Chemistry*, 115(22):1573–1579, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kar:2018:PNC

[KWWH18] Sabyasachi Kar, Yu-Shu Wang, Yang Wang, and Yew Kam Ho. Polarizability of negatively charged helium-like ions interacting with Coulomb and screened Coulomb potentials. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kawatsu:2013:CBB

[KyH13a] Tsutomu Kawatsu and Jun ya Hasegawa. Computational biochemistry and biophysics: Excitation energy transfer in GFP-X-CFP model peptides (X = amino acids): Direct

versus through-bridge energy transfers. *International Journal of Quantum Chemistry*, 113(4):563–568, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kitagawa:2013:CQC

[KYH+13b] Y. Kitagawa, N. Yasuda, H. Hatake, T. Saito, Y. Kataoka, T. Matsui, T. Kawakami, S. Yamanaka, M. Okumura, and K. Yamaguch. Computational quantum chemistry: Combination of approximate spin-projection and spin-restricted calculations based on ONIOM method for geometry optimization of large biradical systems. *International Journal of Quantum Chemistry*, 113(3):290–295, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Koh:2019:GGS

[KYLC19] Pin Wai Koh, Tiem Leong Yoon, Thong Leng Lim, and Yee Hui Robin Chang. The generation of ground-state structures and electronic properties of ternary Al_k Ti_l Ni_m clusters ($k + l + m = 4$) from a two-stage density functional theory global searching approach. *International Journal of Quantum Chemistry*, 119(10):e25884:1–e25884:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kato:2013:CQC

[KYS13] Tetsuya Kato, Yukina Yokoi, and Hideo Sekino. Computational quantum chemistry: Basis set limit computation of dynamic polarizability at near-resonance region. *International Journal of Quantum Chemistry*, 113(3):286–289, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kaliyeva:2017:SCD

[KZA+17] Laura Kaliyeva, Shingis Zhumagali, Nuriya Akhmetova, Amir Karton, and Robert J. O'Reilly. Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C Cl bond dissociation. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2013:TCL

[KZZ13a] Chui-Peng Kong, Zeng-Xia Zhao, and Hong-Xing Zhang. Theoretical computation of low-lying electronic states of HCNS: a CASPT2 study. *International Journal of Quantum Chemistry*, 113(9):1416–1421, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Kong:2013:TSG

[KZZ13b] Chui-Peng Kong, Zeng-Xia Zhao, and Hong-Xing Zhang. Theoretical study of gas phase reactions of important SOA intermediates: (cis- and trans-) BEPOX and β-IEPOX with OH radical. *International Journal of Quantum Chemistry*, 113(8):1162–1170, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lefebvre:2011:ZWR

[LA11] Roland Lefebvre and Osman Atabek. Zero-width resonances and exceptional points in molecular photodissociation. *International Journal of Quantum Chemistry*, 111 (2):272–278, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ladik:2014:LEC

[Lad14] János J. Ladik. Letters to the editor: Comment on "Electronic states of mixed base pairs systems of DNA and the effect of base composition and sequences on the band structures using screw axis translational symmetry". *International Journal of Quantum Chemistry*, 114(4):302, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [XTLA13, XTLA14].

Laestadius:2014:DFP

[Lae14] Andre Laestadius. Density functionals in the presence of magnetic field. *International Journal of Quantum Chemistry*, 114(21):1445–1456, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laikov:2011:IMA

[Lai11] Dimitri N. Laikov. Intrinsic minimal atomic basis representation of molecular electronic wavefunctions. *International Journal of Quantum Chemistry*, 111(12):2851–2867,

October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lakhno:2010:DSH

[Lak10] Victor D. Lakhno. Davydov's solitons in a homogeneous nucleotide chain. *International Journal of Quantum Chemistry*, 110(1):127–137, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lanza:2010:TSL

[Lan10] Giuseppe Lanza. A theoretical study on the LaF_3 molecule embedded in argon matrix. *International Journal of Quantum Chemistry*, 110(2):376–386, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:2010:SCD

[Lar10] Sven Larsson. Superconductivity in cuprates: Details of electron phonon coupling. *International Journal of Quantum Chemistry*, 110(5):1117–1126, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:2011:AC

[Lar11] Sven Larsson. Applications of CASSCF. *International Journal of Quantum Chemistry*, 111(13):3424–3430, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Larsson:2012:MTI

[Lar12] Sven Larsson. Microscopic theory for insulator to metal transition in cuprates. *International Journal of Quantum Chemistry*, 112(7):1829–1837, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lathiotakis:2013:CMB

[Lat13] N. N. Lathiotakis. Correlation measures as benchmarks in reduced density matrix functional theory. *International Journal of Quantum Chemistry*, 113(6):762–765, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ai:2014:TSR

[lAyL14] Li ling Ai and Jing yao Liu. Theoretical study on the reaction of (Z)-$CF_3CH{=}{=}CHCF_3$ with OH radicals. *Inter-*

national Journal of Quantum Chemistry, 114(3):176–182, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lazzeretti:2014:TRI

[Laz14] Paolo Lazzeretti. Tutorial reviews: Invariance of molecular response properties under a coordinate translation. *International Journal of Quantum Chemistry*, 114(20):1364–1392, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ladik:2014:QMB

[LB14a] János J. Ladik and Attila Bende. Quantum molecular biological investigation of the onset of cancer. *International Journal of Quantum Chemistry*, 114(18):1229–1235, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laestadius:2014:HKT

[LB14b] Andre Laestadius and Michael Benedicks. Hohenberg–Kohn theorems in the presence of magnetic field. *International Journal of Quantum Chemistry*, 114(12):782–795, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lutz:2018:IGP

[LB18] Patricia B. Lutz and Craig A. Bayse. Interpreting geometric preferences in π-stacking interactions through molecular orbital analysis. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2019:IEF

[LB19] Qi Luo and Yuxiang Bu. Intriguing electric field effect on magnetic spin couplings in dielectron clathrate hydrates. *International Journal of Quantum Chemistry*, 119 (13):e25916:1–e25916:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lobayan:2016:DED

[LBdV16] Rosana M. Lobayan, Roberto C. Bochicchio, and Carlos Pérez del Valle. Depicting electronic distributions from

accurate computational first principles: On the relationship between the complex patterns of bonding interaction and the back-donation phenomenon. *International Journal of Quantum Chemistry*, 116(24):1851–1861, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lerner:2011:MCF

[LBM11] Dan A. Lerner, Dorothée Berthomieu, and Elaine R. Maia. Modeling of the conformational flexibility and E /Z isomerism of thiazoximic acid and cefotaxime. *International Journal of Quantum Chemistry*, 111(6):1222–1238, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lamichhane:2011:EHM

[LBW11] K. Lamichhane, M. Brack, and P. Winkler. Energies of higher multipole vibrations of fullerenes in a semiclassical approach. *International Journal of Quantum Chemistry*, 111(15):4363–4372, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:DFT

[LBY+14] Jun Li, Hongcun Bai, Nini Yuan, Yuhua Wu, Yujia Ma, Ping Xue, and Yongqiang Ji. Density functional theory studies of $Si_{36}H_{36}$ and $C_{36}H_{36}$ nanocages. *International Journal of Quantum Chemistry*, 114(11):725–730, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Castillo:2012:PBP

[LC12] Alejandro López-Castillo. Prediction of boron–phosphorous nanographene-like material. *International Journal of Quantum Chemistry*, 112(19):3152–3157, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2016:EDP

[LC16] Xinying Li and Junxia Cai. Electron density properties and metallophilic interactions of gold halides AuX_2 and Au_2X (X = F–I): Ab initio calculations. *International Journal of Quantum Chemistry*, 116(18):1350–1357, September 15,

2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Loco:2019:MAL

[LC19] Daniele Loco and Lorenzo Cupellini. Modeling the absorption lineshape of embedded systems from molecular dynamics: a tutorial review. *International Journal of Quantum Chemistry*, 119(1):e25726:1–e25726:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Castillo:2010:SST

[LCB10] Alejandro López-Castillo and Antonio Carlos Borin. Solvatochromic shift of the $\pi \rightarrow \pi^*$ transition in all-*trans*, *cis*-13, *cis*-11, *cis*-9, and *cis*-7 retinal isomers induced by water and methanol. *International Journal of Quantum Chemistry*, 110(11):2076–2087, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2010:CSC

[LCCH10] Min-Hsien Liu, Ken-Fa Cheng, Cheng Chen, and Yaw-Sun Hong. Computational study on the comparative synthesis of energetic FOX-7 derivatives. *International Journal of Quantum Chemistry*, 110(4):813–820, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2011:CSF

[LCCH11] Min-Hsien Liu, Ken-Fa Cheng, Cheng Chen, and Yaw-Sun Hong. Computational study of FOX-7 synthesis in a solvated reaction system. *International Journal of Quantum Chemistry*, 111(9):1859–1869, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leon-Carmona:2012:FRS

[LCG12] Jorge Rafael León-Carmona and Annia Galano. Free radical scavenging activity of caffeine's metabolites. *International Journal of Quantum Chemistry*, 112(21):3472–3478, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:TSMb

[LCH+11] Xiu Hui Lu, Xin Che, Jun Feng Han, Le Yi Shi, and Zhen Xia Lian. Theoretical study of mechanism of extraction reaction between silylene carbene and its derivatives and ethylene oxide. *International Journal of Quantum Chemistry*, 111(10):2306–2310, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lewis:2014:OER

[LCH14] Kristen Lewis, Kari Copeland, and Glake Hill. One-electron redox properties of DNA nucleobases and common tautomers. *International Journal of Quantum Chemistry*, 114(24):1678–1684, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lim:2016:IIG

[LCK+16] Jaechang Lim, Sunghwan Choi, Sungwoo Kang, Jaewook Kim, Kwangwoo Hong, and Woo Youn Kim. Improvement of initial guess via grid-cutting for efficient grid-based density functional calculations. *International Journal of Quantum Chemistry*, 116(19):1397–1403, October 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2010:AXB

[LCL+10a] Wen-Zuo Li, Jian-Bo Cheng, Qing-Zhong Li, Bao-An Gong, and Jia-Zhong Sun. Assignment on the X, A, B, C, and D states of the C_6 H_5 Br^+ cation based on high-level calculations. *International Journal of Quantum Chemistry*, 110(14):2683–2688, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2010:TPH

[LCL+10b] Wen-Zuo Li, Jian-Bo Cheng, Qing-Zhong Li, Bao-An Gong, and Jia-Zhong Sun. Theoretical prediction on $HBeN^-$ and $HNBe^-$ anions using multiconfiguration second-order perturbation theory. *International Journal of Quantum Chemistry*, 110(10):1857–1862, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:CSL

[LCL+11] Wen-Zuo Li, Jian-Bo Cheng, Qing-Zhong Li, Bao-An Gong, and Jia-Zhong Sun. CASPT2 study on low-lying states of HBN and HNB radicals. *International Journal of Quantum Chemistry*, 111(1):123–129, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:HBA

[LCM+11] Nan Lu, Dezhan Chen, Shizhen Mi, Guiqiu Zhang, and Honghong Zhang. The H-Bond activation mechanism and enantioselectivity in stepwise conjugate amine addition promoted by hydroxyl-thiourea catalyst. *International Journal of Quantum Chemistry*, 111(15):4206–4213, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:TSMa

[LCS+11a] Xiu Hui Lu, Xin Che, Le Yi Shi, Jun Feng Han, and Zhen Xia Lian. Theoretical study of mechanism of cycloaddition reaction between dichloro-germylene carbene (Cl_2 Ge C:) and aldehyde. *International Journal of Quantum Chemistry*, 111(5):1055–1063, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:TSMc

[LCS+11b] Xiu Hui Lu, Xin Che, Le Yi Shi, Jun Feng Han, and Zhen Xia Lian. Theoretical study of mechanism of extraction reaction between germylene carbene and its derivatives and thiirane. *International Journal of Quantum Chemistry*, 111(12):3024–3028, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:ADI

[LCT14] Hsueh-Chien Li, Jeng-Da Chai, and Ming-Kang Tsai. Assessment of dispersion-improved exchange-correlation functionals for the simulation of CO_2 binding by alcoholamines. *International Journal of Quantum Chemistry*, 114(12):805–812, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liao:2015:TSS

[LCZ15] Rongbao Liao, Lanlan Chai, and Yun Zhu. A theoretical study on the stability difference of the borane BnHn2- and carborane $C_2B_{n-2}H_n$ ($5 \leq n \leq 7$) clusters. *International Journal of Quantum Chemistry*, 115(4):216–223, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:TIE

[LCZL11] Nan Lu, Dezhan Chen, Guiqiu Zhang, and Qingjian Liu. Theoretical investigation on enantioselective Biginelli reaction catalyzed by natural tartaric acid. *International Journal of Quantum Chemistry*, 111(9):2031–2038, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2015:SNU

[LCZL15] Wei Li, Chihong Chen, Dongbo Zhao, and Shuhua Li. Software news & updates: LSQC: Low scaling quantum chemistry program. *International Journal of Quantum Chemistry*, 115(10):641–646, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2017:TSR

[LD17] Yan Li and Shiwen Du. Theoretical study on the reaction mechanisms and stereoselectivities of DABCO-catalyzed Rauhut–Currier/cyclization reaction of methyl acrylate with 2-benzoyl-3-phenyl-acrylonitrile. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lucas:2011:ITA

[LdAA+11] Jose Maria Lucas, Jaime de Andrés, Margarita Albertí, Josep Maria Bofill, and Antonio Aguilar-Navarro. An ab initio theoretical approach to the gas phase decomposition of C_3 H_7^+ produced in ground state Li^+ + i -C_3 H_7 Cl collisions. *International Journal of Quantum Chemistry*, 111(2):493–504, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Duran:2015:PES

[LDADB+15] David López-Durán, Néstor Aguirre, Gerardo Delgado-Barrio, Pablo Villarreal, Franco Gianturco, and María de Lara-Castells. Potential energy surface and bound states of the $(X^4\Sigma)$KRb-K complex. *International Journal of Quantum Chemistry*, 115(1):19–27, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leite:2012:PSD

[LdBF+12] Thays C. M. Leite, Ana L. F. de Barros, Glaucio B. Ferreira, Antonio C. O. Guerra, and Cássia C. Turci. Photoabsorption spectroscopy of dimethyl sulfoxide at the O1s, C1s, S2s, and S2p regions: a comparison with acetone. *International Journal of Quantum Chemistry*, 112(20):3421–3433, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lazzari-Dean:2015:ERD

[LDKB15] Julia Lazzari-Dean, Anna I. Krylov, and Ksenia B. Bravaya. The effects of resonance delocalization and the extent of π system on ionization energies of model fluorescent proteins chromophores. *International Journal of Quantum Chemistry*, 115(18):1258–1264, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leite:2012:DBN

[LdMCdA+12] Franco Henrique Andrade Leite, José Walkimar de Mesquita Carneiro, Martha Teixeira de Araujo, Moacyr Comar Jr., and Alex Gutterres Taranto. Docking between natural peroxides and heme group by parametric method 6. *International Journal of Quantum Chemistry*, 112(20):3390–3397, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2011:TIS

[LDW+11] Yan Liu, Hongchen Du, Guixiang Wang, Xuedong Gong, Lianjun Wang, and Heming Xiao. Theoretical investigation of solvent effects on tautomeric equilibrium of 2-diazo-4,6-dinitrophenol. *International Journal of Quantum Chem-*

istry, 111(5):1115–1126, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2016:PDF

[LDZG16] Fang Liu, Likai Du, Dongju Zhang, and Jun Gao. Performance of density functional theory on the anisotropic halogen···halogen interactions and potential energy surface: Problems and possible solutions. *International Journal of Quantum Chemistry*, 116(9):710–717, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lehtola:2019:FNHa

[Leh19a] Susi Lehtola. Fully numerical Hartree–Fock and density functional calculations. I. Atoms. *International Journal of Quantum Chemistry*, 119(19):e25945:1–e25945:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lehtola:2019:FNHb

[Leh19b] Susi Lehtola. Fully numerical Hartree–Fock and density functional calculations. II. Diatomic molecules. *International Journal of Quantum Chemistry*, 119(19):e25944:1–e25944:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lehtola:2019:RNR

[Leh19c] Susi Lehtola. A review on non-relativistic, fully numerical electronic structure calculations on atoms and diatomic molecules. *International Journal of Quantum Chemistry*, 119(19):e25968:1–e25968:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lesar:2012:PCR

[Les12] Antonija Lesar. Product channels in the reaction of the CH_3 SO radical with NO_2: DFT and ab initio studies. *International Journal of Quantum Chemistry*, 112(8):1904–1912, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ludena:2011:MBL

[LEU+11] E. V. Ludeña, L. Echevarría, J. M. Ugalde, X. Lopez, and A. Corella-Madueño. Model for a biexciton in a lateral

quantum dot based on exact solutions for the Hookean H_2 molecule. I. Theoretical aspects. *International Journal of Quantum Chemistry*, 111(7–8):1808–1818, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Levy:2010:SCS

[Lev10] Mel Levy. On the simple constrained-search reformulation of the Hohenberg–Kohn theorem to include degeneracies and more (1964–1979). *International Journal of Quantum Chemistry*, 110(15):3140–3144, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Levy:2016:PMT

[Lev16] Mel Levy. Perspective: Mathematical thoughts in DFT. *International Journal of Quantum Chemistry*, 116(11):802–804, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2015:CRC

[LF15] Wenjian Liu and Weihai Fang. Concluding remarks: Concluding remarks. *International Journal of Quantum Chemistry*, 115(11):744, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Latino:2010:APE

[LFF+10] Diogo A. R. S. Latino, Rui P. S. Fartaria, Filomena F. M. Freitas, João Aires-De-Sousa, and Fernando M. S. Silva Fernandes. Approach to potential energy surfaces by neural networks. A review of recent work. *International Journal of Quantum Chemistry*, 110(2):432–445, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:SBB

[LFP+19] Da-Zhi Li, Lin-Yan Feng, Ling Pei, Ming-Zhi Song, Li-Juan Zhang, Hui Wang, and Hua-Jin Zhai. Structures and bonding of B_4O_5 and $B_4O_5^-$ clusters: Emergence of boroxol ring and competition between rhombic B_2O_2 and hexagonal B_3O_3 cores. *International Journal of Quantum Chemistry*, 119(15):e25907:1–e25907:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:CCM

[LFS+11] Shuo Li, J. R. Fried, Jeremy Sauer, John Colebrook, and Douglas S. Dudis. Computational chemistry and molecular simulations of phosphoric acid. *International Journal of Quantum Chemistry*, 111(12):3212–3229, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2018:MSP

[LFTL18] Yan Li, Wenwen Fu, Ruixue Tian, and Changhai Liang. Mechanisms and stereoselectivities of phosphine-catalyzed (3 + 3) cycloaddition reaction between azomethine imine and ynone: a computational study. *International Journal of Quantum Chemistry*, 118(21):e25729:1–e25729:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lagana:2010:PMV

[LG10] Antonio Laganà and Osvaldo Gervasi. A priori molecular virtual reality on EGEE grid. *International Journal of Quantum Chemistry*, 110(2):446–453, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Loos:2012:LOB

[LG12] Pierre-François Loos and Peter M. W. Gill. Leading-order behavior of the correlation energy in the uniform electron gas. *International Journal of Quantum Chemistry*, 112(6): 1712–1716, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2015:PUM

[LG15] Cheng-Wen Liu and Yi Qin Gao. Perspectives: Understanding the microsolvation of salts in molecular clusters. *International Journal of Quantum Chemistry*, 115(9):541–544, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:EAP

[LGHL11] Rui Li, Li-Hua Gan, Qun Hui, and Qian Li. The effects of atom pyramidalization and square distribution on the stability of F_4F_6-$(BN)_n$ polyhedrons. *International Journal of*

Quantum Chemistry, 111(5):983–990, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lei:2019:NLM

[LGL+19] Lan Lei, Xianya Geng, Shuchao Li, Yingjun Peng, and Yuantian Yu. On the normalized Laplacian of Möbius phenylene chain and its applications. *International Journal of Quantum Chemistry*, 119(24):e26044:1–e26044:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lawal:2018:DSA

[LGM+18] Monsurat M. Lawal, Thavendran Govender, Glenn E. M. Maguire, Hendrik G. Kruger, and Bahareh Honarparvar. DFT study of the acid-catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:TSL

[LGP+11] Wen-Zuo Li, Fang Geng, Yu-Wei Pei, Jian-Bo Cheng, Qing-Zhong Li, and Bao-An Gong. Theoretical study on low-lying states of $HAlO^+$ and $HOAl^+$ cations. *International Journal of Quantum Chemistry*, 111(15):4373–4377, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:CSL

[LGP+12] Wen-Zuo Li, Fang-Fang Geng, Yu-Wei Pei, Jian-Bo Cheng, Qing-Zhong Li, and Bao-An Gong. CASPT2 study on low-lying states of HMgO and HOMg. *International Journal of Quantum Chemistry*, 112(4):1209–1214, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lv:2016:TFR

[LGS+16] Jin-Yu Lv, Yuan-Ru Guo, Dong-Mei Su, Ming-Jing Zhang, and Qing-Jiang Pan. Thiocyanate-free ruthenium(II) tetrabenzoporphyrin sensitizers for photoelectrochemical cell: a DFT/TD-DFT probe for stability of axial donor ligands. *International Journal of Quantum Chemistry*, 116

(18):1342–1349, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liang:2011:GPH

[LGW11] Jun-Xi Liang, Zhi-Yuan Geng, and Yong-Cheng Wang. The gas-phase H-abstraction reactions of CCl_3 H with CX^1 $X^{2\cdot-}$ (X^1 X^2 = HF, HCl, HBr, HI, FF, ClCl, BrBr, and II), a DFT study. *International Journal of Quantum Chemistry*, 111(12):3048–3056, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2015:RTS

[LGZC15] Junfeng Li, Xugeng Guo, Yuan Zhao, and Zexing Cao. Reviews: Theoretical studies on excited states of biorelated systems from gas phase to aqueous solution. *International Journal of Quantum Chemistry*, 115(11):680–688, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2015:SEP

[LHL+15] Chang-Geng Luo, Chao-Zheng He, Hua-Yang Li, Gen-Quan Li, Shuai Zhang, and Xu-Yan Liu. Structures and electronic properties of the small rubidium-doped silicon $RbSi_n$ (n = 1–12) clusters. *International Journal of Quantum Chemistry*, 115(1):50–58, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:STE

[LHX+19] Jia Hui Li, Wei Jie Huang, Tianlv Xu, Steven R. Kirk, and Samantha Jenkins. Stress tensor eigenvector following with next-generation quantum theory of atoms in molecules. *International Journal of Quantum Chemistry*, 119(7):e25847:1–e25847:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:BR

[Li11] Xue Li. Book review. *International Journal of Quantum Chemistry*, 111(14):3991, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2015:ROC

[Li15] Xiang-Yuan Li. Reviews: an overview of continuum models for nonequilibrium solvation: Popular theories and new

challenge. *International Journal of Quantum Chemistry*, 115(11):700–721, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2015:FPC

[LIK15] Shixue Liu, Takayoshi Ishimoto, and Michihisa Koyama. First-principles calculation of OH^- /OH adsorption on gold nanoparticles. *International Journal of Quantum Chemistry*, 115(22):1597–1605, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Linderberg:2012:BR

[Lin12] Jan Linderberg. Book review. *International Journal of Quantum Chemistry*, 112(3):937, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lindgren:2014:RDM

[Lin14] Ingvar Lindgren. Review: Development of many-body perturbation theory: How to combine with quantum electrodynamics. *International Journal of Quantum Chemistry*, 114(18):1176–1182, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2014:PRH

[Liu14] Wenjian Liu. Perspectives: Relativistic Hamiltonians. *International Journal of Quantum Chemistry*, 114(15):983–986, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2015:RRA

[Liu15a] Jian Liu. Reviews: Recent advances in the linearized semiclassical initial value representation/classical Wigner model for the thermal correlation function. *International Journal of Quantum Chemistry*, 115(11):657–670, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2015:TRE

[Liu15b] Wenjian Liu. Tutorial reviews: Effective quantum electrodynamics Hamiltonians: a tutorial review. *International Journal of Quantum Chemistry*, 115(10):631–640, May 15,

2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Liu16].

Liu:2016:EEQ

[Liu16] Wenjian Liu. Erratum: Effective quantum electrodynamics Hamiltonians: a tutorial review. *International Journal of Quantum Chemistry*, 116(12):971, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Liu15b].

Laurent:2013:RTD

[LJ13] Adèle D. Laurent and Denis Jacquemin. Review: TD–DFT benchmarks: a review. *International Journal of Quantum Chemistry*, 113(17):2019–2039, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2016:ETC

[LJ16] Jin Yong Lee and Yousung Jung. Editorial: Theoretical chemistry in Korea: Professor Yoon Sup Lee and the early stages of theoretical chemistry in Korea. *International Journal of Quantum Chemistry*, 116(8):561–562, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2018:CSR

[LJK+18] Sung-Sik Lee, Vinod H. Jadhav, Ji-Young Kim, Su-Jin Kim, Dong Wook Kim, and Sungyul Lee. Computational study of S_N2 reactions promoted by crown ether: Contact ion pair versus solvent-separated ion pair mechanism. *International Journal of Quantum Chemistry*, 118 (11):e25547:1–e25547:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:CSX

[LJL+11] Qingzhong Li, Bo Jing, Zhenbo Liu, Wenzuo Li, Jianbo Cheng, Baoan Gong, and Jiazhong Sun. Comparative study of XO$\cdots$ClF and XS$\cdots$ClF (X = H, CH_3, and F) halogen-bonded complexes. *International Journal of Quantum Chemistry*, 111(14):3856–3863, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2012:MSS

[LJSS12] Yu-Fang Liu, Yi Jia, De-Heng Shi, and Jin-Feng Sun. MRCI study on spectroscopic parameters and molecular constants of the ground state of AsP($X\ ^1\Sigma^+$) molecule. *International Journal of Quantum Chemistry*, 112(2):532–539, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:ISS

[LJW+11] Qingzhong Li, Lixia Jiang, Xilin Wang, Wenzuo Li, Jianbo Cheng, and Jiazhong Sun. Ab initio study of the structure, cooperativity, and vibrational properties in the mixed hydrogen-bonded trimers of hydrogen isocyanide and water. *International Journal of Quantum Chemistry*, 111(5): 1072–1080, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lykhin:2016:TRN

[LKd+16] Aleksandr O. Lykhin, Danil S. Kaliakin, Gwen E. dePolo, Alexander A. Kuzubov, and Sergey A. Varganov. Tutorial reviews: Nonadiabatic transition state theory: Application to intersystem crossings in the active sites of metal-sulfur proteins. *International Journal of Quantum Chemistry*, 116 (10):750–761, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Labidi:2011:TAN

[LKDC11] Sofiane Nouar Labidi, Mohammed Benali Kanoun, Marc De Wergifosse, and Benoît Champagne. Theoretical assessment of new molecules for second-order nonlinear optics. *International Journal of Quantum Chemistry*, 111(7–8):1583–1595, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2013:CDD

[LKJ13] Hua-Wei Li, Sabyasachi Kar, and Pinghui Jiang. Calculations of dynamic dipole polarizabilities of Li and Na atoms in Debye plasma using the model potential technique. *International Journal of Quantum Chemistry*, 113(10):1493–1497, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:DMM

[LKLW11] Peng Lu, Xiao-Yu Kuang, Hui-Fang Li, and Huai-Qian Wang. Direct MP2 molecular dynamics studies of H atom reaction with CD_4 and CH_4. *International Journal of Quantum Chemistry*, 111(15):4433–4442, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lan:2013:CUS

[LKN13] You-Zhao Lan, Hong-Lan Kang, and Tao Niu. Comprehensive understanding of size-, shape-, and composition-dependent polarizabilities of Si_m C_n (m, n = 1–4) clusters. *International Journal of Quantum Chemistry*, 113(7): 949–958, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lee:2017:CSV

[LKOS17] Jae Young Lee, Ahhyun Kim, Woo-Suk Oh, and Bonggeun Shong. Computational study on vapor phase coupling reaction between diiso(thio)cyanates with diamines, diols, and dithiols. *International Journal of Quantum Chemistry*, 117 (7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luo:2016:MIR

[LKZ+16] Lun Luo, Xiaohui Kang, Guangli Zhou, Si Chen, Gen Luo, Jingping Qu, and Yi Luo. Mechanistic insights into regioselective polymerization of 1,3-Dienes catalyzed by a bipyridine-ligated iron complex: a DFT study. *International Journal of Quantum Chemistry*, 116(17):1274–1280, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:ITI

[LL11] Da-Zhi Li and Si-Dian Li. An Ab initio theoretical investigation on the geometrical and electronic structures of $BAu_n^{-/0}$ (n = 1−−4) clusters. *International Journal of Quantum Chemistry*, 111(15):4418–4424, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2017:CSS

[LL17] Min-Hsien Liu and Chuan-Wen Liu. Comparative simulation study of chemical synthesis of energetic (R)-1,2,4-butanetriol trinitrate plasticizer. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2018:BRR

[LL18] Zhuo Zhe Li and An Yong Li. $B_4Rg_n^{2+}$ (Rg = He–Rn, n = 1–4): In quest of the potential trapping ability of the aromatic ring. *International Journal of Quantum Chemistry*, 118 (10):e25530:1–e25530:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lima:2019:CSM

[LL19] Adilmo F. Lima and Milan V. Lalic. Comparative study of magnetic and electronic properties of room-temperature polar magnets $ScFeO_3$ and $InFeO_3$. *International Journal of Quantum Chemistry*, 119(7):e25846:1–e25846:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:FPC

[lLBqD+19] Hai long Li, Liang Bian, Fa qin Dong, Mian xin Song, Wei min Li, Frank S. Riehle, Xiao qiang Jiang, Yan hui Lin, Cheng xia Wang, Yu Li, and Wei hui Luo. First-principles calculation of temperature-dependent electronic transitions mechanism in V or Nb substituted $BiFeO_3$. *International Journal of Quantum Chemistry*, 119(24):e26041:1–e26041:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lian:2011:TSS

[LLC+11] Peng Lian, Wei-Peng Lai, Hua-Qiang Cai, Shaojun Qiu, Bo-Zhou Wang, Jian Lv, and Yong-Qiang Xue. Theoretical study on the solvent effect of the nitrosyl cation (NO^+) generating reaction. *International Journal of Quantum Chemistry*, 111(14):3571–3577, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lao:2012:IWF

[LLF+12] Ka-Un Lao, Timm Lankau, Teng-I Fang, Jian-Wei Zou, and Chin-Hui Yu. Interstitial water and the formation of low barrier hydrogen bonds: a computational model study. *International Journal of Quantum Chemistry*, 112(5):1460–1472, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2017:MDD

[LLF17] Yan Li, Tingting Liu, and Wenwen Fu. Mechanisms of DABCO- and DMAP-catalyzed [2 + 4] cycloaddition reactions of methylallenoate with methyleneindolonone: a DFT study. *International Journal of Quantum Chemistry*, 117 (18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:CIB

[LLG+12] Qingzhong Li, Hui Li, Jianhui Gong, Wenzuo Li, and Jianbo Cheng. Competitive interaction between halogen and hydrogen bonds in NH_2Br — HOX (X = F, Cl, and Br) complex. *International Journal of Quantum Chemistry*, 112(11):2429–2434, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lin:2015:SSD

[LLH15] Yen-Chang Lin, Chih-Yuan Lin, and Yew Kam Ho. Spectral/structural data of helium atoms with exponential-cosine-screened Coulomb potentials. *International Journal of Quantum Chemistry*, 115(13):830–836, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2016:FPS

[LLL16] Rui Li, Haibo Li, and Jifeng Liu. First principles study of O_2 dissociation on Pt(111) surface: Stepwise mechanism. *International Journal of Quantum Chemistry*, 116(12):908–914, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2013:ISM

[LLLB13] Xiuhui Lu, Zhenxia Lian, Dongting Liu, and Weijie Bao. Ab initio study of the mechanism of forming a spiro-

heterocyclic ring compound involving Si and Ge from dichlorosilylene germylidene(Cl_2SiGe:) and formaldehyde. *International Journal of Quantum Chemistry*, 113(10): 1562–1567, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liang:2012:VRR

[LLLT12] C. Liang, J. W. Luo, R. F. Li, and N. H. Tu. A visual representation for RNA secondary structure and its application. *International Journal of Quantum Chemistry*, 112 (10):2243–2255, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ledyastuti:2013:CCR

[LLM13] Mia Ledyastuti, Yunfeng Liang, and Toshifumi Matsuoka. Computations of chemical reactions and dynamics: The first-principles molecular dynamics study of quartz–water interface. *International Journal of Quantum Chemistry*, 113(4):401–412, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2013:DSR

[LLP+13] Minjie Li, Weixia Liu, Chunrong Peng, Qinghua Ren, Wencong Lu, and Wei Deng. A DFT study on reaction of eupatilin with hydroxyl radical in solution. *International Journal of Quantum Chemistry*, 113(7):966–974, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lumb:2017:RSB

[LLP17] Sonia Lumb, Shalini Lumb, and Vinod Prasad. Rovibrational spectra of bounded diatomic molecules. *International Journal of Quantum Chemistry*, 117(6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lian:2011:DFT

[LLW+11] Peng Lian, Wei-Peng Lai, Bo-Zhou Wang, Zhong-Xue Ge, and Yong-Qiang Xue. A density functional theory study on diazotization and nitration of 3,5-diamino-1,2,4-triazole. *International Journal of Quantum Chemistry*, 111 (10):2332–2339, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Long:2012:TSI

[LLW+12] Bo Long, Zheng-Wen Long, Yi-Bo Wang, Wei-Jun Zhang, Chao-Yun Long, and Shui-Jie Qin. Theoretical study on HO_2-initiated atmospheric oxidation of halogenated carbonyls. *International Journal of Quantum Chemistry*, 112 (8):1926–1935, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2012:ESW

[LLZ+12] Yunxiang Lu, Haiying Li, Xiang Zhu, Honglai Liu, and Weiliang Zhu. Effects of solvent on weak halogen bonds: Density functional theory calculations. *International Journal of Quantum Chemistry*, 112(5):1421–1430, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2014:RDO

[LLZ+14] Haiying Liu, Genqin Li, Peng Zhao, Gang Chen, and Yuxiang Bu. Rational design of outer-expanded purine analogues as building blocks of DNA-based nanowires with enhanced electronic properties. *International Journal of Quantum Chemistry*, 114(14):911–919, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:UCH

[LLZaH14] Yushuang Li, Qian Liu, Xiaoqi Zheng, and Ping an He. UC-Curve: a highly compact 2D graphical representation of protein sequences. *International Journal of Quantum Chemistry*, 114(6):409–415, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2010:CTS

[LLZZ10] Peng Liu, Jianqiang Liu, Dongju Zhang, and Changqiao Zhang. A comparative theoretical study of the reactivities of the Al^+ and Cu^+ ions toward methylamine and dimethylamine. *International Journal of Quantum Chemistry*, 110 (9):1583–1593, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Limon:2019:SBI

[LMC19] Patricio Limon, Alan Miralrio, and Miguel Castro. Small binary iron-carbon clusters with persistent high magnetic moments. A theoretical characterization. *International Journal of Quantum Chemistry*, 119(14):e25932:1–e25932:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:TIC

[LMCZ11] Nan Lu, Shizhen Mi, Dezhan Chen, and Guiqiu Zhang. Theoretical investigation on chiral cinchona alkaloid salts-catalyzed asymmetric epoxidation of cyclic enones. *International Journal of Quantum Chemistry*, 111(12):2874–2881, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:TST

[LMZ+11] Xiaoyan Li, Lingpeng Meng, Yanli Zeng, Xueying Zhang, and Shijun Zheng. Theoretical study on two types of weak interactions between methylenecyclopropane and XY (X, Y = H, F, Cl, and Br). *International Journal of Quantum Chemistry*, 111(12):3070–3079, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liang:2015:RGT

[LMZY15] Wanzhen Liang, Huili Ma, Hang Zang, and Chuanxiang Ye. Reviews: Generalized time-dependent approaches to vibrationally resolved electronic and Raman spectra: Theory and applications. *International Journal of Quantum Chemistry*, 115(9):550–563, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:GPW

[LNGW14] Peng Li, Wenxia Niu, Tao Gao, and Hongyan Wang. Gas-phase water activation by Th atom: Reaction mechanisms and topological analysis. *International Journal of Quantum Chemistry*, 114(12):760–768, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lundberg:2012:DEH

[LNI12] Marcus Lundberg, Yoshio Nishimoto, and Stephan Irle. Delocalization errors in a hubbard-like model: Consequences

for density-functional tight-binding calculations of molecular systems. *International Journal of Quantum Chemistry*, 112(6):1701–1711, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Levamaki:2018:KLR

[LNV+18] Henrik Levämäki, Ágnes Nagy, Iiro Vilja, Kalevi Kokko, and Levente Vitos. Kullback–Leibler and relative Fisher information as descriptors of locality. *International Journal of Quantum Chemistry*, 118(12):e25557:1–e25557:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lakehal:2013:TIY

[LOHB13] Salima Lakehal, Nadia Ouddai, Douniazed Hannachi, and Mohmed Bououdina. Theoretical investigation of ytterbium trichelates compounds. *International Journal of Quantum Chemistry*, 113(10):1447–1452, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

List:2012:PPX

[LORR+12] Nanna Holmgaard List, Jógvan Magnus Olsen, Tomás Rocha-Rinza, Ove Christiansen, and Jacob Kongsted. Performance of popular XC-functionals for the description of excitation energies in GFP-like chromophore models. *International Journal of Quantum Chemistry*, 112(3):789–800, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lagana:2010:I

[LP10a] Antonio Laganà and Antonino Polimeno. Introduction. *International Journal of Quantum Chemistry*, 110(2):277, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2010:MCC

[LP10b] Xiangzhu Li and Josef Paldus. Multireference coupled-cluster methods for ground and low-lying excited states. A benchmark illustration on CH^+ potentials. *International Journal of Quantum Chemistry*, 110(15):2734–2743, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:TPH

[LPG+12] Wen-Zuo Li, Yu-Wei Pei, F.-F. Geng, Jian-Bo Cheng, Qing-Zhong Li, and Bao-An Gong. Theoretical prediction on $HAlS^+$ and $HSAl^+$ cations using multiconfiguration second-order perturbation theory. *International Journal of Quantum Chemistry*, 112(12):2499–2503, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lombardi:2011:SOC

[LPM+11] A. Lombardi, F. Palazzetti, G. S. Maciel, V. Aquilanti, and M. B. Sevryuk. Simulation of oriented collision dynamics of simple chiral molecules. *International Journal of Quantum Chemistry*, 111(7–8):1651–1658, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

LeBahers:2012:PAG

[LPO+12] Tangui Le Bahers, Thierry Pauporté, Fabrice Odobel, Frédéric Labat, and Ilaria Ciofini. Promising anchoring groups for ZnO-based hybrid materials: a periodic density functional theory investigation. *International Journal of Quantum Chemistry*, 112(9):2062–2071, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lenz:2012:CSC

[LPOP12] Annika Lenz, Anna Pohl, Lars Ojamäe, and Petter Persson. Computational study of the catalytic effect of platinum on the decomposition of DNT. *International Journal of Quantum Chemistry*, 112(7):1852–1858, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2013:BNB

[LQ13] Haichen Li and Yuanyuan Qiao. Bimolecular nature of boron trifluoride catalyzed glycosylation of a galactosyl donor: the role of the acceptor. *International Journal of Quantum Chemistry*, 113(16):1975–1980, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:TUS

[LQZZ12] Yushuang Li, Yufang Qin, Xiaoqi Zheng, and Yu Zhang. Three-unit semicircles curve: a compact 3D graphical representation of DNA sequences based on classifications of nucleotides. *International Journal of Quantum Chemistry*, 112(10):2330–2335, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lajoie:2010:OPA

[LRKM10] Travis W. Lajoie, Jessica J. Ramirez, Dmitri S. Kilin, and David A. Micha. Optical properties of amorphous and crystalline silicon surfaces functionalized with Ag_n adsorbates. *International Journal of Quantum Chemistry*, 110 (15):3005–3014, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Rosa:2019:EPE

[LRMAA19] Sheila López-Rosa, Adrián L. Martín, Juan Antolín, and Juan Carlos Angulo. Electron-pair entropic and complexity measures in atomic systems. *International Journal of Quantum Chemistry*, 119(7):e25861:1–e25861:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lattelais:2011:SGI

[LRP+11] M. Lattelais, O. Risset, J. Pilme, F. Pauzat, Y. Ellinger, F. Sirotti, M. Silly, Ph. Parent, and C. Laffon. The survival of glycine in interstellar ices: a coupled investigation using NEXAFS experiments and theoretical calculations. *International Journal of Quantum Chemistry*, 111(6):1163–1171, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laguna:2017:ITM

[LS17] Humberto G. Laguna and Robin P. Sagar. Information theoretical measures from cumulative and survival densities in quantum systems. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:IPS

[LS19] Xin Li and Wanling Shen. The influence of pore structure on reaction mechanism of propylene dimerization in zeolite: a theoretical viewpoint. *International Journal of Quantum Chemistry*, 119(16):e25962:1–e25962:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ludena:2018:LPP

[LSC+18] Eduardo V. Ludeña, Edison X. Salazar, Mauricio H. Cornejo, Darío E. Arroyo, and Valentin V. Karasiev. The Liu–Parr power series expansion of the Pauli kinetic energy functional with the incorporation of shell-inducing traits: Atoms. *International Journal of Quantum Chemistry*, 118 (15):e25601:1–e25601:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lopez-Sosa:2019:NCD

[LSCMSFC19] Luis López-Sosa, Heriberto Cruz-Martínez, Omar Solorza-Feria, and Patrizia Calaminici. Nickel and copper doped palladium clusters from a first-principles perspective. *International Journal of Quantum Chemistry*, 119(22): e26013:1–e26013:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2014:BSR

[LSG+14] Shi Liu, Sriraj Srinivasan, Michael C. Grady, Masoud Soroush, and Andrew M. Rappe. Backbiting and β-scission reactions in free-radical polymerization of methyl acrylate. *International Journal of Quantum Chemistry*, 114(5):345–360, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2019:EGP

[LSKM19] Fang Liu, David M. Sanchez, Heather J. Kulik, and Todd J. Martínez. Exploiting graphical processing units to enable quantum chemistry calculation of large solvated molecules with conductor-like polarizable continuum models. *International Journal of Quantum Chemistry*, 119(1):e25760:1–e25760:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lei:2008:IET

[LSL+08] Yibo Lei, Bingbing Suo, Anyang Li, Yusheng Dou, Yubin Wang, and Zhenyi Wen. Involvement of excited triplet state in the photodissociation of cyclobutane. *International Journal of Quantum Chemistry*, 108(4):788–796, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2016:TRU

[LSP+16] Li Li, John C. Snyder, Isabelle M. Pelaschier, Jessica Huang, Uma-Naresh Niranjan, Paul Duncan, Matthias Rupp, Klaus-Robert Müller, and Kieron Burke. Tutorial reviews: Understanding machine-learned density functionals. *International Journal of Quantum Chemistry*, 116(11): 819–833, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

LaPorta:2010:RFO

[LSR+10a] Felipe A. La Porta, Regis T. Santiago, Teodorico C. Ramalho, Matheus P. Freitas, and Elaine F. F. Da Cunha. The role of the Frontier orbitals in acid–base chemistry of organic amines probed by ab initio and chemometric techniques. *International Journal of Quantum Chemistry*, 110 (11):2015–2023, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [LSR+11].

Lee:2010:DFE

[LSR10b] Jung-Goo Lee, Celeste Sagui, and Christopher Roland. Dimerization free energy of vancomycin-group antibiotics and the cooperative effect: a density functional approach. *International Journal of Quantum Chemistry*, 110(15): 2894–2902, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

LaPorta:2011:ERF

[LSR+11] Felipe A. La Porta, Regis T. Santiago, Teodorico C. Ramalho, Matheus P. Freitas, and Elaine F. F. Da Cunha. Erratum: The role of the frontier orbitals in acid–base chemistry of organic amines probed by ab initio and chemometric techniques. *International Journal of Quantum Chemistry*, 111(15):4505, December 2011. CODEN

IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [LSR+10a].

Li:2013:CBB

[LSR+13] Xichen Li, Eduardo M. Sproviero, Ulf Ryde, Victor S. Batista, and Guangju Chen. Computational biochemistry and biophysics: Theoretical EXAFS studies of a model of the oxygen-evolving complex of photosystem II obtained with the quantum cluster approach. *International Journal of Quantum Chemistry*, 113(4):474–478, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Laguna:2019:EKL

[LSS19] Humberto G. Laguna, Saúl J. C. Salazar, and Robin P. Sagar. Entropic Kullback–Leibler type distance measures for quantum distributions. *International Journal of Quantum Chemistry*, 119(19):e25984:1–e25984:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:MDK

[LSW19] Shuchao Li, Wanting Sun, and Shujing Wang. Multiplicative degree-Kirchhoff index and number of spanning trees of a zigzag polyhex nanotube TUHC$[2n, 2]$. *International Journal of Quantum Chemistry*, 119(17):e25969:1–e25969:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leite:2010:SNA

[LTdSJ+10] Franco Henrique A. Leite, Alex G. Taranto, Manoelito C. dos Santos Junior, Alexsandro Branco, Martha T. de Araujo, and José Walkimar de M. Carneiro. Search for new antimalarial compounds obtained from natural sources by molecular modeling. *International Journal of Quantum Chemistry*, 110(11):2057–2066, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2018:MSG

[LTL18] Yan Li, Ruixue Tian, and Changhai Liang. Mechanistic study on gold(I)-catalyzed crosscoupling of diazo compounds: a DFT study. *International Journal of Quantum*

Chemistry, 118(14):e25581:1–e25581:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2010:TSE

[Lu10] Shen-Zhuang Lu. Theoretical study of electron transfer in uranyl(VI)–uranyl(V) complexes in solution. *International Journal of Quantum Chemistry*, 110(9):1756–1763, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2015:CBI

[Lu15] Lilin Lu. Can B3LYP be improved by optimization of the proportions of exchange and correlation functionals? *International Journal of Quantum Chemistry*, 115(8):502–509, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lungu:2013:LER

[Lun13a] Radu P. Lungu. Letters to the Editor: Reply on "Comment on 'Statistical physics of a mesoscopic fermion system inside a rectangular box'". *International Journal of Quantum Chemistry*, 113(8):1244, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Lun13b, Tou13].

Lungu:2013:SPM

[Lun13b] Radu P. Lungu. Statistical physics of a mesoscopic fermion system inside a rectangular box. *International Journal of Quantum Chemistry*, 113(8):1234–1242, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comments [Tou13, Lun13a].

Luzanov:2008:MCR

[Luz08] Anatoliy V. Luzanov. Matrix-covariant representation of high-order configuration interaction and coupled cluster theories. *International Journal of Quantum Chemistry*, 108 (4):671–695, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2011:SFQ

[Luz11a] A. V. Luzanov. Spin-free quantum chemistry: What one can gain from Fock's cyclic symmetry. *International Jour-*

nal of Quantum Chemistry, 111(15):4042–4066, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2011:QFA

[Luz11b] Anatoliy V. Luzanov. Quantum fidelity for analyzing atoms and fragments in molecule: Application to similarity, chirality, and aromaticity. *International Journal of Quantum Chemistry*, 111(10):2196–2220, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2012:SSS

[Luz12] A. V. Luzanov. Some spin and spin-free aspects of Coulomb correlation in molecules. *International Journal of Quantum Chemistry*, 112(17):2915–2923, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2013:NRM

[Luz13] Anatoliy V. Luzanov. Nonstationarity and related measures for time-dependent Hartree–Fock and multiconfigurational models. *International Journal of Quantum Chemistry*, 113(23):2489–2505, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:AIB

[LV12] Yong Q. Li and António J. C. Varandas. Accurate ab initio-based double many-body expansion adiabatic potential energy surface for the 2^2 A′ state of NH_2 by extrapolation to the complete basis set limit. *International Journal of Quantum Chemistry*, 112(17):2932–2939, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Levine:2016:ESI

[LV16] Benjamin G. Levine and Sergey A. Varganov. Editorial: Special issue on excited states in complex systems. *International Journal of Quantum Chemistry*, 116(10):737–738, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lata:2019:ERQ

[LV19] Suman Lata and Vikas. Exploring the role of quantum-mechanical descriptors in the concentration-dependent adsorption of aromatic organic compounds by multiwalled carbon nanotubes. *International Journal of Quantum Chemistry*, 119(5):e25825:1–e25825:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Leitao:2014:EPL

[LVdSdM14] Ezequiel F. V. Leitão, Elizete Ventura, Otávio L. de Santana, and Silmar A. do Monte. Electronic properties of the low-lying spin states of dimethylnitrosamine coordinated to Fe(III) heme models: an ab initio study. *International Journal of Quantum Chemistry*, 114(8):508–520, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lories:2012:DII

[LVP12a] Xavier Lories, Jacques Vandooren, and Daniel Peeters. Definition of an isodesmicity index from G3B3 energy components. *International Journal of Quantum Chemistry*, 112 (2):540–550, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lories:2012:IDR

[LVP12b] Xavier Lories, Jacques Vandooren, and Daniel Peeters. Isomerization of dehydrofulvene radicals to the phenyl radical, and application to the growth of polycyclic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 112(8):1959–1967, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:DFT

[LW11] Zhi-Ming Li and Quan-Rui Wang. A density functional theory study on the Diels–Alder reactions with vinylallenes as dienes. *International Journal of Quantum Chemistry*, 111(14):3805–3815, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2013:TSE

[LW13] Nan Lu and Huatian Wang. Theoretical study of enantiomeric and geometric control in chiral guanidine-catalyzed asymmetric 1,4-addition of 5H-oxazol-4-ones. *International Journal of Quantum Chemistry*, 113(20):2267–2276, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2015:TIP

[LW15] Nan Lu and Huatian Wang. A theoretical investigation on palladium-catalyzed one-pot coupling of aryl iodides, alkynes, and amines through C N bond cleavage for the synthesis of indole derivatives. *International Journal of Quantum Chemistry*, 115(6):361–368, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2018:OAS

[LW18] Nannan Liu and Jian Wang. Odd aromatic Si_4 ring stabilized by V — V bond passing through it: May π-bonding form without σ-bonding as precondition? *International Journal of Quantum Chemistry*, 118(24):e25788:1–e25788:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2010:TSM

[LWC+10] Xiu Hui Lu, Wei Rong Wu, Xin Che, Jun Feng Han, and Le Yi Shi. Theoretical study of mechanism of cycloaddition reaction between dimethylmethylene carbene and formaldehyde. *International Journal of Quantum Chemistry*, 110(6):1273–1278, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lozano:2012:TMA

[LWH+12] N. B. H. Lozano, K. C. Weber, K. M. Honorio, R. V. C. Guido, A. D. Andricopulo, and A. B. F. Da Silva. Theoretical models for the antitrypanosomal activity of thiosemicarbazone derivatives. *International Journal of Quantum Chemistry*, 112(20):3364–3370, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2010:TSG

[LWJL10] Anjie Liu, Dongling Wu, Dianzeng Jia, and Lang Liu. Theoretical studies on geometry, solvent effect, and photochromic mechanism of two bis-heterocyclic compounds containing pyrazolone ring. *International Journal of Quantum Chemistry*, 110(7):1360–1367, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:DFT

[LWL+12] Haibin Li, Shuixing Wu, Yi Liao, Zhongmin Su, Yuhe Kan, and Xueling Tang. Density functional theory studies on structures and absorption spectra of $[Au(tpy)Cl]^{2+}$ and its derivatives: Role of basis set, functional, solvent effect, and spin orbit effect. *International Journal of Quantum Chemistry*, 112(6):1642–1653, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:SBR

[LWL19] Zhuo Zhe Li, Mei Wen, and An Yong Li. Stability and bonding in rare gas inserted interhalogens $FRgXF_n$ (X = Br and I, n = 0 and 2). *International Journal of Quantum Chemistry*, 119(15):e25940:1–e25940:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2013:ICE

[LWWZ13] Dan Li, Yuliang Wang, Jun Wang, and Yingtao Zhao. Influence of collision energy and reagent vibrational excitation on the dynamics of the reaction H + LiH. *International Journal of Quantum Chemistry*, 113(21):2379–2384, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:DFS

[LWX+14] Qingzheng Li, Houyuan Wang, Haiping Xia, Shihao Wei, and Jianhui Yang. Density functional study of hydrogen adsorption and diffusion on Ni-loaded graphene and graphene oxide. *International Journal of Quantum Chemistry*, 114 (13):879–884, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2013:RRT

[LWY13] Chun Li, Liming Wang, and Zong-Chao Yan. Recursion relations for the three-electron subsidiary integral $W(l, m, n; \alpha, \beta, \gamma)$. *International Journal of Quantum Chemistry*, 113(9):1307–1315, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:NLM

[LWY19] Shuchao Li, Wei Wei, and Shiqun Yu. On normalized Laplacians, multiplicative degree-Kirchhoff indices, and spanning trees of the linear [n]phenylenes and their dicyclobutadieno derivatives. *International Journal of Quantum Chemistry*, 119(8):e25863:1–e25863:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2014:TSC

[LWZ+14] Wenfang Liu, Bingqiang Wang, Caiyun Zhang, Xiaofen Yin, and Jian Zhang. Theoretical study on a chemosensor for fluoride anion-based on a urea derivative. *International Journal of Quantum Chemistry*, 114(2):138–144, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2013:ISC

[LXD13] Nan-Nan Liu, Jing Xu, and Yi-Hong Ding. Inverse sandwich complexes based on low-valent group 13 elements and cyclobutadiene: a theoretical investigation on E-C_4H_4 - E (E = Al, Ga, In, Tl). *International Journal of Quantum Chemistry*, 113(7):1018–1025, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:TSMd

[LXLL11] Xiu Hui Lu, Ping Ping Xiang, Zhen Xia Lian, and Yong Qing Li. Theoretical study of mechanism of cycloaddition reaction between dimethyl-silylene carbene [$(CH_3)_2Si{=}{=}C$:] and formaldehyde. *International Journal of Quantum Chemistry*, 111(14):3664–3672, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2012:TSS

[LXW+12] Liuxia Liu, Ying Xue, Xin Wang, Xiang Chu, and Mingli Yang. Theoretical study of static (Hyper)polarizabilities of twisted intramolecular charge transfer chromophores. *International Journal of Quantum Chemistry*, 112(4):1086–1096, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2014:TIA

[LXW+14] Qiang Li, Sheng-Xian Xu, Jing-Lan Wang, Hong-Ying Xia, Feng Zhao, and Yi-Bo Wang. Theoretical insights into the absorption and emission properties of blue luminescent copper(I) complexes based on the pyrazolyl–pyridine ligands. *International Journal of Quantum Chemistry*, 114 (24):1685–1691, December 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lyakh:2014:SAT

[Lya14] Dmitry I. Lyakh. Scale-adaptive tensor algebra for local many-body methods of electronic structure theory. *International Journal of Quantum Chemistry*, 114(23):1607–1618, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lyakh:2019:DSV

[Lya19] Dmitry I. Lyakh. Domain-specific virtual processors as a portable programming and execution model for parallel computational workloads on modern heterogeneous high-performance computing architectures. *International Journal of Quantum Chemistry*, 119(12):e25926:1–e25926:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2018:TAC

[LYD+18] Feifei Lu, Lihua Yang, Yaru Dang, Qingzhong Li, and Xiaoyan Li. Theoretical assessing on the coordination mode and bonding in heteronuclear group-13 dimetallocene. *International Journal of Quantum Chemistry*, 118 (3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2012:SON

[LYL+12] Yan Liu, Guo-Chun Yang, Chun-Guang Liu, Shi-Ling Sun, and Yong-Qing Qiu. Second-order nonlinear optical responses switching of N∧N∧N ruthenium carboxylate complexes with proton-electron transfer. *International Journal of Quantum Chemistry*, 112(3):779–788, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2017:CBS

[LYR+17] Xiaojun Li, Xiaohui Yang, Hongjiang Ren, Ping Sun, and Zhenhua Fang. The chemical bonding and spectral assignments of rhodium(III)-catalyzed closo-dodecaborate complexes: Ab initio study. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:DPR

[LYS+19] Ming-Yang Li, Hang Yin, Ming-Yue Sui, Fei Wang, Yan-Hui Liu, and Guang-Yan Sun. In-depth probe of researching interfacial charge transfer process for organic solar cells: a promising bisadduct fullerene derivatives acceptor. *International Journal of Quantum Chemistry*, 119(15): e25938:1–e25938:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:SOS

[LYW11] Wei Li, Feng Yang, and Zhengdong Wang. Structure and optical spectra of bis(pyrrol-2-ylmethyleneamine) complexes: A DFT and TDDFT study of the self-assembly complexes of bis(pyrrol-2-ylmethyleneamine) ligands linked by alkyl spacers with Cu(II). *International Journal of Quantum Chemistry*, 111(9):2099–2108, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2019:RMP

[LYW+19] Ying Li, Le Yang, Zhan Wei, Qinghua Hou, Lanlan Li, and Peng Jin. Robust metal-pentagon interactions in the Th-based endohedral metallofullerenes revealed by DFT calculations. *International Journal of Quantum Chemistry*, 119

(6):e25826:1–e25826:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Luzanov:2010:EIE

[LZ10] A. V. Luzanov and O. A. Zhikol. Electron invariants and excited state structural analysis for electronic transitions within CIS, RPA, and TDDFT models. *International Journal of Quantum Chemistry*, 110(4):902–924, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lei:2012:BEA

[LZ12] Hong-Wen Lei and Hong Zhang. Boundary effect on the adsorption properties of H_2 on charged MgC_aH_b complex. *International Journal of Quantum Chemistry*, 112(2):566–574, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2010:TSI

[LZB10] Da-Zhi Li, Shi-Guo Zhang, and He Bian. Theoretical study of the inhibitive properties of a group of benzimidazoles. *International Journal of Quantum Chemistry*, 110(9):1772–1777, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lu:2011:NMS

[LZD+11] Junming Lu, Bo Zhang, Qingming Deng, Jinan Wang, Yunxiang Lu, and Weiliang Zhu. The nature and magnitude of specific halogen bonds between iodoperfluorobenzene and heterocyclic systems. *International Journal of Quantum Chemistry*, 111(10):2352–2358, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2013:CAA

[LZFZ13] Wenliang Li, Hongsheng Zhai, Yan Feng, and JuanJuan Zhao. A comparison of attack angle dependence of exchange channel of reaction H + HS ($v = 0, 1$; $j = 0$) on $3A''$ and $3A'$ surfaces. *International Journal of Quantum Chemistry*, 113(24):2629–2633, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2015:SNO

[LZW+15] Weiqi Li, Xin Zhou, Qiang Wang, Zhuang Xiong, and Wei Quan Tian. Structural, nonlinear optical, and vibration properties of the $C_{40}H_{10}$ buckybowl modified with nitrogen atoms. *International Journal of Quantum Chemistry*, 115(21):1553–1560, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2018:DSR

[LZW+18] Zhenhua Li, Kan Zhang, Weihan Wang, Baowei Wang, and Xinbin Ma. DFT study into the reaction mechanism of CO methanation over pure MoS_2. *International Journal of Quantum Chemistry*, 118(16):e25643:1–e25643:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2011:NSE

[LZZ+11] Zhi-Feng Li, Yuan-Cheng Zhu, Guo-Fang Zuo, Hui-An Tang, and Hong-Yü Li. A novel single-electron sodium bond system of $H_3C\cdots NaY$ (Y = H, OH, F, CCH, CN, and NC). *International Journal of Quantum Chemistry*, 111(3):570–577, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Li:2012:QCM

[LZZ12] Xue Li, Qing-Chuan Zheng, and Hong-Xing Zhang. Quantum chemical modeling of 1,1-proton transfer reaction catalyzed by a cofactor-independent α-methylacyl-CoA racemase. *International Journal of Quantum Chemistry*, 112 (2):619–624, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Lin:2013:IIT

[LZZ+13] He Lin, Shun-Guan Zhu, Lin Zhang, Xin-Hua Peng, Peng-Yuan Chen, and Hong-Zhen Li. Intermolecular interactions, thermodynamic properties, crystal structure, and detonation performance of HMX/NTO cocrystal explosive. *International Journal of Quantum Chemistry*, 113 (10):1591–1599, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2017:TIS

[LZZ+17] Xian-He Liu, Zeng-Xia Zhao, Wei Zhang, Ting-Ting Yin, and Hong-Xing Zhang. Theoretical investigation on the spectroscopic properties of furylfulgide with different substituents and design of novel bis-furylfulgimide photochromes. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Liu:2019:NST

[LZZ19] Jia-Bao Liu, Jing Zhao, and Zhongxun Zhu. On the number of spanning trees and normalized Laplacian of linear octagonal-quadrilateral networks. *International Journal of Quantum Chemistry*, 119(17):e25971:1–e25971:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mattsson:2010:SFS

[MA10] Ann E. Mattsson and Rickard Armiento. The subsystem functional scheme: The Armiento-Mattsson 2005 (AM05) functional and beyond. *International Journal of Quantum Chemistry*, 110(12):2274–2282, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohajeri:2011:OES

[MA11a] Afshan Mohajeri and Mojtaba Alipour. On the optical, electronic, and structural properties of zinc sulfide nanoclusters. *International Journal of Quantum Chemistry*, 111(14):3841–3850, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohajeri:2011:ZSN

[MA11b] Afshan Mohajeri and Mojtaba Alipour. Zinc selenide nanoclusters: Static dipole polarizability and electronic properties. *International Journal of Quantum Chemistry*, 111 (14):3888–3896, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matamala:2012:SMC

[MA12] Adelio R. Matamala and Alejandro A. Alarcón. A simple model for the calculation of HOMO and LUMO energy

levels of benzocatafusenes. *International Journal of Quantum Chemistry*, 112(5):1316–1322, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2014:HSK

[Ma14] Haibo Ma. Hydration structure of Na^+, K^+, F^-, and Cl^- in ambient and supercritical water: a quantum mechanics/ molecular mechanics study. *International Journal of Quantum Chemistry*, 114(15):1006–1011, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Magliano:2012:MDS

[MAD12] A. Magliano, M. Anselmi, and A. Di Nola. Molecular dynamics study of aggregation of amyloidogenic peptides in explicit water. *International Journal of Quantum Chemistry*, 112(7):1844–1851, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mironov:2019:MPE

[MAF19] Vladimir Mironov, Yuri Alexeev, and Dmitri G. Fedorov. Multithreaded parallelization of the energy and analytic gradient in the fragment molecular orbital method. *International Journal of Quantum Chemistry*, 119(12): e25937:1–e25937:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Magnani:2014:PSM

[Mag14] Nicola Magnani. Perspective: Spectroscopic and magnetic investigations of actinide-based nanomagnets. *International Journal of Quantum Chemistry*, 114(12):755–759, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maiti:2014:RAM

[Mai14] Amitesh Maiti. Review: Atomistic modeling toward high-efficiency carbon capture: a brief survey with a few illustrative examples. *International Journal of Quantum Chemistry*, 114(3):163–175, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Makri:2015:PQC

[Mak15] Nancy Makri. Perspectives: Quantum-classical path integral: a rigorous approach to condensed phase dynamics. *International Journal of Quantum Chemistry*, 115(18): 1209–1214, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mamedov:2013:UAT

[Mam13] B. A. Mamedov. Unified analytical treatment for calculation of the two-dimensional Franck–Condon factors using the Duschinsky transformation. *International Journal of Quantum Chemistry*, 113(9):1372–1375, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mamedov:2014:IGP

[Mam14] Bahtiyar A. Mamedov. Israfil I. Guseinov: a pioneer of the quantum theory of atomic, molecular, and nuclear systems*. *International Journal of Quantum Chemistry*, 114 (5):361–366, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Musavi:2015:RTN

[MAN15] Seyed Majid Musavi, Javad Amani, and Parva Noruzi. Reaching for two new stable ambiphilic quinoline-derived N-heterocyclic carbenes at DFT level. *International Journal of Quantum Chemistry*, 115(4):224–230, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mandelshtam:2016:LEC

[Man16] Vladimir A. Mandelshtam. Letters to the Editor: Comment on "Benchmarking compressed sensing, super-resolution, and filter diagonalization" (Int. J. Quantum Chem. 2016, **116**, 1097). *International Journal of Quantum Chemistry*, 116(23):1814–1817, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [MBSAG16a, MBSAG16b].

Manzoor:2017:CSO

[MANP17] Taniya Manzoor, Summera Asmi, Saba Niaz, and Altaf Hussain Pandith. Computational studies on opto-

electronic and charge transfer properties of some perylene-based donor-π-acceptor systems for dye sensitized solar cell applications. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meneses:2010:TSR

[MAP+10] Lorena Meneses, Andrea Araya, Fernanda Pilaquinga, Michelle Espín, Pamela Carrillo, and Freddy Sánchez. Theoretical studies of reactivity and selectivity in some organic reactions. *International Journal of Quantum Chemistry*, 110(13):2360–2370, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morcillo:2018:IPH

[MAPS18] Milagros F. Morcillo, José M. Alcaraz-Pelegrina, and Antonio Sarsa. Ionization probability of the hydrogen atom suddenly released from confinement. *International Journal of Quantum Chemistry*, 118(12):e25563:1–e25563:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maroulis:2011:BLD

[Mar11] George Maroulis. Bond length dependence of the polarizability and hyperpolarizability of boron hydride. *International Journal of Quantum Chemistry*, 111(4):807–818, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maroulis:2012:QPC

[Mar12] George Maroulis. Quantifying the performance of conventional DFT methods on a class of difficult problems: The interaction (hyper)polarizability of two water molecules as a test case. *International Journal of Quantum Chemistry*, 112(9):2231–2241, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martens:2013:CFM

[Mar13] Craig C. Martens. Concepts and fundamental methods in molecular simulations: Coherent quantum processes in thermal and nonequilibrium environments. *International Journal of Quantum Chemistry*, 113(3):316–325, February

5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Masunov:2010:TSC

[Mas10] Artëm E. Masunov. Theoretical spectroscopy of carbocyanine dyes made accurate by frozen density correction to excitation energies obtained by TD–DFT. *International Journal of Quantum Chemistry*, 110(15):3095–3100, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Massa:2011:BR

[Mas11] Lou Massa. Book Review. *International Journal of Quantum Chemistry*, 111(12):3251, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Masiello:2014:PMT

[Mas14] David J. Masiello. Perspective: Multiscale theory and simulation of plasmon-enhanced molecular optical processes. *International Journal of Quantum Chemistry*, 114(21): 1413–1420, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mathar:2002:MCT

[Mat02] Richard J. Mathar. Mutual conversion of three flavors of Gaussian type orbitals. *International Journal of Quantum Chemistry*, 90(1):227–243, ???? 2002. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Mat10].

Mathar:2010:EMC

[Mat10] Richard J. Mathar. Erratum: Mutual conversion of three flavors of Gaussian type orbitals. *International Journal of Quantum Chemistry*, 110(4):962, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Mat02].

Mammino:2019:DMP

[MAT19] Liliana Mammino and Luis Alvarez-Thon. Different mutual positions of double bonds in open carbon chains and corresponding information from magnetically induced current densities. *International Journal of Quantum Chemistry*,

119(18):e25941:1–e25941:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Momen:2018:RWI

[MAW+18] Roya Momen, Alireza Azizi, Lingling Wang, Ping Yang, Tianlv Xu, Steven R. Kirk, Wenxuan Li, Sergei Manzhos, and Samantha Jenkins. The role of weak interactions in characterizing peptide folding preferences using a QTAIM interpretation of the Ramachandran plot $(\varphi - \psi)$. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mayer:2014:PEA

[May14] István Mayer. Perspectives: Effective atomic orbitals: a tool for understanding electronic structure of molecules. *International Journal of Quantum Chemistry*, 114(16):1041–1047, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukherjee:2012:RRM

[MB12] Neetik Mukherjee and Kamal Bhattacharyya. Rayleigh–Ritz method for excited quantum states via nonlinear variations without constraints: Role of supersymmetry. *International Journal of Quantum Chemistry*, 112(4):960–971, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales-Bayuelo:2013:UER

[MB13] Alejandro Morales-Bayuelo. Understanding the electronic reorganization in the thermal isomerization reaction of trans-3,4-dimethylcyclobutene. Origins of outward pseudodiradical $2n + 2\pi$ torquoselectivity. *International Journal of Quantum Chemistry*, 113(10):1534–1543, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marquez:2014:SVI

[MB14] Maria Belén Márquez and Silvia Antonia Brandán. A structural and vibrational investigation on the antiviral deoxyribonucleoside thymidine agent in gas and aqueous solution phases. *International Journal of Quantum Chemistry*, 114

(3):209–221, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohajeri:2015:INI

[MB15] Afshan Mohajeri and Nafiseh Bitaab. Investigating the nature of intermolecular and intramolecular bonds in noble gas containing molecules. *International Journal of Quantum Chemistry*, 115(3):165–171, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Messaoudi:2013:ERT

[MBA+13] Sabri Messaoudi, Bechir Bejaoui, Fourat Akrout, Malika Bel Hassen, and Cherif Sammari. Exploration of the reactivity of N_2O_5 with two $Si(OH)_4$ monomers using electronic structure methods. *International Journal of Quantum Chemistry*, 113(11):1633–1640, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mostafa:2019:DGR

[MBA+19] Rola Mostafa, Éric Brémond, Carlo Adamo, Ilaria Ciofini, Christophe Morell, and Henry Chermette. Does the gradient-regulated connection improve the description of correlated metal bond properties? *International Journal of Quantum Chemistry*, 119(6):e25831:1–e25831:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales-Bayuelo:2012:TSC

[MBBT+12] Alejandro Morales-Bayuelo, Rosa Baldiris, Juan Torres, Juan E. Torres, and Ricardo Vivas-Reyes. Theoretical study of the chemical reactivity and molecular quantum similarity in a series of derivatives of 2-adamantylthiazolidine-4-one using density functional theory and the topo-geometrical superposition approach. *International Journal of Quantum Chemistry*, 112(14):2681–2687, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Majid:2019:FPS

[MBKH19] Abdul Majid, Amber Batool, Salah Ud-Din Khan, and Sajjad Haider. First-principles study of vibrational properties of $TiSiO_4$ clusters. *International Journal of Quantum*

Chemistry, 119(14):e25924:1–e25924:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muchova:2018:MDM

[MBS+18] Eva Muchová, Michal Bezek, Jirí Suchan, Radek Cibulka, and Petr Slavícek. Molecular dynamics and metadynamics simulations of [2 + 2] photocycloaddition. *International Journal of Quantum Chemistry*, 118(10):e25534:1–e25534:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Markovich:2016:BCS

[MBSAG16a] Thomas Markovich, Samuel M. Blau, Jacob N. Sanders, and Alán Aspuru-Guzik. Benchmarking compressed sensing, super-resolution, and filter diagonalization. *International Journal of Quantum Chemistry*, 116(14):1097–1106, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [Man16] and response [MBSAG16b].

Markovich:2016:LER

[MBSAG16b] Thomas Markovich, Samuel M. Blau, Jacob N. Sanders, and Alán Aspuru-Guzik. Letters to the Editor: Response to: "Comment on benchmarking compressed sensing, super-resolution, and filter diagonalization". *International Journal of Quantum Chemistry*, 116(23):1818–1821, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Man16, MBSAG16a].

Morales-Bayuelo:2018:ATS

[MBSMJC18] Alejandro Morales-Bayuelo, Jesús Sánchez-Márquez, Gourhari Jana, and Pratim Kumar Chattaraj. Analyzing torquoselectivity in a series of unusual ring-opening reactions through bond reactivity indices and the adaptive natural density partitioning method. *International Journal of Quantum Chemistry*, 118(23):e25778:1–e25778:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morales-Bayuelo:2012:QMS

[MBTVR12] Alejandro Morales-Bayuelo, Juan Torres, and Ricardo Vivas-Reyes. Quantum molecular similarity analysis and

quantitative definition of catecholamines with respect to biogenic monoamines associated: Scale alpha and beta of quantitative convergence. *International Journal of Quantum Chemistry*, 112(14):2637–2642, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maciel:2011:IQC

[MC11a] Bruna C. M. Maciel and Puspitapallab Chaudhuri. An ab initio quantum chemical characterization of structure and vibrational spectra of anthranilic acid. *International Journal of Quantum Chemistry*, 111(7–8):1709–1718, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marmorino:2011:BEE

[MC11b] M. G. Marmorino and Kayleigh Cassella. Bounds to electronic expectation values for atomic and molecular systems. *International Journal of Quantum Chemistry*, 111 (14):3588–3596, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendez:2012:SBB

[MC12] Mariano Méndez and Andrés Cedillo. Stability and bonding in the borane–H_2 complexes. *International Journal of Quantum Chemistry*, 112(22):3564–3569, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazumdar:2014:RCP

[MC14] Sumitendra Mazumdar and Rudolf Torsten Clay. Review: The chemical physics of unconventional superconductivity. *International Journal of Quantum Chemistry*, 114(16): 1053–1059, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mangondo:2017:ORS

[MC17] Paidamwoyo Mangondo and Ignacy Cukrowski. On the origin of the relative stability of Zn^{II} NTA and Zn^{II} NTPA metal complexes. An insight from the IQA, IQF, and π-FARMS methods. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Munoz-Castro:2018:FHR

[MC18a] Alvaro Muñoz-Castro. Fulfilling the $2(N+1)^2$ Hirsch rule in smaller hollow fullerenes. Evaluation of long-range magnetic behavior and NMR patterns of C_{28}, C_{28}^{4-}, C_{24} N_4, and $C_{28}H_4$. *International Journal of Quantum Chemistry*, 118(19):e25645:1–e25645:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Munoz-Castro:2018:SMU

[MC18b] Alvaro Muñoz-Castro. A superatomic molecule under the spin-orbit coupling: Insights from the electronic properties in the thiolate-protected Au_{38} $(SR)_{24}$ cluster. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martins-Costa:2011:SSD

[MCARL11] Marilia Martins-Costa, Josep M. Anglada, and Manuel F. Ruiz-López. Structure, stability, and dynamics of hydrogen polyoxides. *International Journal of Quantum Chemistry*, 111(7–8):1543–1554, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marquez:2012:DSG

[MCC12] Edgar Marquez, Tania Cordova, and Gabriel Chuchani. DFT study of the gas-phase thermal decomposition kinetics of 2-ethoxypyridine into 2-pyridone. *International Journal of Quantum Chemistry*, 112(3):724–730, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McCoy:2013:CMS

[McC13a] Anne B. McCoy. Computations of molecular structure, properties and spectroscopies: Potential energy surfaces and properties of ICN^- and ICN. *International Journal of Quantum Chemistry*, 113(3):366–374, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Montero-Campillo:2013:MAS

[MCC13b] M. Merced Montero-Campillo and M. Natália D. S. Cordeiro. Mechanism of aziridination of styrene catalyzed

by copper(I) bis(oxazoline). *International Journal of Quantum Chemistry*, 113(16):2002–2011, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Macleod-Carey:2019:ABP

[MCCGM+19] Desmond Macleod-Carey, Giovanni F. Caramori, Raúl Guajardo-Maturana, Dayan Paez-Hernandez, Alvaro Muñoz-Castro, and Ramiro Arratia-Perez. Advances in bonding and properties of inorganic systems from relativistic calculations in Latin America. *International Journal of Quantum Chemistry*, 119(2):e25777:1–e25777:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Makshakova:2011:GVF

[MCE11] Olga Makshakova, Denis Chachkov, and Elena Ermakova. Geometry and vibrational frequencies of the helical polypeptide complexes with ligand molecules. *International Journal of Quantum Chemistry*, 111(11):2525–2539, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Munoz-Castro:2017:AAX

[MCK17] Alvaro Muñoz-Castro and R. Bruce King. Au_{10}^{2+} and Au_6 X_4^{2+} clusters: Superatomic molecules bearing an SP^3-hybrid Au_6 core. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mavromoustakos:2011:PIL

[MCKD11] Thomas Mavromoustakos, Petros Chatzigeorgiou, Catherine Koukoulitsa, and Serdar Durdagi. Partial interdigitation of lipid bilayers. *International Journal of Quantum Chemistry*, 111(6):1172–1183, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mi:2011:DSS

[MCL11] Shizhen Mi, Dezhan Chen, and Nan Lu. DFT study of the structure and property of small organic hole-transporting molecules. *International Journal of Quantum Chemistry*, 111(9):2039–2044, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marchal:2010:GSA

[MCP10] Rémi Marchal, Philippe Carbonnière, and Claude Pouchan. A global search algorithm of minima exploration for the investigation of low lying isomers of clusters from DFT-based potential energy surface. A theoretical study of Si_n and Si_{n-1} Al clusters. *International Journal of Quantum Chemistry*, 110(12):2256–2259, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muniz:2016:DFT

[MCRS16] Jesús Muñiz, Roger Castillo, José B. Robles, and Enrique Sansores. Density functional theory study of the reactivity and electronic structure of the transesterification of triacetin in biodiesel production via a sulfated zirconia heterogeneous catalysis. *International Journal of Quantum Chemistry*, 116(13):988–999, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mota:2011:TMN

[MCV11] V. C. Mota, P. J. S. B. Caridade, and A. J. C. Varandas. Toward the modeling of the NO_2 ($^2A''$) manifold. *International Journal of Quantum Chemistry*, 111(14):3776–3785, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohallem:2011:IDM

[MD11] Josée R. Mohallem and Leonardo G. Diniz. Isotopic dipole moments in water clusters. *International Journal of Quantum Chemistry*, 111(7–8):1493–1497, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malbouisson:2012:QMH

[MdAdCS12] Luiz A. C. Malbouisson, Micael D. de Andrade, and Antonio M. de C. Sobrinho. Quadrupole moment of the hydrogen fluoride using the multireference Hartree–Fock CI method. *International Journal of Quantum Chemistry*, 112 (20):3409–3413, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Manzhos:2015:RNN

[MDC15] Sergei Manzhos, Richard Dawes, and Tucker Carrington. Reviews: Neural network-based approaches for building high dimensional and quantum dynamics-friendly potential energy surfaces. *International Journal of Quantum Chemistry*, 115(16):1012–1020, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melendez:2016:TSG

[MDNDO+16] Francisco J. Melendez, J. Sergio Durand-Niconoff, Miguel A. Domínguez-Ortiz, Oscar García-Barradas, Norma A. Caballero, and Enrique González. Theoretical study of global and local reactivities of coumarin and its hydroxylated derivatives. *International Journal of Quantum Chemistry*, 116(9):663–669, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martini:2012:NPP

[MDP12] María Florencia Martini, Edgardo Aníbal Disalvo, and Mónica Pickholz. Nicotinamide and picolinamide in phospholipid monolayers. *International Journal of Quantum Chemistry*, 112(20):3289–3295, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Molina-Espiritu:2013:ITA

[MEEA+13] Moyocoyani Molina-Espíritu, Rodolfo O. Esquivel, Juan Carlos Angulo, Juan Antolín, Cristina Iuga, and Jesús S. Dehesa. Information-theoretical analysis for the S_N2 exchange reaction $CH_3Cl + F^-$. *International Journal of Quantum Chemistry*, 113(24):2589–2599, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mennucci:2015:EFF

[MEF+15] Benedetta Mennucci, Odile Eisenstein, Heike Fliegl, Kathrin H. Hopmann, Trygve Helgaker, and Kenneth Ruud. Editorial: FemEx — female excellence in theoretical and computational chemistry. *International Journal of Quantum Chemistry*, 115(18):1195–1196, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendizabal:2010:TSA

[Men10] Fernando Mendizabal. Theoretical study of Au_3 (CH_3 N $COCH_3)_{3n}$ · 2,4,7-trinitro-9-fluorenone ($n = 1, 2$) complexes. *International Journal of Quantum Chemistry*, 110 (6):1279–1286, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mennucci:2015:PMA

[Men15] Benedetta Mennucci. Perspectives: Modeling absorption and fluorescence solvatochromism with QM/Classical approaches. *International Journal of Quantum Chemistry*, 115(18):1202–1208, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Merchan:2011:RDL

[Mer11] Manuela Merchán. In remembrance of Dr. Luis Serrano-Andrés. *International Journal of Quantum Chemistry*, 111(13):3261–3262, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Metropoulos:2011:CMA

[Met11] Aristophanes Metropoulos. Can methylene amidogene and its isomers be formed by a concerted reaction? *International Journal of Quantum Chemistry*, 111(3):624–630, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malaspina:2011:ESF

[MFB11] Thaciana Malaspina, Eudes Eterno Fileti, and Erick Leite Bastos. Effect of solute flexibility and polarization on the solvatochromic shift of a brominated merocyanine dye in water: a sequential MD/QM study. *International Journal of Quantum Chemistry*, 111(7–8):1607–1615, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martins:2012:IBB

[MFK+12] Mateus J. F. Martins, Ary R. Ferreira, Elena Konstantinova, Heitor A. de Abreu, Wladmir F. Souza, Sandra S. X. Chiaro, Luís G. Dias, and Alexandre A. Leitão. Interactions between 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid and γ-Al_2O_3 (100) surface calculated by

density functional theory. *International Journal of Quantum Chemistry*, 112(19):3234–3239, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendez-Fragoso:2010:LSH

[MFLK10] R. Méndez-Fragoso and E. Ley-Koo. Lamé spheroconal harmonics in atoms and molecules. *International Journal of Quantum Chemistry*, 110(15):2765–2774, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendez-Fragoso:2011:HAS

[MFLK11] R. Méndez-Fragoso and E. Ley-Koo. The hydrogen atom in a semi-infinite space with an elliptical cone boundary. *International Journal of Quantum Chemistry*, 111(12):2882–2897, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitrushchenkov:2012:IOL

[MFLP12] Alexander O. Mitrushchenkov, Guido Fano, Roberto Linguerri, and Paolo Palmieri. On the importance of orbital localization in QC-DMRG calculations. *International Journal of Quantum Chemistry*, 112(6):1606–1619, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mombru:2018:PCR

[MFM18] Dominique Mombrú, Ricardo Faccio, and Alvaro W. Mombrú. Possible causes for rippling in a multivacancy graphene system. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mejia:2018:ADA

[MFOH18] Leopoldo Mejía, Franklin Ferraro, Edison Osorio, and Cacier Z. Hadad. Activation and diffusion of ammonia borane hydrogen on gold tetramers. *International Journal of Quantum Chemistry*, 118(13):e25567:1–e25567:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marques:2010:SAA

[MFR10] Alexandra T. Marques, Pedro A. Fernandes, and Maria João Ramos. Structural analysis of ABAD point mutations causing 2-methyl-3-hydroxylbutyryl-coA deficiency. *International Journal of Quantum Chemistry*, 110(1):148–160, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2018:EOP

[MFZ+18] Qiangqiang Meng, Lele Fan, Lei Zhu, Ning Xu, and Qinfang Zhang. Electronic and optical properties of α-MoO_3 /TiO_2 heterostructures: a DFT study. *International Journal of Quantum Chemistry*, 118(18):e25681:1–e25681:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Motiu:2010:FFH

[MG10] Stefan Motiu and Valentin Gogonea. [fe–fe]-hydrogenase reactivated by residue mutations as bridging carbonyl rearranges: A QM/MM study. *International Journal of Quantum Chemistry*, 110(14):2705–2718, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Micera:2012:EFB

[MG12] Giovanni Micera and Eugenio Garribba. The effect of the functional, basis set, and solvent in the simulation of the geometry and spectroscopic properties of $VIVO^{2+}$ complexes. chemical and biological applications. *International Journal of Quantum Chemistry*, 112(12):2486–2498, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mierzwa:2018:ESM

[MGB18] Grzegorz Mierzwa, Agnieszka J. Gordon, and Slawomir Berski. The electronic structure of molecules with the B — F and B — Cl bond in light of the topological analysis of electron localization function: Possibility of multiple bonds? *International Journal of Quantum Chemistry*, 118(24):e25781:1–e25781:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2011:TSS

[MGD11] Bhaskar Mondal, Deepanwita Ghosh, and Abhijit K. Das. Theoretical study of [Si,O,C,O] species: Prediction of new species on triplet potential energy surface. *International Journal of Quantum Chemistry*, 111(3):606–615, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2011:GEA

[MGK+11] Svetlana V. Malinovskaya, Alexander V. Glushkov, Olga Yu. Khetselius, Yury M. Lopatkin, Andrey V. Loboda, Ludmila V. Nikola, Andrey A. Svinarenko, and Tat'Yana B. Perelygina. Generalized energy approach for calculating electron collision cross-sections for multicharged ions in a plasma: Debye shielding model. *International Journal of Quantum Chemistry*, 111(2):288–296, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Madhavan:2012:VAC

[MGK+12] Thirumurthy Madhavan, Changdev G. Gadhe, Gugan Kothandan, Kyeong Lee, and Seung Joo Cho. Various atomic charge calculation schemes of CoMFA on HIF-1 inhibitors of moracin analogs. *International Journal of Quantum Chemistry*, 112(4):995–1005, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Masliy:2019:FAT

[MGK19] Alexey N. Masliy, Tatiana N. Grishaeva, and Andrey M. Kuznetsov. Formation of aqua and tetraammine Cu(II) complexes inside the cavities of cucurbit[6,8]urils: a DFT forecast. *International Journal of Quantum Chemistry*, 119 (9):e25877:1–e25877:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Madsen:2011:DMP

[MGM11] Marianne Sloth Madsen, Allan Gross, and Kurt V. Mikkelsen. Determining molecule–particle reaction parameters. *International Journal of Quantum Chemistry*, 111 (7–8):1740–1747, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Masia:2014:PFM

[MGN14] Marco Masia, Elvira Guàrdia, and Paolo Nicolini. Perspectives: The force matching approach to multiscale simulations: Merits, shortcomings, and future perspectives. *International Journal of Quantum Chemistry*, 114(16):1036–1040, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Munoz-Garcia:2016:POP

[MGP16] Ana B. Muñoz-García and Michele Pavone. Perspective: From oxide to proton conduction: a quantum-chemical perspective on the versatility of $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$-based materials. *International Journal of Quantum Chemistry*, 116(21):1501–1506, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miralrio:2017:TSS

[MHHPR+17] Alan Miralrio, Arturo Hernández-Hernández, Jose A. Pescador-Rojas, Enrique Sansores, Pablo A. López-Pérez, Francisco Martínez-Farías, and Eduardo Rangel Cortes. Theoretical study of the stability and properties of magic numbers $(m = 5, n = 2)$ and $(m = 6, n = 3)$ of bimetallic bismuth–copper nanoclusters; Bi_m Cu_n. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maeda:2015:RIR

[MHO+15] Satoshi Maeda, Yu Harabuchi, Yuriko Ono, Tetsuya Taketsugu, and Keiji Morokuma. Reviews: Intrinsic reaction coordinate: Calculation, bifurcation, and automated search. *International Journal of Quantum Chemistry*, 115(5):258–269, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mejrissi:2018:CTI

[MHOG18] Leila Mejrissi, Héla Habli, Brahim Oujia, and Florent Xavier Gadéa. Charge transfer ionic character illustration for strontium hydride ion through a diabatic investigation. *International Journal of Quantum Chemistry*, 118(18):e25680:1–e25680:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maruyama:2008:IIH

[MHT+08] Youhei Maruyama, Kenta Hongo, Masanori Tachikawa, Yoshiyuki Kawazoe, and Hiroshi Yasuhara. Ab initio interpretation of Hund's rule for the methylene molecule: Variational optimization of its molecular geometries and energy component analysis. *International Journal of Quantum Chemistry*, 108(4):731–743, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malenov:2018:IMI

[MHZ18] Dusan P. Malenov, Michael B. Hall, and Snezana D. Zarić. Influence of metal ion on chelate-aryl stacking interactions. *International Journal of Quantum Chemistry*, 118(16): e25629:1–e25629:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mehranfar:2019:URN

[MIKH19] Aliyeh Mehranfar, Mohammad Izadyar, Mohammad Khavani, and Mohammad Reza Housaindokht. Understanding the role of noncovalent interactions on the rate of some Diels-Alder reactions in different solvents. *International Journal of Quantum Chemistry*, 119(9):e25878:1–e25878:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Militzer:2012:BEP

[Mil12] B. Militzer. Bonding and electronic properties of ice at high pressure. *International Journal of Quantum Chemistry*, 112(1):314–320, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minami:2013:FDF

[MIN13] Takuya Minami, Soichi Ito, and Masayoshi Nakano. Frontiers in density functional theory: Functional dependence of excitation energy for pentacene/C_{60} model complex in the nonempirically tuned long-range corrected density functional theory. *International Journal of Quantum Chemistry*, 113(3):252–256, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitin:2011:ICW

[Mit11a] Alexander V. Mitin. Ab initio calculations of weakly bonded He_2 and Be_2 molecules by MRCI method with pseudo-natural molecular orbitals. *International Journal of Quantum Chemistry*, 111(11):2560–2567, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitin:2011:EAA

[Mit11b] Alexander V. Mitin. Effect of amino acid polarization in force field biomolecular calculations. *International Journal of Quantum Chemistry*, 111(11):2555–2559, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitin:2011:LTI

[Mit11c] Alexander V. Mitin. Lagrange-type iterative methods for calculation of extreme eigenvalues of generalized eigenvalue problem with large symmetric matrices. *International Journal of Quantum Chemistry*, 111(11):2545–2554, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moraes:2011:NFF

[MJ11] Tatiana F. Moraes and Itamar Borges Jr. Nuclear Fukui functions and the deformed atoms in molecules representation of the electron density: Application to gas-Phase RDX (hexahydro-1,3,5-trinitro-1,3,5- triazine) electronic structure and decomposition. *International Journal of Quantum Chemistry*, 111(7–8):1444–1452, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Milovanovic:2014:TIG

[MJ14] Milan Z. Milovanović and Stanka V. Jerosimić. Theoretical investigation of geometry and stability of small lithium-iodide Li_nI (n = 2–6) clusters. *International Journal of Quantum Chemistry*, 114(3):192–208, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mahler:2016:RAP

[MJ16a] Andrew Mahler and Benjamin G. Janesko. Revisiting alternative pathways in the Fischer–Tropsch process: Accurate density functional theory calculations on "magic" Ru_{12} clusters. *International Journal of Quantum Chemistry*, 116 (20):1451–1458, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mehmood:2016:EDR

[MJ16b] Arshad Mehmood and Benjamin G. Janesko. The electron delocalization range in stretched bonds. *International Journal of Quantum Chemistry*, 116(23):1783–1795, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muhammed:2019:EFA

[MJM19] Mufasila M. Muhammed, Joicy John, and Junais H. Mokkath. Electric field amplification of plasmon-molecule hybrids revealed by first-principles time dependent density functional theory calculations. *International Journal of Quantum Chemistry*, 119(23):e26021:1–e26021:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitikiri:2018:MLT

[MJSC18] Praveen Mitikiri, Gourhari Jana, Shamik Sural, and Pratim K. Chattaraj. A machine learning technique toward generating minimum energy structures of small boron clusters. *International Journal of Quantum Chemistry*, 118 (17):e25672:1–e25672:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mammino:2010:AAE

[MK10a] Liliana Mammino and Mwadham M. Kabanda. Adducts of acylphloroglucinols with explicit water molecules: Similarities and differences across a sufficiently representative number of structures. *International Journal of Quantum Chemistry*, 110(13):2378–2390, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mammino:2010:CSC

[MK10b] Liliana Mammino and Mwadham M. Kabanda. A computational study of the carboxylic acid of phloroglucinol in vacuo and in water solution. *International Journal of Quantum Chemistry*, 110(3):595–623, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mammino:2011:IIH

[MK11] Liliana Mammino and Mwadham M. Kabanda. Interplay of intramolecular hydrogen bonds, OH orientations, and symmetry factors in the stabilization of polyhydroxybenzenes. *International Journal of Quantum Chemistry*, 111 (14):3701–3716, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mammino:2012:CSP

[MK12] Liliana Mammino and Mwadham M. Kabanda. Computational study of the patterns of weaker intramolecular hydrogen bonds stabilizing acylphloroglucinols. *International Journal of Quantum Chemistry*, 112(14):2650–2658, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mirzaie-Khalilabadi:2019:NCD

[MKD19] Elahe Mirzaie-Khalilabadi and Maryam Dehestani. Nonadiabatic coupling and diabatic electronic population dynamics on 1^1A_2 and 1^1B_1 states of ozone molecule. *International Journal of Quantum Chemistry*, 119(19):e25993:1–e25993:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monajjemi:2011:SSE

[MKHM11] M. Monajjemi, M. Khosravi, B. Honarparvar, and F. Mollaamin. Substituent and solvent effects on the structural bioactivity and anticancer characteristic of catechin as a bioactive constituent of green tea. *International Journal of Quantum Chemistry*, 111(12):2771–2777, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitin:2011:ESC

[MKM11] Alexander V. Mitin, James D. Kubicki, and Kenneth M. Merz, Jr. Electronic structure, chemical bonding, and oxidation numbers of first-row transition metals in [$MePIm_2$] complexes and their cations. *International Journal of Quantum Chemistry*, 111(14):3630–3642, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mineva:2013:TDM

[MKSG13] Tzonka Mineva, Sailaja Krishnamurty, Dennis R. Salahub, and Annick Goursot. Temperature dependence of the molecular conformations of dilauroyl phosphatidylcholine: a density functional study. *International Journal of Quantum Chemistry*, 113(5):631–636, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mu:2011:DFI

[MKW11] Dan Mu, Wei-Xin Kong, and Song Wang. A density functional investigation of the reaction mechanism of H_2 O + HCNO. *International Journal of Quantum Chemistry*, 111 (1):165–173, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moradi:2010:FES

[MLB+10] Mahmoud Moradi, Jung-Goo Lee, Volodymyr Babin, Christopher Roland, and Celeste Sagui. Free energy and structure of polyproline peptides: an ab initio and classical molecular dynamics investigation. *International Journal of Quantum Chemistry*, 110(15):2865–2879, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2012:DFT

[MLB+12] Jose R. Mora, Jesus Lezama, Neydher Berroteran, Tania Cordova, and Gabriel Chuchani. Density functional theory and ab initio study on the reaction mechanisms of the homogeneous, unimolecular elimination kinetics of selected 1-chloroalkenes in the gas phase. *International Journal of Quantum Chemistry*, 112(24):3729–3738, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Manzoni:2011:DFT

[MLC+11] V. Manzoni, M. L. Lyra, B. S. Cavada, N. Saker Neto, and V. N. Freire. Density functional theory study of the electronic properties of naphthofuranquinone compounds with antitrypanocidal activity. *International Journal of Quantum Chemistry*, 111(7–8):1270–1279, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moskalenko:2010:CPC

[MLDP10] S. A. Moskalenko, M. A. Liberman, E. V. Dumanov, and I. V. Podlesny. Collective properties and combined quantum transitions of two-dimensional magnetoexcitons. *International Journal of Quantum Chemistry*, 110(1):177–194, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moon:2017:SOI

[MLK17] Jiwon Moon, Jeong Sik Lim, and Joonghan Kim. Spin-orbit ab initio and density functional theory investigation of bismuth monoboronyl, BiBO. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marques:2010:ETS

[MLPT10] Alberto D. S. Marques, Chhiu T. Lin, Luiza G. Pereira, and Yuji Takahata. Experimental and theoretical studies of 2-amino-3-methylimidazo[4,5-f]quinoline derivatives: Cooked-food mutagens. *International Journal of Quantum Chemistry*, 110(11):2047–2056, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mang:2010:TDL

[MLW10] Chaoyong Mang, Caiping Liu, and Kechen Wu. Theoretical determination of lowest structures of all-metal aromatic clusters M_4L_2 (M = Al, Ga, In, Tl; L = Li, Na, K, Rb, Cs). *International Journal of Quantum Chemistry*, 110(5): 1127–1135, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2014:DFT

[MLW+14] Guangcai Ma, Yulin Li, Lixin Wei, Yongjun Liu, and Chengbu Liu. A density functional theory study on the catalytic mechanism of hydroxycinnamoyl-CoA hydratase-lyase. *International Journal of Quantum Chemistry*, 114 (4):249–254, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Musho:2016:TOE

[MLW16] Terence Musho, Jiangtian Li, and Nianqiang Wu. Thermodynamics of the oxygen evolution electrocatalysis in a functionalized UiO-66 metal-organic frameworks. *International Journal of Quantum Chemistry*, 116(15):1153–1159, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2016:EPP

[MLY+16] Nana Ma, Shujun Li, Likai Yan, Wenyong Wang, Yongqing Qiu, and Guisheng Zhang. Electronic properties of polyoxometalate derivatives $[(C_2B_9H_{11})\ M'M_5O_{18}]^{n-}$ (M' = Ti^{IV}, Mo^{VI}, W^{VI}; M = Mo^{VI}, W^{VI}): Protonation, electronic spectra, and redox properties. *International Journal of Quantum Chemistry*, 116(5):396–404, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minicozzi:2010:CIP

[MM10] V. Minicozzi and S. Morante. Is Cu involved in prion oligopeptide stability? Experiments and numerical simulations. *International Journal of Quantum Chemistry*, 110 (3):656–680, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mirzaei:2011:CSA

[MM11] Maryam Mirzaei and Mahmoud Mirzaei. A computational study of aluminum phosphide nanotubes. *International Journal of Quantum Chemistry*, 111(14):3851–3855, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Motaghiani:2013:DFS

[MM13] Shahram Motaghiani and Kavoos Mirabbaszadeh. Density functional study of platinum polyyne monomer, oligomer, and polymer: Ground state geometrical and electronic structures. *International Journal of Quantum Chemistry*, 113(11):1650–1659, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melo:2019:RCE

[MM19] Juan I. Melo and Alejandro F. Maldonado. Relativistic corrections to the electric field gradient given by linear response elimination of the small component formalism. *International Journal of Quantum Chemistry*, 119(15): e25935:1–e25935:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mujica-Martinez:2010:MBT

[MMA10] C. A. Mujica-Martínez and J. C. Arce. Mini-bandstructure tailoring in π-conjugated periodic block copolymers using the envelope crystalline-orbital method. *International Journal of Quantum Chemistry*, 110(13):2532–2540, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minaev:2013:RDS

[MMÅ13] Boris F. Minaev, N. Arul Murugan, and Hans Ågren. Reviews: Dioxygen spectra and bioactivation. *International Journal of Quantum Chemistry*, 113(14):1847–1867, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meng:2012:SHD

[MMBK12] Qingguo Meng, P. Stanley May, Mary T. Berry, and Dmitri Kilin. Sequential hydrogen dissociation from a charged $Pt_{13}H_{24}$ cluster modeled by ab initio molecular dynamics. *International Journal of Quantum Chemistry*, 112(24): 3896–3903, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Medvedev:2019:EAV

[MMC+19] Alexander G. Medvedev, Alexey A. Mikhaylov, Ivan Yu. Chernyshov, Mikhail V. Vener, Ovadia Lev, and Petr V.

Prikhodchenko. Effect of aluminum vacancies on the H_2O_2 or H_2O interaction with a gamma-AlOOH surface. A solid-state DFT study. *International Journal of Quantum Chemistry*, 119(13):e25920:1–e25920:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melendez:2011:SVA

[MMCN+11] F. J. Melendez, C. Muñoz-Caro, A. Niño, J. Sandoval-Lira, and A. Rangel-Huerta. Structural and vibrational analysis of the OH torsional motion in difluorohydroxyborane. *International Journal of Quantum Chemistry*, 111(15):4389–4399, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Merino:2019:TCL

[MMCNV19] Gabriel Merino, Alvaro Muñoz-Castro, Marco Antonio Chaer Nascimento, and Alberto Vela. Theoretical chemistry in Latin America. *International Journal of Quantum Chemistry*, 119(2):e25852:1–e25852:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muhammad:2013:CMN

[MMF+13] Shabbir Muhammad, Takuya Minami, Hitoshi Fukui, Kyohei Yoneda, Shu Minamide, Ryohei Kishi, Yasuteru Shigeta, and Masayoshi Nakano. Computational meso- and nano-science: Comparative study of diradical characters and third-order nonlinear optical properties of linear/cyclic acenes versus phenylenes. *International Journal of Quantum Chemistry*, 113(4):592–598, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mai:2015:RGM

[MMG15] Sebastian Mai, Philipp Marquetand, and Leticia González. Reviews: a general method to describe intersystem crossing dynamics in trajectory surface hopping. *International Journal of Quantum Chemistry*, 115(18):1215–1231, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2011:RMG

[MML+11a] José R. Mora, Edgar Márquez, Jesus Lezama, Tania Córdova, and Gabriel Chuchani. The reaction mechanism of the gas-phase thermal decomposition kinetics of neopentyl halides: A DFT study. *International Journal of Quantum Chemistry*, 111(15):4011–4019, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moura:2011:CBO

[MML11b] Renaldo T. Moura, Jr., Oscar L. Malta, and Ricardo L. Longo. The chemical bond overlap plasmon as a tool for quantifying covalency in solid state materials and its applications to spectroscopy. *International Journal of Quantum Chemistry*, 111(7–8):1626–1638, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazur:2016:SNU

[MMŁ+16] Grzegorz Mazur, Marcin Makowski, Roman Łazarski, Radosław Włodarczyk, Ewa Czajkowska, and Michał Glanowski. Software news & updates: Automatic code generation for quantum chemistry applications. *International Journal of Quantum Chemistry*, 116(18):1370–1381, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2012:DSH

[MMM+12] Jose R. Mora, David J. Marquez, Edgar Marquez, Marcos Loroño, Tania Cordova, and Gabriel Chuchani. DFT studies of homogeneous catalysis in the gas phase: Dehydration kinetics of several tertiary alcohols with hydrogen chloride. *International Journal of Quantum Chemistry*, 112 (1):78–88, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mendez:2016:DIM

[MMM16] Alejandra M. P. Mendez, Darío M. Mitnik, and Jorge E. Miraglia. Depurated inversion method for orbital-specific exchange potentials. *International Journal of Quantum Chemistry*, 116(24):1882–1890, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [Cin20] and reply [MMM20].

Magers:2019:HMC

[MMM19] D. Brandon Magers, Andrew K. Magers, and David H. Magers. The *s*-homodesmotic method for the computation of conventional strain energies of bicyclic systems and individual rings within these systems. *International Journal of Quantum Chemistry*, 119(8):e25864:1–e25864:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mitnik:2020:RCD

[MMM20] D. M. Mitnik, A. M. P. Mendez, and J. E. Miraglia. Reply to "Comment on 'Depurated Inversion Method for Orbital-Specific Exchange Potentials'". *International Journal of Quantum Chemistry*, 120(4):e26102:1–e26102:??, February 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Cin20].

Markovic:2012:SRB

[MMMM12] Zoran S. Marković, Svetlana Marković, Jasmina M. Dimitrić Marković, and Dejan Milenković. Structure and reactivity of baicalein radical cation. *International Journal of Quantum Chemistry*, 112(8):2009–2017, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muller:2011:HTT

[MMP11] Thomas J. Müller and Florian Müller-Plathe. Heat transport through a biological membrane—An asymmetric property? Technical issues of nonequilibrium molecular dynamics methods. *International Journal of Quantum Chemistry*, 111(7–8):1403–1418, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Macchiagodena:2018:NAM

[MMP+18a] Marina Macchiagodena, Giordano Mancini, Marco Pagliai, Gianni Cardini, and Vincenzo Barone. New atomistic model of pyrrole with improved liquid state properties and structure. *International Journal of Quantum Chemistry*, 118(9):e25554:1–e25554:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazzone:2018:QMD

[MMP+18b] Gloria Mazzone, Tiziana Marino, Paolo Piazzetta, Fortuna Ponte, Mario Prejanò, Emilia Sicilia, and Marirosa Toscano. Quantum mechanical DFT elucidation of CO_2 catalytic conversion mechanisms: Three examples. *International Journal of Quantum Chemistry*, 118(9):e25572:1–e25572:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marino:2010:IRC

[MMR+10] Tiziana Marino, Donatella Mazzuca, Nino Russo, Marirosa Toscano, and Andre Grand. On the interaction of rubidium and cesium mono-, strontium and barium bi-cations with DNA and RNA bases. A theoretical study. *International Journal of Quantum Chemistry*, 110(1):138–147, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mora:2010:SES

[MMRRA10] M. A. Mora, M. A. Mora-Ramírez, and Manuel F. Rubio-Arroyo. Structural and electronic study of neutral, positive, and negative small rhodium clusters [Rh_n, $Rh_n{}^+$, and $Rh_n{}^-$]. *International Journal of Quantum Chemistry*, 110(13):2541–2547, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muya:2019:TIR

[MMSC19] Jules Tshishimbi Muya, Biswa Ranjan Meher, Subash Chandra Sahoo, and Hoeil Chung. A theoretical insight into the role of counter anions and their interactions in nitropentaamminecobalt(III) toward linkage isomerism-induced photochemical motion. *International Journal of Quantum Chemistry*, 119(14):e25929:1–e25929:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miyakawa:2013:MDS

[MMT+13] Takeshi Miyakawa, Ryota Morikawa, Masako Takasu, Kimikazu Sugimori, Taku Mizukami, Kazutomo Kawaguchi, Hiroaki Saito, and Hidemi Nagao. Molecular dynamics simulations of the Hras-GTP complex and the Hras-GDP complex. *International Journal of Quantum Chemistry*,

113(21):2333–2337, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Milovanovic:2019:TEI

[MMV+19] Branislav Milovanović, Milan Milovanović, Suzana Velicković, Filip Veljković, Aleksandra Perić-Grujić, and Stanka Jerosimić. Theoretical and experimental investigation of geometry and stability of small potassium-iodide K_nI (n = 2–6) clusters. *International Journal of Quantum Chemistry*, 119(22):e26009:1–e26009:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matczak:2019:FHT

[MMW19] Piotr Matczak, Grzegorz Mlostoń, and Wolfgang Weigand. Ferrocenyl hetaryl thioketones: a computational study of their conformational stability. *International Journal of Quantum Chemistry*, 119(24):e26033:1–e26033:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazur:2011:DTS

[MMWA11] Grzegorz Mazur, Marcin Makowski, Radosław Włodarczyk, and Yuriko Aoki. Dressed TDDFT study of low-lying electronic excited states in selected linear polyenes and diphenylopolyenes. *International Journal of Quantum Chemistry*, 111(4):819–825, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meraj:2012:EDP

[MNC12] Gulafroz Meraj, Mahadevappa Naganathappa, and Ajay Chaudhari. Energetics during proton transfer process in hydrated zündel ion complex. *International Journal of Quantum Chemistry*, 112(5):1439–1448, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mishra:2013:CCR

[MNE+13] Himanshu Mishra, Robert J. Nielsen, Shinichi Enami, Michael R. Hoffmann, Agustín J. Colussi, and William A. Goddard III. Computations of chemical reactions and dynamics: Quantum chemical insights into the dissociation of nitric acid on the surface of aqueous electrolytes. *International Journal of Quantum Chemistry*, 113(4):413–417,

February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Manzoor:2019:EED

[MNP19] Taniya Manzoor, Saba Niaz, and Altaf Hussain Pandith. Exploring the effect of different coumarin donors on the optical and photovoltaic properties of azo-bridged push-pull systems: a theoretical approach. *International Journal of Quantum Chemistry*, 119(18):e25979:1–e25979:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Motapon:2011:SDD

[MNS11] O. Motapon, S. A. Ndengue, and K. D. Sen. Static and dynamic dipole polarizabilities and electron density at origin: Ground and excited states of hydrogen atom confined in multiwalled fullerenes. *International Journal of Quantum Chemistry*, 111(15):4425–4432, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Man:2017:ICH

[MNV+17] Nguyen Thi Hong Man, Pham Le Nhan, Vien Vo, Duong Tuan Quang, and Nguyen Tien Trung. An insight into C H$\cdots$N hydrogen bond and stability of the complexes formed by trihalomethanes with ammonia and its monohalogenated derivatives. *International Journal of Quantum Chemistry*, 117(6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Medina:2019:NEN

[MNZPT19] Leidy Y. Medina, Francisco Núñez-Zarur, and Jhon F. Pérez-Torres. Nonadiabatic effects in the nuclear probability and flux densities through the fractional Schrödinger equation. *International Journal of Quantum Chemistry*, 119(16):e25952:1–e25952:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mejia:2011:EEW

[MOE+11] Sol M. Mejía, Juan F. Orrego, Juan F. Espinal, Patricio Fuentealba, and Fanor Mondragón. Exploration of the $(\text{ethanol})_4$–water heteropentamers potential energy surface by simulated annealing and Ab initio molecular dynamics. *International Journal of Quantum Chemistry*, 111(12):

3080–3096, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murakami:2012:DFS

[MOH+12] Yoshinori Murakami, Tatsuo Oguchi, Kohtaro Hashimoto, Akihiro Nakamura, Yasuyuki Sakai, and Hiromitsu Ando. Density functional study of the phenylethyl + O_2 reaction: Kinetic analysis for the low-temperature autoignition of ethylbenzenes. *International Journal of Quantum Chemistry*, 112(8):1968–1983, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melaccio:2011:UQM

[MOLF11] Federico Melaccio, Massimo Olivucci, Roland Lindh, and Nicolas Ferré. Unique QM/MM potential energy surface exploration using microiterations. *International Journal of Quantum Chemistry*, 111(13):3339–3346, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morgon:2011:TSA

[Mor11] Nelson H. Morgon. Theoretical study of the anthropogenic greenhouse gas (SF_5CF_3) and analysis of the reaction of SF_6 with CF. *International Journal of Quantum Chemistry*, 111(7–8):1555–1561, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morgon:2012:EFP

[Mor12] Nelson H. Morgon. Enthalpies of formation of phosphorus and oxygen compounds determined by the correlation consistent composite approach. *International Journal of Quantum Chemistry*, 112(19):3256–3260, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Morgan:2013:BRA

[Mor13] John D. Morgan III. Book review: *Advances in quantum chemistry: Unstable states in the continuous spectra, part 2: Interpretation, theory, and applications*. *International Journal of Quantum Chemistry*, 113(7):1047–1048, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mostafanejad:2014:TRB

[Mos14] Mohammad Mostafanejad. Tutorial reviews: Basics of the spin Hamiltonian formalism. *International Journal of Quantum Chemistry*, 114(22):1495–1512, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazilov:2010:MMG

[MOSK10] Elisey Mazilov, Evgeniya Ogurtsova, Alexander Shamov, and Grigorii Khrapkovskii. The monomolecular mechanism of the gas-phase thermal decomposition of primary N-nitramines. *International Journal of Quantum Chemistry*, 110(4):939–945, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matsuoka:2013:CMS

[MOY13] Takahide Matsuoka, Sayo Oonishi, and Satoshi Yabushita. Computations of molecular structure, properties and spectroscopies: Theoretical study on angular momentum polarization parameters, branching ratios, and anisotropy parameters of chlorine atoms from photodissociation of iodine monochloride. *International Journal of Quantum Chemistry*, 113(3):375–381, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martini:2012:MDS

[MP12] M. Florencia Martini and Mónica Pickholz. Molecular dynamics study of uncharged bupivacaine enantiomers in phospholipid bilayers. *International Journal of Quantum Chemistry*, 112(20):3341–3345, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukherjee:2011:NES

[MPB11] Neetik Mukherjee, Ranjit K. Pathak, and Kamal Bhattacharyya. Near-exact supersymmetric partner potentials: Construction and exploitation. *International Journal of Quantum Chemistry*, 111(14):3597–3607, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovskaya:2010:ISC

[MPC10] S. Malinovskaya, V. Patel, and T. Collins. Internal state cooling with a femtosecond optical frequency comb. *International Journal of Quantum Chemistry*, 110(15):3080–3085, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meyer:2010:MIC

[MPD+10] A. Meyer, W. F. Perger, R. Demichelis, B. Civalleri, and R. Dovesi. Magnetic interactions in Ca_3 Fe_2 Ge_3 O_{12} and Ca_3 Cr_2 Ge_3 O_{12} garnets. An ab initio all-electron quantum mechanical simulation. *International Journal of Quantum Chemistry*, 110(12):2192–2201, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mandal:2015:TDN

[MPD+15] Subhajit Mandal, Sudip Pan, Dibakar Deb, Santanab Giri, Soma Duley, Slavko Radenković, David L. Cooper, Patrick Bultinck, Anakuthil Anoop, Manish Bhattacharjee, and Pratim K. Chattaraj. Three-dimensional networks containing rectangular Sr_4 and Ba_4 units: Synthesis, structure, bonding, and potential application for Ne gas separation. *International Journal of Quantum Chemistry*, 115 (20):1501–1510, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Musa:2011:NNA

[MPE11] Klefah A. K. Musa, Viraja R. Palwai, and Leif A. Eriksson. New nonsteroidal anti-inflammatory molecules with reduced photodegradation side effects and enhanced COX-2 selectivity. *International Journal of Quantum Chemistry*, 111(6):1184–1195, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Markova:2015:HSM

[MPE15] Nadezhda Markova, Ljupco Pejov, and Venelin Enchev. A Hybrid statistical mechanics — quantum chemical model for proton transfer in 5-azauracil and 6-azauracil in water solution. *International Journal of Quantum Chemistry*, 115 (8):477–485, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monge-Palacios:2019:FAC

[MPGGS19] Manuel Monge-Palacios, Edwing Grajales-González, and Subram M. Sarathy. Formic acid catalyzed keto-enol tautomerizations for C_2 and C_3 enols: Implications in atmospheric and combustion chemistry. *International Journal of Quantum Chemistry*, 119(21):e25954:1–e25954:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maurel:2012:IMO

[MPJ12] François Maurel, Aurélie Perrier, and Denis Jacquemin. Ab initio modeling of optical spectra in pH-sensitive diarylethenes. *International Journal of Quantum Chemistry*, 112(4):1122–1133, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moin:2011:CDA

[MPL+11] Syed Tarique Moin, Andreas B. Pribil, Len Herald V. Lim, Thomas S. Hofer, Bernhard R. Randolf, and Bernd M. Rode. Carbon dioxide in aqueous environment—A quantum mechanical charge field molecular dynamics study. *International Journal of Quantum Chemistry*, 111(7–8): 1370–1378, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Magoulas:2015:SPG

[MPM15] Ilias Magoulas, Aristotle Papakondylis, and Aristides Mavridis. Structural parameters of the ground states of the quasi-stable diatomic anions CO^-, BF^-, and BCl^- as obtained by conventional Ab Initio methods. *International Journal of Quantum Chemistry*, 115(12):771–778, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marrero-Ponce:2011:BES

[MPMCM+11] Yovani Marrero-Ponce, Eugenio R. Martínez, Gerardo M. Casañola-Martín, Facundo Pérez-Giménez, Yunaimy Echevería Díaz, Ramon Garcia-Domenech, and José E. Rodriguez Brogues. Bond-extended stochastic and nonstochastic bilinear indices. I. QSPR/QSAR applications to the description of properties/activities of small-medium size organic compounds. *International Journal of Quantum Chemistry*,

111(1):8–34, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monari:2010:HSS

[MPRB+10] Antonio Monari, Jose Pitarch-Ruiz, Gian Luigi Bendazzoli, Stefano Evangelisti, and Jose Sanchez-Marin. High-spin states in tetrahedral X_4 clusters (X = H, Li, Na, K). *International Journal of Quantum Chemistry*, 110(4):874–884, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Monge-Palacios:2012:APE

[MPRCEG12] M. Monge-Palacios, C. Rangel, J. C. Corchado, and J. Espinosa-García. Analytical potential energy surface for the reaction with intermediate complexes NH_3 + Cl $\rightarrow$ NH_2 + HCl: Application to the kinetics study. *International Journal of Quantum Chemistry*, 112(8):1887–1903, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mosyagin:2011:EIT

[MPT11] N. S. Mosyagin, A. N. Petrov, and A. V. Titov. The effect of the iterative triple and quadruple cluster amplitudes on the adiabatic potential curve in the coupled cluster calculations of the ground electronic state of the Yb dimer. *International Journal of Quantum Chemistry*, 111(14):3793–3798, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marino:2012:SBP

[MPTR12] Tiziana Marino, Matej Pavelka, Marirosa Toscano, and Nino Russo. Structural and binding properties of metal ion chelators relevant to Alzheimer's disease. A theoretical investigation. *International Journal of Quantum Chemistry*, 112(9):2109–2114, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mosyagin:2013:GRE

[MPTZ13] Nikolai S. Mosyagin, Aleksander N. Petrov, Anatoly V. Titov, and Andrei V. Zaitsevskii. Generalized relativistic effective core potential calculations of the adiabatic potential curve and spectroscopic constants for the ground

electronic state of the Ca_2 molecule. *International Journal of Quantum Chemistry*, 113(20):2277–2281, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Medina:2011:FSA

[MPV+11] J. S. Medina, R. Prosmiti, P. Villarreal, G. Delgado-Barrio, J. V. Alemán, B. González, and G. Winter. Filtered stress autocorrelation functions of liquid water models. *International Journal of Quantum Chemistry*, 111(2):375–386, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Meyer:2010:MIE

[MPZWD10] A. Meyer, F. Pascale, C. M. Zicovich-Wilson, and R. Dovesi. Magnetic interactions and electronic structure of uvarovite and andradite garnets. An ab initio all-electron simulation with the CRYSTAL06 program. *International Journal of Quantum Chemistry*, 110(2):338–351, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miranda-Quintana:2017:IHC

[MQA17] Ramón Alain Miranda-Quintana and Paul W. Ayers. Interpolating Hamiltonians in chemical compound space. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miranda-Quintana:2013:DTQ

[MQG13] Ramón Alain Miranda-Quintana and Marco Martínez González. Deflation techniques in quantum chemistry: Excited states from ground states. *International Journal of Quantum Chemistry*, 113(22):2478–2488, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mercier:2011:CDM

[MR11] Yannick Mercier and Mar Reguero. Comparison of the deactivation mechanism of 5-fluorouracil with that of its parent system, uracil: The need of the use of the MS-CASPT2 method. *International Journal of Quantum Chemistry*,

111(13):3405–3415, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malinovsky:2012:GSQ

[MR12] Vladimir S. Malinovsky and Sergey Rudin. Geometric single-qubit gates for an electron spin in a quantum dot. *International Journal of Quantum Chemistry*, 112(24):3744–3749, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukherjee:2018:FIC

[MR18a] Neetik Mukherjee and Amlan K. Roy. Fisher information in confined isotropic harmonic oscillator. *International Journal of Quantum Chemistry*, 118(21):e25727:1–e25727:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukherjee:2018:IEM

[MR18b] Neetik Mukherjee and Amlan K. Roy. Information-entropic measures in free and confined hydrogen atom. *International Journal of Quantum Chemistry*, 118(15):e25596:1–e25596:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murugan:2011:MSN

[MRÅ11] Natarajan Arul Murugan, Zilvinas Rinkevicius, and Hans Ågren. Modeling solvatochromism of Nile red in water. *International Journal of Quantum Chemistry*, 111(7–8):1521–1530, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miyashita:2015:SNU

[MRS15] Naoyuki Miyashita, Suyong Re, and Yuji Sugita. Software news and updates: REIN: Replica-exchange INterface for simulating protein dynamics and function. *International Journal of Quantum Chemistry*, 115(5):325–332, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Marino:2011:IMC

[MRT11] Tiziana Marino, Nino Russo, and Marirosa Toscano. Interaction of the Mn^{2+}, Co^{2+}, Ni^{2+}, and Zn^{2+} with prion protein HGGGW pentapeptide model. *International Journal*

of Quantum Chemistry, 111(6):1152–1162, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miroshnychenko:2010:EDD

[MS10] K. V. Miroshnychenko and A. V. Shestopalova. The effect of drug-DNA interactions on the intercalation site formation. *International Journal of Quantum Chemistry*, 110(1): 161–176, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

March:2012:PTD

[MS12] Norman H. March and Richard H. Squire. Phase transitions driven by quasiparticle interactions. II. *International Journal of Quantum Chemistry*, 112(1):89–98, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mahadevi:2014:MHB

[MS14a] A. Subha Mahadevi and G. Narahari Sastry. Modulation of hydrogen bonding upon ion binding: Insights into cooperativity. *International Journal of Quantum Chemistry*, 114(2):145–153, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miralrio:2014:ESS

[MS14b] Alan Miralrio and Luis Enrique Sansores. Electronic structure and stability of binary and ternary aluminum-bismuth-nitrogen nanoclusters. *International Journal of Quantum Chemistry*, 114(14):931–942, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohan:2014:ABE

[MS14c] Neetha Mohan and Cherumuttathu H. Suresh. Accurate binding energies of hydrogen, halogen, and dihydrogen bonded complexes and cation enhanced binding strengths. *International Journal of Quantum Chemistry*, 114(13):885–894, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miralrio:2017:SSE

[MS17] Alan Miralrio and Luis Enrique Sansores. Structures, stabilities, and electronic properties of fullerene C_{36} with en-

dohedral atomic Sc, Y, and La: a dispersion-corrected DFT study. *International Journal of Quantum Chemistry*, 117 (6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mukherjee:2019:TSR

[MSAB19] Bijit Mukherjee, K. R. Shamasundar, Satrajit Adhikari, and Michael Baer. Topological studies related to molecular systems formed during the Big Bang: H_3^+ as an example. *International Journal of Quantum Chemistry*, 119(16): e25949:1–e25949:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondragon-Solorzano:2018:SUV

[MSBF18] Gustavo Mondragón-Solórzano and Joaquín Barroso-Flores. Spectroscopical UV–Vis implications of an intramolecular η^2-Mg coordination in bacteriochlorophyll-a from the Fenna–Matthews=-Olson complex. *International Journal of Quantum Chemistry*, 118(17):e25663:1–e25663:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Matamala:2010:DOD

[MSC10] Adelio R. Matamala, Cristian A. Salas, and José F. Cariñena. Degeneracy in one-dimensional quantum mechanics: a case study. *International Journal of Quantum Chemistry*, 110(7):1317–1321, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Makarova:2016:CSS

[MSG16] Maria V. Makarova, Sergey G. Semenov, and Olga A. Guskova. Computational study of structure, electronic, and microscopic charge transport properties of small conjugated diketopyrrolopyrrole-thiophene molecules. *International Journal of Quantum Chemistry*, 116(20):1459–1466, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Malhado:2013:CFM

[MSH13] João Pedro Malhado, Riccardo Spezia, and James T. Hynes. Concepts and fundamental methods in molecular simulations: Conical intersection structure and dynamics for a model protonated Schiff base photoisomerization in

solution. *International Journal of Quantum Chemistry*, 113 (3):296–305, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mhin:2011:TII

[MSK11] Byung Jin Mhin, Hyun-Il Seo, and Seung-Joon Kim. Theoretical investigation on the IR spectra of four-membered silicon oxide ring. *International Journal of Quantum Chemistry*, 111(14):3755–3760, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mizukami:2012:SES

[MSK+12] Taku Mizukami, Hiroaki Saito, Shuhei Kawamoto, Takeshi Miyakawa, Masashi Iwayama, Masako Takasu, and Hidemi Nagao. Solvation effect on the structural change of a globular protein: a molecular dynamics study. *International Journal of Quantum Chemistry*, 112(1):344–350, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Minyaev:2016:PSD

[MSM16] Ruslan M. Minyaev, Andrey G. Starikov, and Vladimir I. Minkin. Perspectives: Supermolecular design: From molecules to solid states. *International Journal of Quantum Chemistry*, 116(4):259–264, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melichercik:2018:CGF

[MSNP18] Miroslav Melicherčík, Denisa Suchá, Pavel Neogrády, and Michal Pitoňák. Off-center Gaussian functions: Applications toward larger basis sets, post-second-order correlation treatment, and truncated virtual orbital space in investigations of noncovalent interactions. *International Journal of Quantum Chemistry*, 118(14):e25580:1–e25580:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muniz:2013:RAB

[MSOV13] Jesús Muñiz, Enrique Sansores, Alfredo Olea, and Edgar Valenzuela. The role of aromaticity on the building of nanohybrid materials functionalized with metalated (Au(III), Ag(III), Cu(III)) extended porphyrins and single-walled carbon nanohorns: a theoretical study. *Interna-*

tional Journal of Quantum Chemistry, 113(7):1034–1046, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Muniz:2011:EAA

[MSRn+11] Jesús Muñiz, Enrique Sansores, J. A. Reyes-nava, V.-H. Ramos-sanchez, and Alfredo Olea. Effects of the Au(I)–Au(I) closed-shell attraction on the electronic and phosphorescent properties in a series of coordination compounds: a theoretical study. *International Journal of Quantum Chemistry*, 111(15):4378–4388, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mazurek:2011:FCL

[MSS11] Aleksander P. Mazurek and Nina Sadlej-Sosnowska. Is fullerene C_{60} large enough to host an aromatic molecule? *International Journal of Quantum Chemistry*, 111(10): 2398–2405, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miranda:2010:HSP

[MSVMCI10] A. Miranda, F. A. Serrano, R. Vázquez-Medina, and M. Cruz-Irisson. Hydrogen surface passivation of Si and Ge nanowires: a semiempirical approach. *International Journal of Quantum Chemistry*, 110(13):2448–2454, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Miyagi:2012:IFM

[MSY+12] Satoshi Miyagi, Satoshi Sawamura, Eri Yoshikawa, Kenichi Dedachi, Satoshi Itoh, Mitsuko Ishihara-Sugano, and Noriyuki Kurita. Ab initio fragment molecular orbital calculations on specific interactions between aryl hydrocarbon receptor and dioxin. *International Journal of Quantum Chemistry*, 112(1):289–299, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McDowell:2010:SMH

[MT10] Sean A. C. McDowell and Ajit J. Thakkar. A simple model of hydrogen bonding with particular application to trends in hydrogen-bonded dimers. *International Journal of Quantum Chemistry*, 110(8):1506–1513, July 2010. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

McCarthy:2011:EPE

[MT11] Shane P. McCarthy and Ajit J. Thakkar. Electron-pair extracule densities for low-lying excited states of He and Li^+. *International Journal of Quantum Chemistry*, 111(4): 753–759, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martins:2012:OSD

[MTL+12] João B. L. Martins, Carlton A. Taft, Elson Longo, Elton A. S. de Castro, Wiliam F. da Cunha, José R. S. Politi, and Ricardo Gargano. ONIOM study of dissociated hydrogen and water on ZnO surface. *International Journal of Quantum Chemistry*, 112(19):3223–3227, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Maslakov:2019:NCB

[MTR+19] Konstantin I. Maslakov, Yury A. Teterin, Mikhail V. Ryzhkov, Aleksej J. Popel, Anton Yu. Teterin, Kirill E. Ivanov, Stepan N. Kalmykov, Vladimir G. Petrov, and Ian Farnan. The nature of the chemical bond in UO_2. *International Journal of Quantum Chemistry*, 119(24):e26040:1–e26040:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mondal:2015:EMA

[MTS15] Saptarsi Mondal, Avula Uday Teja, and Prashant Chandra Singh. Effect of microhydration on the atmospherically important metastable carbonyl sulfide anion: Structure, energetic, and infrared study. *International Journal of Quantum Chemistry*, 115(12):785–795, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mueller:2012:BR

[Mue12] Guido Mueller. Book Review. *International Journal of Quantum Chemistry*, 112(3):938–939, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mejia-Urueta:2012:DFS

[MUNZVR12] Rafael Mejia-Urueta, Francisco Nuñez-Zarur, and Ricardo Vivas-Reyes. Density functional study on electronic structures and reactivity in carbazol-oxadiazole dyads used in organic light emitting diodes. *International Journal of Quantum Chemistry*, 112(16):2808–2815, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Melendez:2010:TST

[MUPC10] F. J. Melendez, Omar Urzúa, M. Judith Percino, and Victor M. Chapela. A theoretical study on three conformational structures of 2,6-distyrylpyridine. *International Journal of Quantum Chemistry*, 110(4):838–849, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Murrell:2012:OLD

[Mur12] John N. Murrell. The origins and later developments of molecular orbital theory. *International Journal of Quantum Chemistry*, 112(17):2875–2879, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Moncada:2013:HIE

[MURR13] Félix Moncada, Lalita S. Uribe, Jonathan Romero, and Andrés Reyes. Hydrogen isotope effects on covalent and noncovalent interactions: the case of protonated rare gas clusters. *International Journal of Quantum Chemistry*, 113 (10):1556–1561, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mohallem:2019:PME

[MVA19] José R. Mohallem, Paulo F. G. Velloso, and Antonio F. C. Arapiraca. Probing molecular environments with a fictitious isotopic dipole. *International Journal of Quantum Chemistry*, 119(13):e25917:1–e25917:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mandra:2013:DNR

[MVC13] Salvatore Mandrà, Stéphanie Valleau, and Michele Ceotto. Deep nuclear resonant tunneling thermal rate constant calculations. *International Journal of Quantum Chemistry*, 113(12):1722–1734, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Martinez:2018:HIP

[MVG18] Ana Martínez, Rubicelia Vargas, and Annia Galano. How to identify promising metal scavengers? *d*-penicillamine with copper as a study case. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mulugeta:2015:SES

[MW15] Yonas Mulugeta and Hagos Woldeghebriel. Size effect on the structural and electronic properties of lead telluride clusters. *International Journal of Quantum Chemistry*, 115 (4):197–207, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mattsson:2016:TRD

[MW16] Ann E. Mattsson and John M. Wills. Tutorial reviews: Density functional theory for *d*- and *f*-electron materials and compounds. *International Journal of Quantum Chemistry*, 116(11):834–846, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mao:2015:RTI

[MWH15] Yu Mao, Hai-Feng Wang, and P. Hu. Reviews: Theoretical investigation of NH_3-SCR processes over zeolites: a review. *International Journal of Quantum Chemistry*, 115(10):618–630, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2018:BDF

[MXC18] Fangfang Ma, Hong-Bin Xie, and Jingwen Chen. Benchmarking of DFT functionals for the kinetics and mechanisms of atmospheric addition reactions of OH radicals with phenyl and substituted phenyl-based organic pollutants. *International Journal of Quantum Chemistry*, 118

(10):e25533:1–e25533:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Madugula:2017:MDP

[MY17] Sita Sirisha Madugula and Soujanya Yarasi. Molecular design of porphyrin dyes for dye sensitized solar cells: a quantitative structure property relationship study. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mysovsky:2012:SRH

[Mys12] Andrey S. Mysovsky. Spectral representation of Hartree–Fock exchange operator. *International Journal of Quantum Chemistry*, 112(4):986–994, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ma:2010:IBR

[MYZ+10] Ke-Sheng Ma, Jin-Mao You, Zheng-Yu Zhou, Chun-Fang Su, and Xiang-Xiang Wang. Interaction between RNA segment (adenine-uracil) and model of protein unit (formamide): a density-functional theory study. *International Journal of Quantum Chemistry*, 110(7):1425–1431, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Makiabadi:2013:IIU

[MZB+13] Batoul Makiabadi, Mohammad Zakarianejad, Sotoodeh Bagheri, Hamid Reza Masoodi, and Raziyeh Sadaat Aghaie. Intermolecular interactions in uracil–nitrous acid complexes: structures, binding energy, topological properties, and nuclear magnetic resonance study. *International Journal of Quantum Chemistry*, 113(21):2361–2371, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mo:2017:EEM

[MZLM17] Lixin Mo, Yanli Zeng, Xiaoyan Li, and Lingpeng Meng. The enhancing effects of molecule X (X = PH_2Cl, SHCl, ClCl) on chalcogen–chalcogen interactions in cyclic trimers Y $\cdots$ Y $\cdots$ X (Y = SHCl, SeHCl). *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Mosyagin:2016:RGR

[MZST16] Nikolai S. Mosyagin, Andrei V. Zaitsevskii, Leonid V. Skripnikov, and Anatoly V. Titov. Reviews: Generalized relativistic effective core potentials for actinides. *International Journal of Quantum Chemistry*, 116(4):301–315, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nazari:2012:APF

[NA12] Fariba Nazari and Narjes Ansari. Adsorption of polyfunctional 5-fluorouracil and 2,4-dithio-5-fluorouracil on Au(111) surface: Structure, energy, and electronic transmission. *International Journal of Quantum Chemistry*, 112 (10):2287–2293, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naghma:2014:TSC

[NA14] Rahla Naghma and Bobby Antony. Total scattering cross sections for ethylene by electron impact for incident electron energies from 1 to 2000 eV. *International Journal of Quantum Chemistry*, 114(4):271–277, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2010:PPD

[Nag10] Á. Nagy. The Pauli potential from the differential virial theorem. *International Journal of Quantum Chemistry*, 110 (12):2117–2120, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2015:FSI

[Nag15] Ágnes Nagy. Fisher and Shannon information in orbital-free density functional theory. *International Journal of Quantum Chemistry*, 115(19):1392–1395, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2016:EAD

[Nag16a] Á. Nagy. Editorial: Advances in DFT. *International Journal of Quantum Chemistry*, 116(11):801, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2016:EED

[Nag16b] Ágnes Nagy. Euler equation for descriptors of the spherically symmetric Coulomb systems. *International Journal of Quantum Chemistry*, 116(11):862–866, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2017:TTD

[Nag17] Ágnes Nagy. Thermodynamical transcription of the density functional theory with constant temperature. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ndassa:2017:URR

[NAK+17] Ibrahim Mbouombouo Ndassa, Abel Idrice Adjieufack, Joseph Mbadcam Ketcha, Slawomir Berski, Mar Ríos-Gutiérrez, and Luis R. Domingo. Understanding the reactivity and regioselectivity of [3 + 2] cycloaddition reactions between substituted nitrile oxides and methyl acrylate. A molecular electron density theory study. *International Journal of Quantum Chemistry*, 117(24):??, December 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2012:DTS

[Nal12] Roman F. Nalewajski. Direct (through-space) and indirect (through-bridge) components of the chemical bond multiplicities. *International Journal of Quantum Chemistry*, 112(11):2355–2370, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2013:SED

[Nal13] Roman F. Nalewajski. Separation of energies of the direct (through-space) and indirect (through-bridge) interactions in SCF LCAO MO theory. *International Journal of Quantum Chemistry*, 113(6):766–770, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nalewajski:2015:PPC

[Nal15] Roman F. Nalewajski. Perspectives: Phase/current information descriptors and equilibrium states in molecules. *In-*

ternational Journal of Quantum Chemistry, 115(19):1274–1288, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2019:CNP

[Nas19] Marco Antonio Chaer Nascimento. The consequences of neglecting permutation symmetry in the description of many-electrons systems. *International Journal of Quantum Chemistry*, 119(2):e25765:1–e25765:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [Fer19].

Ng:2017:IEI

[NB17] Yee-Hong Ng and Ryan P. A. Bettens. Improving on equilibrium isotropic nuclear shielding constants. *International Journal of Quantum Chemistry*, 117(1):15–23, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikolaienko:2019:LOO

[NB19] Tymofii Y. Nikolaienko and Leonid A. Bulavin. Localized orbitals for optimal decomposition of molecular properties. *International Journal of Quantum Chemistry*, 119(3): e25798:1–e25798:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nelin:2010:RBC

[NBI+10] C. J. Nelin, P. S. Bagus, E. S. Ilton, S. A. Chambers, H. Kuhlenbeck, and H.-J. Freund. Relationships between complex core level spectra and materials properties. *International Journal of Quantum Chemistry*, 110(15):2752–2764, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2012:HBB

[NBL12] Renata X. D. Nascimento, Márcia K. D. L. Belarmino, and Nathália B. D. Lima. Hydrogen bonds between pyrazine and RCOOH (R = H, CH_3, and C_6H_5): a theoretical study. *International Journal of Quantum Chemistry*, 112 (19):3147–3151, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naji:2014:EMP

[NBL+14] Sufyan Naji, Adil Belhaj, Hicham Labrim, Mohamed Bhihi, Abdelilah Benyoussef, and Abdallah El Kenz. Electronic and magnetic properties of iron adsorption on graphene with double hexagonal geometry. *International Journal of Quantum Chemistry*, 114(7):463–467, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nazmutdinov:2016:RME

[NBZG16] Renat R. Nazmutdinov, Michael D. Bronshtein, Tamara T. Zinkicheva, and Dmitrii V. Glukhov. Reviews: Modeling of electron transfer across electrochemical interfaces: State-of-the art and challenges for quantum and computational chemistry. *International Journal of Quantum Chemistry*, 116(3):189–201, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naganathappa:2011:SCA

[NC11] Mahadevappa Naganathappa and Ajay Chaudhari. Spectroscopic characterization of aminoacetonitrile, its ions and protonated aminoacetonitrile using quantum chemical methods. *International Journal of Quantum Chemistry*, 111(9):2064–2071, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagurniak:2018:AEI

[NCMC+18] Glaucio R. Nagurniak, Giovanni F. Caramori, Alvaro Muñoz-Castro, Renato L. T. Parreira, and Éder H. da Silva. The ability of Ex^2Box^{4+} to interact with guests containing π-electron-rich and π-electron-poor moieties. *International Journal of Quantum Chemistry*, 118(15): e25607:1–e25607:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nazari:2010:SEH

[ND10] Fariba Nazari and Zohreh Doroodi. The substitution effect on heavy versions of cyclobutadiene. *International Journal of Quantum Chemistry*, 110(8):1514–1528, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nadvorny:2011:HBC

[ND11] Daniela Nadvorny and João Bosco P. Da Silva. Hydrogen bond complexes of hydantoin: a theoretical study. *International Journal of Quantum Chemistry*, 111(7–8):1436–1443, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakazato:2010:ACS

[NDH10] Daniel T. I. Nakazato, Eduardo L. De Sá, and Roberto L. A. Haiduke. An atomic charge study of highly ionic diatomic molecular systems. *International Journal of Quantum Chemistry*, 110(9):1729–1737, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nguyen:2019:CML

[NDLC19] Quang Van Nguyen, Sandip De, Junhong Lin, and Volkan Cevher. Chemical machine learning with kernels: the impact of loss functions. *International Journal of Quantum Chemistry*, 119(9):e25872:1–e25872:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Noel:2012:ESD

[NDM+12] Y. Noël, M. De La Pierre, L. Maschio, M. Rérat, C. M. Zicovich-Wilson, and R. Dovesi. Electronic structure, dielectric properties and infrared vibrational spectrum of fayalite: an ab initio simulation with an all-electron Gaussian basis set and the B3LYP functional. *International Journal of Quantum Chemistry*, 112(9):2098–2108, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nguyen:2010:AEG

[NDP10] Kiet A. Nguyen, Paul N. Day, and Ruth Pachter. Analytical energy gradients of Coulomb-attenuated time-dependent density functional methods for excited states. *International Journal of Quantum Chemistry*, 110(12): 2247–2255, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nordholm:2011:ERE

[NE11] Sture Nordholm and William Eek. Ergodicity and rapid electron delocalization — The dynamical mechanism of atomic reactivity and covalent bonding. *International Journal of Quantum Chemistry*, 111(9):2072–2088, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nurazar:2015:SCD

[NEEV15] Roghaye Nurazar, Zahra Fallah Ebrahimi, Mehdi D. Esrafili, and Esmail Vessally. Sensing and catalytic decomposition of hydrogen peroxide by silicon carbide nanotubes: a DFT study. *International Journal of Quantum Chemistry*, 115(8):471–476, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nemeth:2014:PMD

[Ném14] Károly Németh. Perspectives: Materials design by quantum-chemical and other theoretical/computational means: Applications to energy storage and photoemissive materials. *International Journal of Quantum Chemistry*, 114(16):1031–1035, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nesbet:2010:SDI

[Nes10] R. K. Nesbet. Six decades of interacting electrons. *International Journal of Quantum Chemistry*, 110(15):3136–3139, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nest:2011:CEE

[Nes11] M. Nest. Can electron equilibration in excited Na_8 clusters be interpreted as thermalization? *International Journal of Quantum Chemistry*, 111(2):505–509, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Netz:2012:BDI

[Net12] Paulo Augusto Netz. Benzothiadiazoles as DNA intercalators: Docking and simulation. *International Journal of Quantum Chemistry*, 112(20):3296–3302, October 15,

2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nascimento:2011:SVD

[NF11] D. L. Nascimento and A. L. A. Fonseca. A 2D spinless version of Dirac's equation written in a noninertial frame of reference. *International Journal of Quantum Chemistry*, 111(7–8):1361–1369, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niu:2010:TIS

[NFD+10] Yuzhong Niu, Shengyu Feng, Yunqiao Ding, Rongjun Qu, Dengxu Wang, and Jianjun Han. Theoretical investigation on sulfur-containing chelating resin-divalent metal complexes. *International Journal of Quantum Chemistry*, 110 (10):1982–1993, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niu:2011:TSI

[NFQ+11] Yuzhong Niu, Shengyu Feng, Rongjun Qu, Yunqiao Ding, Dengxu Wang, and Yike Wang. Theoretical study on the interaction of sulfur- and aminopyridine-containing chelating resins with Hg(II) and Pb(II). *International Journal of Quantum Chemistry*, 111(5):991–1001, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Navarro:2011:TES

[NG11] Jesús Navarro and Rafael Guardiola. Thermal effects on small para-hydrogen clusters. *International Journal of Quantum Chemistry*, 111(2):463–471, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ng:2012:OQE

[Ng12] Andrew Ng. Outstanding questions in electron–ion energy relaxation, lattice stability, and dielectric function of warm dense matter. *International Journal of Quantum Chemistry*, 112(1):150–160, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasertayoob:2011:TRQ

[NGS11] Payam Nasertayoob, Mohammad Goli, and Shant Shahbazian. Toward a regional quantum description of the positronic systems: Primary considerations. *International Journal of Quantum Chemistry*, 111(9):1970–1981, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nold:2011:TEH

[NH11] Christopher P. Nold and John D. Head. Theoretical exploration of hydrogen loss from AlH_3 and Al_2H_6. *International Journal of Quantum Chemistry*, 111(7–8):1639–1645, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakanishi:2018:PSG

[NH18] Waro Nakanishi and Satoko Hayashi. Perturbed structures generated using coordinates derived from compliance constants in internal vibrations for QTAIM dual functional analysis: Intrinsic dynamic nature of interactions. *International Journal of Quantum Chemistry*, 118(11):e25590:1–e25590:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Noureddine:2012:TSH

[NHB12] Issaoui Noureddine, Ghalla Houcine, and Oujia Brahim. Theoretical study of hydrogen and deuterium bond in glutaric acid crystal dimer. *International Journal of Quantum Chemistry*, 112(4):1006–1015, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Najafabadi:2012:IHA

[NHG+12] Reza Izadi Najafabadi, Mohammad Reza Housaindokht, Mohammad Sadegh Sadeghi Googheri, Mohsen Sargolzaei, and Mohammad Izadyar. The influence of hydrophobic amino acid side groups on the acidity of the aromatic imidazole ring of histidine: a theoretical study. *International Journal of Quantum Chemistry*, 112(14):2675–2680, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nicolaides:2011:SPS

[Nic11] Cleanthes A. Nicolaides. State- and property-specific quantum chemistry: Basic characteristics, and sample applications to atomic, molecular, and metallic ground and excited states of beryllium. *International Journal of Quantum Chemistry*, 111(13):3347–3361, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nicolaides:2014:PQC

[Nic14] Cleanthes A. Nicolaides. Perspectives: Quantum chemistry and its "ages". *International Journal of Quantum Chemistry*, 114(15):963–982, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikolaev:2011:EMO

[Nik11] A. V. Nikolaev. Expansion of the π-molecular orbitals of the C_{60} fullerene in spherical harmonics. *International Journal of Quantum Chemistry*, 111(11):2478–2481, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakamura:2019:PEL

[NIK19] Taiji Nakamura, Akira Imanishi, and Takako Kudo. Planarity of ethylene/linear polyene analogues focused on π-electron holding ability of the components. *International Journal of Quantum Chemistry*, 119(24):e26029:1–e26029:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nozaki:2016:TSA

[NIT16] Hiroo Nozaki, Kazuhide Ichikawa, and Akitomo Tachibana. Theoretical study of atoms by the electronic kinetic energy density and stress tensor density. *International Journal of Quantum Chemistry*, 116(7):504–514, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowroozi:2012:EOC

[NJA+12] A. Nowroozi, P. Mohammadzadeh Jahani, N. Asli, H. Hajiabadi, S. Dahmardeh, and H. Raissi. Evaluation of the origin of conformational and tautomeric preferences in *N*-formylformamide — a quantum chemical study. *Inter-*

national Journal of Quantum Chemistry, 112(2):489–497, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2013:CMN

[NKF+13] Masayoshi Nakano, Ryohei Kishi, Hitoshi Fukui, Takuya Minami, Kyohei Yoneda, Shu Minamide, Yudai Inoue, Taishi Yamada, Soichi Ito, Shabbir Muhammad, Yasuteru Shigeta, Takashi Kubo, and Benoît Champagne. Computational meso- and nano-science: Diradicalology in third-order nonlinear optical systems: Second hyperpolarizabilities of acetylene-linked phenalenyl-based superpolyenes. *International Journal of Quantum Chemistry*, 113(4):585–591, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakajima:2015:SNU

[NKKN15] Takahito Nakajima, Michio Katouda, Muneaki Kamiya, and Yutaka Nakatsuka. Software news and updates: NTChem: a high-performance software package for quantum molecular simulation. *International Journal of Quantum Chemistry*, 115(5):349–359, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakatomi:2019:SIM

[NKWT19] Taiki Nakatomi, Shoichi Koido, Yuya Watabe, and Toshiyuki Takayanagi. Spin-inversion mechanisms in the reactions of transition metal cations (Sc^+, Ti^+, V^+, Cr^+, Mn^+, Fe^+, Co^+, Ni^+, and Cu^+) with OCS in the gas phase: a perspective from automated reaction path search calculations. *International Journal of Quantum Chemistry*, 119 (11):e25908:1–e25908:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nguyen:2011:TSI

[NL11] Ngoc Ha Nguyen and Minh Cam Le. Theoretical study of the interaction between C_2 H_5 OH and mordenite zeolite by periodic density functional theory method. *International Journal of Quantum Chemistry*, 111(12):3151–3166, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nieto-Malagon:2012:EPE

[NMHPVG12] Guillermo Nieto-Malagón, Julio M. Hernández-Pérez, Rubicelia Vargas, and Jorge Garza. Electrostatic potential effects of β-cyclodextrin on optical properties of the 4-dimethyl-aminobenzonitrile. *International Journal of Quantum Chemistry*, 112(21):3552–3557, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niaz:2014:TIC

[NMIP14] Saba Niaz, Taniya Manzoor, Nasarul Islam, and Altaf Hussain Pandith. Theoretical investigations on C_2H_4Nb complex as a potential hydrogen storage system, using Møller–Plesset (MP2) and density functional theory. *International Journal of Quantum Chemistry*, 114(7):449–457, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakanishi:2010:SDP

[NMS+10] Yasuyuki Nakanishi, Toru Matsui, Yasuteru Shigeta, Yasutaka Kitagawa, Toru Saito, Yusuke Kataoka, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Sequence-dependent proton-transfer reaction in stacked GC pair III: The influence of proton transfer to conductivity. *International Journal of Quantum Chemistry*, 110 (12):2221–2230, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikodem:2014:LBW

[NMSR14] Astrid Nikodem, Alexei V. Matveev, Thomas M. Soini, and Notker Rösch. Load balancing by work-stealing in quantum chemistry calculations: Application to hybrid density functional methods. *International Journal of Quantum Chemistry*, 114(12):813–822, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nychyporenko:2014:SLM

[NMV+14] Oleg S. Nychyporenko, Olga P. Melnyk, Olexandr O. Viniychuk, Tetiana M. Pinchuk-Rugal, Volodymyr A. Brusentsov, Elena L. Pavlenko, Oksana P. Dmytrenko, Nikolay P. Kulish, and Olexiy D. Kachkovsky. Shape and

location of multiple charge carriers in linear π-electron systems. *International Journal of Quantum Chemistry*, 114 (6):416–428, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2017:DSDb

[NNSN17] Masahiko Nakano, Ryota Nakamura, Junji Seino, and Hiromi Nakai. Development of spin-dependent relativistic open-shell Hartree–Fock theory with time-reversal symmetry (II): the restricted open-shell approach. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakarada:2018:MIH

[NP18] Đura Nakarada and Milena Petković. Mechanistic insights on how hydroquinone disarms OH and OOH radicals. *International Journal of Quantum Chemistry*, 118(4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowroozi:2011:CBI

[NRGS11] Alireza Nowroozi, Hossain Roohi, Mohammad Sadegh Sadeghi Ghoogheri, and Mohseneh Sheibaninia. The competition between the intramolecular hydrogen bond and π-electron delocalization in trifluoroacetylacetone — a theoretical study. *International Journal of Quantum Chemistry*, 111 (3):578–585, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowroozi:2011:RIH

[NRHJ11] A. Nowroozi, H. Raissi, H. Hajiabadi, and P. Mohammadzadeh Jahani. Reinvestigation of intramolecular hydrogen bond in malonaldehyde derivatives: an ab initio, AIM and NBO study. *International Journal of Quantum Chemistry*, 111(12):3040–3047, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nochebuena:2015:VWI

[NRI15] Jorge Nochebuena, Ana Ramírez, and Joel Ireta. On the van der Waals interactions and the stability of polypeptide chains in helical conformations. *International Journal of Quantum Chemistry*, 115(22):1613–1620, November 15,

2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowroozi:2011:NSI

[NRP+11] A. Nowroozi, H. Roohi, M. Poorsargol, P. Mohammadzadeh Jahani, H. Hajiabadi, and H. Raissi. NH$\cdots$S and SH$\cdots$N intramolecular hydrogen bond in β-thioaminoacrolein: a quantum chemical study. *International Journal of Quantum Chemistry*, 111(12):3008–3016, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nowroozi:2011:CTP

[NRS+11] Alireza Nowroozi, Hossein Roohi, Mohseneh Sheibaninia, Mohammad Sadegh Sadeghi Ghoogheri, and Heidar Raissi. Conformational and tautomeric preferences in 3-aminoacrylaldehyde: a theoretical study. *International Journal of Quantum Chemistry*, 111(3):586–595, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagaraju:2010:CSF

[NS10a] M. Nagaraju and G. Narahari Sastry. Comparative study on formamide–water complex. *International Journal of Quantum Chemistry*, 110(10):1994–2003, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nasertayoob:2010:RFQ

[NS10b] Payam Nasertayoob and Shant Shahbazian. Revisiting the foundations of the quantum theory of atoms in molecules: The subsystem variational procedure and the finite nuclear models. *International Journal of Quantum Chemistry*, 110 (6):1188–1196, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nagy:2013:FWF

[NS13] Péter R. Nagy and Ágnes Szabados. Frontiers in wave function theory: Unitary perturbation theory applied to multiconfigurational reference functions. *International Journal of Quantum Chemistry*, 113(3):230–238, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nabi:2019:ICL

[NS19] Fathola A. Nabi and Alireza Shayesteh. Ab initio calculations on low-lying electronic states of PdH. *International Journal of Quantum Chemistry*, 119(17):e25967:1–e25967:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakano:2017:DSDa

[NSN17] Masahiko Nakano, Junji Seino, and Hiromi Nakai. Development of spin-dependent relativistic open-shell Hartree–Fock theory with time-reversal symmetry (I): the unrestricted approach. *International Journal of Quantum Chemistry*, 117(10):??, May 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakai:2015:SIA

[NT15] Hiromi Nakai and Takao Tsuneda. Special issue article: Preface. *International Journal of Quantum Chemistry*, 115 (5):245–246, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naskar:2018:ESB

[NTCG18] Pulak Naskar, Srijeeta Talukder, Pinaki Chaudhury, and Subhasree Ghosh. The effect of stochastic barrier fluctuation on semiclassical transmission probability and Shannon entropy of a symmetric double well potential. *International Journal of Quantum Chemistry*, 118(17):e25667:1–e25667:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nemukhin:2013:PQC

[NTCK13] Alexander Nemukhin, Igor Topol, Jack Collins, and Maria Khrenova. Perspectives: Quantum chemistry in studies of fluorescent and photosensing proteins. *International Journal of Quantum Chemistry*, 113(14):1828–1832, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naskar:2019:CID

[NTGC19] Pulak Naskar, Srijeeta Talukder, Subhasree Ghosh, and Pinaki Chaudhury. Controlling the isomerization dynamics of iodide acetonitrile dimer complex by optimally de-

signed electromagnetic field: a wave packet based approach. *International Journal of Quantum Chemistry*, 119 (14):e25927:1–e25927:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nguyen:2010:DFT

[NTNL10] Ngoc Ha Nguyen, Thanh Hue Tran, Minh Tho Nguyen, and Minh Cam Le. Density functional theory study of the oxidative dehydrogenation of propane on the (001) surface of V_2 O_5. *International Journal of Quantum Chemistry*, 110(14):2653–2670, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nikolaev:2010:MIE

[NVI10] Alexander V. Nikolaev, Bart Verberck, and Galina V. Ionova. Molecular interaction energies and optimal configuration of a cubane dimer. *International Journal of Quantum Chemistry*, 110(5):1063–1069, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nicolas-Vazquez:2013:NAP

[NVPCJ+13] Inés Nicolás-Vázquez, Guadalupe Pérez-Caballero, Annia Galano Jiménez, Georgina Guzmán Rangel, and René Miranda Ruvalcaba. A novel azocompound, 2-(4-phenylazoaniline)-4-phenylphenol: Spectroscopic and quantum-chemical approach. *International Journal of Quantum Chemistry*, 113(8):1107–1115, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Naumkin:2012:BCC

[NW12] Fedor Y. Naumkin and David J. Wales. Beryllium cluster cages endohedrally doped by hydrogen: $H_2@Be_n$ ($8 \leq n \leq 14$). *International Journal of Quantum Chemistry*, 112(18): 3068–3075, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niu:2011:MAR

[NWQX11] Ying-Yu Niu, Rong Wang, Ming-Hui Qiu, and Jun-Ling Xiu. Multiphoton association reaction He + $H^+ \rightarrow HeH^+$ steered by ultra-short laser pulse. *International Journal of Quantum Chemistry*, 111(9):2117–2122, August 5,

2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nakai:2013:PSI

[NYA+13] Hiromi Nakai, Kazunari Yoshizawa, Koji Ando, Takahito Nakajima, and Erkki J. Brändas. Preface: Special issue: Seventh Congress of the International Society for Theoretical Chemical Physics. *International Journal of Quantum Chemistry*, 113(3):171–172, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nyman:2014:TRC

[Nym14] Gunnar Nyman. Tutorial review: Computational methods of quantum reaction dynamics. *International Journal of Quantum Chemistry*, 114(18):1183–1198, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nishihara:2010:UMM

[NYS+10] Satomich Nishihara, Shusuke Yamanaka, Tohru Saito, Yasutaka Kitagawa, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. UNO- and ULO-MRCC(Mk), AP-UCC and AP-UBD approaches to diradical systems. *International Journal of Quantum Chemistry*, 110(15):3015–3026, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ndambuki:2013:AUT

[NZ13] Sylvester Ndambuki and Tom Ziegler. An analysis of unsupported triple and quadruple metal–metal bonds between two homonuclear group 6 transition elements based on the combined natural orbitals for chemical valence and extended transition state method. *International Journal of Quantum Chemistry*, 113(6):753–761, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Nunez-Zarur:2010:DFS

[NZAVR10] Francisco Núñez-Zarur, Eduardo Arguello, and Ricardo Vivas-Reyes. Density functional study on electronic structures and reactivity in methyl-substituted chelates used in organic light-emitting diodes. *International Journal of Quantum Chemistry*, 110(9):1622–1636, August 5, 2010.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Niu:2015:GPA

[NZLG15] Wenxia Niu, Hong Zhang, Peng Li, and Tao Gao. Gas-phase ammonia activation by Th, Th^+, and Th^{2+}: Reaction mechanisms, bonding analysis, and rate constant calculations. *International Journal of Quantum Chemistry*, 115(1):6–18, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orgaz:2012:HHI

[OA12] Emilio Orgaz and Andrea Aburto. Hydrogen–hydrogen interaction in the $LaNiInH_{4/3}$ hydride. *International Journal of Quantum Chemistry*, 112(21):3490–3497, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Otaki:2013:CMS

[OA13] Hiroki Otaki and Koji Ando. Computations of molecular structure, properties and spectroscopies: Atoms-in-molecules analysis of the effect of intermolecular interactions on dielectric properties in hydrogen-bonded material 5-bromo-9-hydroxyphenalenone. *International Journal of Quantum Chemistry*, 113(3):386–392, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Omidyan:2019:POP

[OAA19] Reza Omidyan, Maryam Abbasi, and Gholamhassan Azimi. Photophysical and optoelectronic properties of a platinum(II) complex and its derivatives, designed as a highly efficient OLED emitter: a theoretical study. *International Journal of Quantum Chemistry*, 119(3):e25793:1–e25793:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

OBrien:2017:CSP

[OAC17] Joseph Senan O'Brien, Matthew J. Allen, and Gerardo Andrés Cisneros. Computational study of pH-responsive di-lanthanide complexes. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017.

CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ona:2013:OLC

[OAT+13] Ofelia B. Oña, Diego R. Alcoba, William Tiznado, Alicia Torre, and Luis Lain. An orbital localization criterion based on the topological analysis of the electron localization function. *International Journal of Quantum Chemistry*, 113(9):1401–1408, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oliveira:2019:MOS

[OB19] Marco A. S. Oliveira and Itamar Borges, Jr. On the molecular origin of the sensitivity to impact of cyclic nitramines. *International Journal of Quantum Chemistry*, 119(8):e25868:1–e25868:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortiz:2010:DSF

[OCB+10] E. Ortiz, A. Cuán, C. Badillo, C. M. Cortés-Romero, Q. Wang, and L. Noreña. DFT study of ferroelectric properties of the copolymers: Poly(vinylideneflouride-trifluoroethylene) and poly(vinylidene fluoride-chlorotrifluoroethylene). *International Journal of Quantum Chemistry*, 110(13): 2411–2417, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ortolan:2019:CCS

[OCGM+19] Alexandre O. Ortolan, Nicholas D. Charistos, Raul Guajardo-Maturana, Carolina Olea Ulloa, Giovanni F. Caramori, Renato L. T. Parreira, and Alvaro Muñoz-Castro. On the cation-π capabilities of small all sp^2-carbon host structures. Evaluation of $[6.8]_3$ cyclacene from relativistic DFT calculations. *International Journal of Quantum Chemistry*, 119(4):e25811:1–e25811:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oliveira:2018:LCH

[OCL+18] Igor M. Oliveira, Marcos A. Castro, Salviano A. Leão, Tertius L. Fonseca, and Renato B. Pontes. Li_4 C_4 H_2 N_2: a molecule with large hyperpolarizabilities and electride characteristic. *International Journal of Quantum Chemistry*,

118(21):e25661:1–e25661:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozkan:2012:RCA

[OD12] Ilker Ozkan and Yavuz Dede. Reactions of ^{1}S, ^{1}D, and ^{3}P carbon atoms with water. Oxygen abstraction and intermolecular formaldehyde generation mechanisms: An MCSCF study. *International Journal of Quantum Chemistry*, 112(4):1165–1184, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozkaya:2016:CTF

[OD16] Sibel Ozkaya and Gokcen Birlik Demirel. Chemisorption of thiol-functionalized metallocene molecules on Si(111)–Ag$\sqrt{3} \times \sqrt{3}$ surface: a density functional theory study. *International Journal of Quantum Chemistry*, 116(1):35–41, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ozdemiir:2011:QCI

[ÖEDB11] Namik Özdemiır, Biılge Eren, Muharrem Dıınçer, and Yunus Bekdemiır. Quantum-chemical, IR, NMR, and X-ray diffraction studies on 2-(4-chlorophenyl)-1-methyl-1H-benzo[d]imidazole. *International Journal of Quantum Chemistry*, 111(12):3112–3124, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Orenha:2019:HDP

[OG19] Renato P. Orenha and Sergio E. Galembeck. How does the pH influences the Ru–NO coordination compounds? *International Journal of Quantum Chemistry*, 119(20): e25999:1–e25999:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Opoku:2018:USE

[OGvSG18] Francis Opoku, Krishna Kuben Govender, Cornelia Gertina Catharina Elizabeth van Sittert, and Penny Poomani Govender. Understanding the synergistic effects, optical and electronic properties of ternary Fe/C/S-doped TiO_2 anatase within the DFT + U approach. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2012:TSH

[OH12] Taku Onishi and Trygve Helgaker. A theoretical study on hydrogen transport mechanism in $SrTio_3$ perovskite. *International Journal of Quantum Chemistry*, 112(1):201–207, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2013:CMN

[OH13] Taku Onishi and Trygve Helgaker. Computational meso- and nano-science: a theoretical study on the hydrogen transport mechanism in $SrTiO_3$ perovskite. II. Scandium doping at titanium site. *International Journal of Quantum Chemistry*, 113(4):599–604, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ou:2019:BCR

[OH19] Jen-Hao Ou and Yew Kam Ho. Benchmark calculations of Rényi, Tsallis entropies, and Onicescu information energy for ground state helium using correlated Hylleraas wave functions. *International Journal of Quantum Chemistry*, 119(14):e25928:1–e25928:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ono:2013:FMS

[OHDA13] Junichi Ono, Kim Hyeon-Deuk, and Koji Ando. Frontiers in molecular simulations: Semiquantal molecular dynamics simulations of hydrogen-bond dynamics in liquid water using spherical Gaussian wave packets. *International Journal of Quantum Chemistry*, 113(3):356–365, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2013:NCT

[Oht13] Katsuhisa Ohta. Nonsingular constraints in time-dependent variational principle for parametrized wave functions. *International Journal of Quantum Chemistry*, 113 (2):161–170, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

OReilly:2016:DHA

[OK16] Robert J. O'Reilly and Amir Karton. A dataset of highly accurate homolytic N — Br bond dissociation energies ob-

tained by means of W2 theory. *International Journal of Quantum Chemistry*, 116(1):52–60, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Osella:2019:EEC

[OK19] Silvio Osella and Stefan Knippenberg. Environmental effects on the charge transfer properties of Graphene quantum dot based interfaces. *International Journal of Quantum Chemistry*, 119(10):e25882:1–e25882:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okumura:2010:DCH

[OKK10] Mitsutaka Okumura, Yasutaka Kitagawa, and Takashi Kawakami. DFT calculations for the heterojunction effect between metal clusters and the stabilizer molecules. *International Journal of Quantum Chemistry*, 110(15):2903–2911, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

OReilly:2012:HCH

[OKR12] Robert J. O'Reilly, Amir Karton, and Leo Radom. NH and NCl homolytic bond dissociation energies and radical stabilization energies: an assessment of theoretical procedures through comparison with benchmark-quality W2w data. *International Journal of Quantum Chemistry*, 112 (8):1862–1878, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olsen:2011:CMP

[Ols11a] Jeppe Olsen. The CASSCF method: a perspective and commentary. *International Journal of Quantum Chemistry*, 111(13):3267–3272, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olson:2011:ATS

[Ols11b] John A. Olson. Atomic term symbols via partitioning techniques. *International Journal of Quantum Chemistry*, 111 (12):2844–2850, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ostojic:2013:TSC

[OMĐ13a] Bojana D. Ostojić, Slobodan Mišić, and Dragana S. Đordević. A theoretical study of conformational flexibility, magnetic properties, and polarizabilities of trimethylnaphthalenes. *International Journal of Quantum Chemistry*, 113(15):1890–1898, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Otsuka:2013:CBB

[OM13b] Takao Otsuka and Tsuyoshi Miyazaki. Computational biochemistry and biophysics: a quantum chemistry study of Ds–Pa unnatural DNA base pair. *International Journal of Quantum Chemistry*, 113(4):504–509, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olvera-Neria:2011:NOA

[ONBP11] O. Olvera-Neria, V. Bertin, and E. Poulain. The nitric oxide adsorption on gold neutral, cation, and anion atoms: a comparative ab initio MRCI–MRPT2 studies. *International Journal of Quantum Chemistry*, 111(9):2054–2063, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2010:ECC

[Oni10] Taku Onishi. The effects of counter cation on oxide ion conductivity: In the case of Sr-doped $LaAlO_3$ perovskite. *International Journal of Quantum Chemistry*, 110(15):2912–2917, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onishi:2012:MDN

[Oni12] Taku Onishi. A material design on new sodium ion conductor for sodium-sulfur battery. I. $NaAlO(CN)_2$ and $Na_xAl_{1-x/3}$ $(CN)_3$ perovskite. *International Journal of Quantum Chemistry*, 112(24):3777–3781, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Okumura:2013:CSP

[ONK+13] Mitsutaka Okumura, Yasuyuki Nakanishi, Keiji Kinoshita, Satoru Yamada, Yasutaka Kitagawa, Takashi Kawakami,

Shunsuke Yamanaka, Toru Amaya, and Toshikazu Hirao. Computations of structures, properties and functions of complex systems: Theoretical investigation for the stability of the concave-bound cyclopentadienyl iron complex of sumanene. *International Journal of Quantum Chemistry*, 113(4):437–442, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Onate:2019:FIU

[OOI+19] Clement A. Onate, Michael C. Onyeaju, Akpan N. Ikot, Osarodion Ebomwonyi, and John O. A. Idiodi. Fisher information and uncertainty relations for potential family. *International Journal of Quantum Chemistry*, 119(19): e25991:1–e25991:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oller:2018:GLR

[OPAVM18] Javier Oller, Patricia Pérez, Paul W. Ayers, and Esteban Vöhringer-Martinez. Global and local reactivity descriptors based on quadratic and linear energy models for α, β-unsaturated organic compounds. *International Journal of Quantum Chemistry*, 118(20):e25706:1–e25706:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Olivares-Pilon:2017:HHH

[OPC17] Horacio Olivares-Pilón and Salvador A. Cruz. The H, H_2^+, and HeH^{2+} systems confined by an impenetrable spheroidal cavity: Revisited study via the Lagrange-mesh approach. *International Journal of Quantum Chemistry*, 117(17):??, September 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohanessian:2011:RPZ

[OPF11] Gilles Ohanessian, Delphine Picot, and Gilles Frison. Reactivity of polynuclear zinc-thiolate sites. *International Journal of Quantum Chemistry*, 111(6):1239–1247, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Osadchuk:2014:ICC

[OPP+14] Irina Osadchuk, Tõnis Pehk, Anne Paju, Margus Lopp, Mario Öeren, and Toomas Tamm. Isomers and conformers

of complexes of Ti(O i Pr)$_4$ with cyclopentane-1,2-dione: NMR study and DFT calculations. *International Journal of Quantum Chemistry*, 114(15):1012–1018, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ogloblya:2010:PCC

[OPS10] O. V. Ogloblya, Yu. I. Prylutskyy, and Yu. M. Strzhemechny. Peculiarities of conductance of carbon nanotube-based quantum dots. *International Journal of Quantum Chemistry*, 110(1):195–201, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oung:2018:UQT

[ORJ18] Sangwar Wadtey Oung, Julian Rudolph, and Christoph R. Jacob. Uncertainty quantification in theoretical spectroscopy: the structural sensitivity of X-ray emission spectra. *International Journal of Quantum Chemistry*, 118(2): ??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2010:I

[ÖS10a] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 110(15):2721, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohta:2010:ILP

[OS10b] Katsuhisa Ohta and Toshikazu Sakai. Intuitive local picture for spin polarization of chemical bonds. *International Journal of Quantum Chemistry*, 110(6):1172–1187, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2012:I

[ÖS12a] N. Y. Öhrn and J. R. Sabin. Introduction. *International Journal of Quantum Chemistry*, 112(1):1, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohrn:2012:SIS

[ÖS12b] N. Y. Öhrn and J. R. Sabin. Special issue: 2012 Sanibel Symposium. *International Journal of Quantum Chemistry*,

112(24):3721, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Owen:2012:CTA

[OSJ+12] Michael C. Owen, Milán Szó´ri, Balázs Jojárt, Bela Viskolcz, and Imre G. Csizmadia. Conformational and thermodynamic analysis of the COXIB scaffold using quantum chemical calculations. *International Journal of Quantum Chemistry*, 112(3):922–936, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oba:2014:TIP

[OT14] Yuki Oba and Masanori Tachikawa. Theoretical investigation of a positron binding to an aspartame molecule using the ab initio multicomponent molecular orbital approach. *International Journal of Quantum Chemistry*, 114 (17):1146–1149, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Osmushko:2016:ADM

[OVT+16] Ivan S. Osmushko, Vitaliy I. Vovna, Sergey A. Tikhonov, Yuriy V. Chizhov, and Irina V. Krauklis. Application of DFT for the modeling of the valence region photoelectron spectra of boron and *d*-element complexes and macromolecules. *International Journal of Quantum Chemistry*, 116(4):325–332, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Oruganti:2018:TRQ

[OWD18] Baswanth Oruganti, Jun Wang, and Bo Durbeej. Tutorial reviews: Quantum chemical design of rotary molecular motors. *International Journal of Quantum Chemistry*, 118 (1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Owens:2017:SSS

[Owe17] Frank J. Owens. Structure and stability of solvation complexes of trimethyl phosphate and dimethyl methyl phosphonate. *International Journal of Quantum Chemistry*, 117 (7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Partovi-Azar:2016:IPQ

[PABSK16] Pouya Partovi-Azar, Matthias Berg, Simone Sanna, and Thomas D. Kühne. Improved parameterization of the quantum harmonic oscillator model based on localized Wannier functions to describe van der Waals interactions in density functional theory. *International Journal of Quantum Chemistry*, 116(15):1160–1165, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poltev:2010:DSP

[PAD+10] Valeri I. Poltev, Victor M. Anisimov, Victor I. Danilov, Tanja van Mourik, Alexandra Deriabina, Eduardo González, Maria Padua, Dolores Garcia, Francisco Rivas, and Nina Polteva. DFT study of polymorphism of the DNA double helix at the level of dinucleoside monophosphates. *International Journal of Quantum Chemistry*, 110(13):2548–2559, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pomogaev:2015:SEP

[PAKA15] Vladimir A. Pomogaev, Pavel V. Avramov, Alex A. Kuzubov, and Victor Ya. Artyukhov. Structure and electronic properties of hollow-caged C_{60} fullerene-derived $(MN_4)_nC_{6(10-n)}$ (M = Zn, Mg, Fe, n = 1–6) complexes. *International Journal of Quantum Chemistry*, 115(4):239–244, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palacios:2010:KIR

[Pal10] José Luis Palacios. On the Kirchhoff index of regular graphs. *International Journal of Quantum Chemistry*, 110 (7):1307–1309, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pandey:2016:TIR

[Pan16] Krishna K. Pandey. Theoretical insights into the relative bonding of normal and abnormal N-heterocyclic carbenes in $[PdCl_2\ (NHC^R)_2]$ and $[PdCl_2\ (NHC^R)(aNHC^R)]$ (R = H, Ph, Mes). *International Journal of Quantum Chemistry*, 116(7):537–546, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2019:CCD

[Pan19] Yong Pan. Cr concentration driving the structural, mechanical, and thermodynamic properties of Cr–Al compounds from first-principles calculations. *International Journal of Quantum Chemistry*, 119(15):e25943:1–e25943:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Posada-Amarillas:2016:CSS

[PAPCMM+16] Alvaro Posada-Amarillas, Rafael Pacheco-Contreras, Sharity Morales-Meza, Mario Sanchez, and J. Christian Schön. Computational studies of stable hexanuclear Cu_l Ag_m Au_n $(l+m+n = 6; l, m, n > 0)$ clusters. *International Journal of Quantum Chemistry*, 116(13):1006–1015, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pathak:2015:SHP

[Pat15] Arup Kumar Pathak. Stepwise hydration of phosphate anion: a microscopic theory connecting domain of instability and stability. *International Journal of Quantum Chemistry*, 115(7):413–418, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puzzarini:2010:BCM

[PB10] Cristina Puzzarini and Vincenzo Barone. Benchmark calculations for molecules in the gas phase: State-of-the-art coupled-cluster computations. *International Journal of Quantum Chemistry*, 110(3):637–655, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piccardo:2015:GVP

[PBB15] Matteo Piccardo, Julien Bloino, and Vincenzo Barone. Generalized vibrational perturbation theory for rotovibrational energies of linear, symmetric and asymmetric tops: Theory, approximations, and automated approaches to deal with medium-to-large molecular systems. *International Journal of Quantum Chemistry*, 115(15):948–982, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Persson:2012:I

[PBL12] Petter Persson, Tore Brinck, and Roland Lindh. Introduction. *International Journal of Quantum Chemistry*, 112 (7):1759, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez-Badell:2010:MMH

[PBM10] Yoana Pérez-Badell and Luis A. Montero. Multiple minima hypersurfaces studies of aluminosilicate hydration. *International Journal of Quantum Chemistry*, 110(3):586–594, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Polyak:2018:AUG

[PBR18] Iakov Polyak, Michael J. Bearpark, and Michael A. Robb. Application of the unitary group approach to evaluate spin density for configuration interaction calculations in a basis of S^2 eigenfunctions. *International Journal of Quantum Chemistry*, 118(12):e25559:1–e25559:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putz:2013:EKH

[PC13] Mihai V. Putz and Pratim K. Chattaraj. Electrophilicity kernel and its hierarchy through softness in conceptual density functional theory. *International Journal of Quantum Chemistry*, 113(18):2163–2171, September 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Penotti:2016:CRS

[PC16] Fabio E. Penotti and David L. Cooper. Combining rival π-space descriptions of O_3 and of SO_2. *International Journal of Quantum Chemistry*, 116(9):718–730, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paschoal:2014:NXX

[PCD14] Diego Paschoal, Marcello F. Costa, and Hélio F. Dos Santos. NLO-X (X = I–III): New Gaussian basis sets for prediction of linear and nonlinear electric properties. *International Journal of Quantum Chemistry*, 114(12):796–804,

June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paiva:2018:SNI

[PCF+18] Pedro Paiva, Inês P. D. Costa, Cleide E. Ferreira, Pedro Ferreira, Andreia T. Pereira, Nuno M. F. S. A. Cerqueira, Pedro A. Fernandes, and Maria J. Ramos. Studies on neuraminidase inhibition. *International Journal of Quantum Chemistry*, 118(9):e25592:1–e25592:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Penotti:2019:RSD

[PCK19] Fabio E. Penotti, David L. Cooper, and Peter B. Karadakov. Is the S_2 N_2 ring a singlet diradical? Critical analysis of alternative valence bond descriptions. *International Journal of Quantum Chemistry*, 119(7):e25845:1–e25845:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parreira:2012:HBR

[PCMG12] Renato L. T. Parreira, Giovanni F. Caramori, Nelson H. Morgon, and Sérgio E. Galembeck. Hydrogen bond and the resonance effect on the formamide–water complexes. *International Journal of Quantum Chemistry*, 112(5):1401–1420, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palermo:2008:RAR

[PCML08] Nicholas Y. Palermo, József Csontos, Richard F. Murphy, and Sándor Lovas. Role of aromatic residues in stabilizing the secondary and tertiary structure of avian pancreatic polypeptide. *International Journal of Quantum Chemistry*, 108(4):814–819, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pipolo:2011:CFE

[PCR+11] Silvio Pipolo, Roberto Cammi, Antonio Rizzo, Chiara Cappelli, Benedetta Mennucci, and Jacopo Tomasi. Cavity field effects within a polarizable continuum model of solvation: Application to the calculation of electronic circular dichroism spectra of R-(+)-3-methyl-cyclopentanone. *International Journal of Quantum Chemistry*, 111(4):826–

838, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peng:2019:CCS

[PCV19] Chong Peng, Justus A. Calvin, and Edward F. Valeev. Coupled-cluster singles, doubles and perturbative triples with density fitting approximation for massively parallel heterogeneous platforms. *International Journal of Quantum Chemistry*, 119(12):e25894:1–e25894:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paidarova:2011:TUF

[PD11] Ivana Paidarová and Philippe Durand. Towards a unified formulation of dynamics and thermodynamics II. Dissipative processes and entropy production. *International Journal of Quantum Chemistry*, 111(2):237–244, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Papamokos:2014:TAM

[PDNC14] George Papamokos, Jens Dreyer, Luciano Navarini, and Paolo Carloni. Trapping acrylamide by a Michael addition: a computational study of the reaction between acrylamide and niacin. *International Journal of Quantum Chemistry*, 114(9):553–559, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palin:2014:RCS

[PDR+14] Erika J. Palin, Martin T. Dove, Simon A. T. Redfern, Joaquín Ortega-Castro, Claro Ignacio Sainz-Díaz, and Alfonso Hernández-Laguna. Reviews: Computer simulations of cations order-disorder in 2:1 dioctahedral phyllosilicates using cation-exchange potentials and Monte Carlo methods. *International Journal of Quantum Chemistry*, 114(19): 1257–1286, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pavlov:2011:ETF

[PE11] Mikhail Pavlov and Alexander Ermilov. The electronic terms of the finite-length nanotubes, generated by edge states: A CASSCF study. *International Journal of Quantum Chemistry*, 111(11):2592–2601, September 2011. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pearson:2011:NPA

[Pea11] Ralph G. Pearson. A new property of atom energies. *International Journal of Quantum Chemistry*, 111(12):2727–2731, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paixao:2012:TSI

[PEA+12] Nathália Magalhães Paixão, Lucas Fagundes Esteves, Cleber Paulo Andrada Anconi, Clebio Soares Nascimento Jr., Wagner Batista De Almeida, Hélio Ferreira Dos Santos, and Luiz Antônio Sodré Costa. Theoretical study of inclusion of a dinuclear platinum(II) complex in α, β, and γ-cyclodextrins. *International Journal of Quantum Chemistry*, 112(20):3403–3408, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pedone:2016:RRA

[Ped16] Alfonso Pedone. Reviews: Recent advances in solid-state NMR computational spectroscopy: the case of aluminosilicate glasses. *International Journal of Quantum Chemistry*, 116(21):1520–1531, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Percus:2010:RIA

[Per10a] J. K. Percus. The role of inequalities in the analysis of many-body systems. *International Journal of Quantum Chemistry*, 110(15):2996–3004, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perger:2010:FPC

[Per10b] W. F. Perger. First-principles calculation of second-order elastic constants and equations of state for lithium azide, LiN_3, and lead azide, $Pb(N_3)_2$. *International Journal of Quantum Chemistry*, 110(10):1916–1922, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pernal:2018:TRC

[Per18] Katarzyna Pernal. Tutorial reviews: Correlation energy from random phase approximations: a reduced density

matrices perspective. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Polkehn:2018:RQD

[PETB18] Matthias Polkehn, Pierre Eisenbrandt, Hiroyuki Tamura, and Irene Burghardt. Reviews: Quantum dynamical studies of ultrafast charge separation in nanostructured organic polymer materials: Effects of vibronic interactions and molecular packing. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PereiradosSantos:2013:IBD

[PFdM13] Marcos Andre Pereira dos Santos, Wiliam Ferreira da Cunha, Pedro Henrique de Oliveira Neto, and Geraldo Magela e Silva. Influence of bipolaron density on the transport properties of thermalized organic conductors. *International Journal of Quantum Chemistry*, 113(23):2540–2545, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perez-Gonzalez:2012:SAM

[PGG12] Adriana Pérez-González and Annia Galano. On the ˙OH and ˙OOH scavenging activity of 3-methyl-1-pyridin-2-yl-5-pyrazolone: Comparisons with its parent compound, edaravone. *International Journal of Quantum Chemistry*, 112 (21):3441–3448, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pacheco-Garcia:2010:ESE

[PGGRMP10] C. Pacheco-García, J. García-Ravelo, J. Morales, and J. J. Peña. Exactly solvable effective mass Schrödinger equation with Coulomb-like potential. *International Journal of Quantum Chemistry*, 110(15):2880–2885, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2015:BSS

[PGMGRM15] José Juan Peña, Jesús García-Martínez, Jesus García-Ravelo, and Jesus Morales. Bound state solutions of D-dimensional Schrödinger equation with exponential-type potentials. *International Journal of Quantum Chemistry*,

115(3):158–164, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paukku:2012:QTM

[PH12] Y. Paukku and G. Hill. Quantum topological molecular descriptors in QSAR analysis of organophosphorus compounds. *International Journal of Quantum Chemistry*, 112 (5):1343–1352, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pham:2019:ISL

[Pha19] Tuan Anh Pham. Ab initio simulations of liquid electrolytes for energy conversion and storage. *International Journal of Quantum Chemistry*, 119(1):e25795:1–e25795:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pandith:2013:CAQ

[PI13] Altaf Hussain Pandith and Nasarul Islam. Comparative assessment of QSTR models based on density functional, Hartree–Fock, AM1, and PM3 methods for acute toxicity of aliphatic compounds toward *Vibrio fischeri*. *International Journal of Quantum Chemistry*, 113(6):830–839, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Provorse:2016:TRE

[PI16] Makenzie R. Provorse and Christine M. Isborn. Tutorial reviews: Electron dynamics with real-time time-dependent density functional theory. *International Journal of Quantum Chemistry*, 116(10):739–749, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pierloot:2011:TMC

[Pie11] K. Pierloot. Transition metals compounds: Outstanding challenges for multiconfigurational methods. *International Journal of Quantum Chemistry*, 111(13):3291–3301, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piela:2012:IIS

[Pie12] Lucjan Piela. Intermolecular interactions — from some general features to conformational autocatalysis. *Interna-*

tional Journal of Quantum Chemistry, 112(18):3091–3097, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2013:NOF

[Pir13] M. Piris. A natural orbital functional based on an explicit approach of the two-electron cumulant. *International Journal of Quantum Chemistry*, 113(5):620–630, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Prats:2018:GCA

[PIS18] Hèctor Prats, Francesc Illas, and Ramón Sayós. General concepts, assumptions, drawbacks, and misuses in kinetic Monte Carlo and microkinetic modeling simulations applied to computational heterogeneous catalysis. *International Journal of Quantum Chemistry*, 118(9):e25518:1–e25518:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pitaevskii:2012:APD

[Pit12] L. P. Pitaevskii. On analytical properties of the diamagnetic permeability in the presence of the spatial dispersion. *International Journal of Quantum Chemistry*, 112 (18):2998–3001, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2019:SCA

[PJ19] Vladimir I. Pupyshev and Henry E. Montgomery Jr. On the shell-confined atom problem. *International Journal of Quantum Chemistry*, 119(10):e25887:1–e25887:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Preat:2008:TST

[PJP08] Julien Preat, Denis Jacquemin, and Eric A. Perpète. Tayloring standard TDDFT approaches for computing UV/Vis transitions in thiocarbonyl chromophores. *International Journal of Quantum Chemistry*, 108(4):762–773, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Preat:2010:UVS

[PJP10] Julien Preat, Denis Jacquemin, and Eric A. Perpète. A UV/VIS spectra investigation of pH-sensitive dyes using time-dependent density functional theory. *International Journal of Quantum Chemistry*, 110(12):2147–2154, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Parameswari:2013:ECC

[PK13a] Azhagesan Renuga Parameswari and Poomani Kumaradhas. Exploring the conformation, charge density distribution and the electrostatic properties of galanthamine molecule in the active site of AChE using DFT and AIM theory. *International Journal of Quantum Chemistry*, 113 (8):1200–1208, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pishtshev:2013:ASB

[PK13b] Aleksandr Pishtshev and Mihhail Klopov. Assessing structural bonding aspects of multiband superconductors through impurity-induced local lattice distortions: a case study on MgB_2. *International Journal of Quantum Chemistry*, 113(5):643–650, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poloni:2016:PTG

[PK16] Roberta Poloni and Jihan Kim. Perspectives: Thermodynamics of gas adsorption in MOFs using ab initio calculations. *International Journal of Quantum Chemistry*, 116 (8):569–572, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pogany:2014:TSP

[PKK14] Peter Pogány, Attila Kovács, and Rudy J. M. Konings. Theoretical study of Pu and Am tetracarbide molecules. *International Journal of Quantum Chemistry*, 114(9):587–597, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pooja:2016:QIE

[PKK+16] Pooja, R. Kumar, G. Kumar, R. Kumar, and Anil Kumar. Quantum information entropy of Eckart potential. *In-*

ternational Journal of Quantum Chemistry, 116(19):1413–1418, October 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pelloni:2011:SGT

[PL11] Stefano Pelloni and Paolo Lazzeretti. Stagnation graphs and topological models of magnetic-field induced electron current density for some small molecules in connection with their magnetic symmetry. *International Journal of Quantum Chemistry*, 111(2):356–367, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2018:KIM

[PL18a] Yingui Pan and Jianping Li. Kirchhoff index, multiplicative degree-Kirchhoff index and spanning trees of the linear crossed hexagonal chains. *International Journal of Quantum Chemistry*, 118(24):e25787:1–e25787:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putikam:2018:NMI

[PL18b] Raghunath Putikam and Ming-Chang Lin. A novel mechanism for the isomerization of N_2 O_4 and its implication for the reaction with H_2 O and acid rain formation. *International Journal of Quantum Chemistry*, 118(12):e25560:1–e25560:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pliego:2018:MNF

[Pli18] Josefredo R. Pliego, Jr. Mechanism of nucleophilic fluorination promoted by bis-tert-alcohol-functionalized crown-6-calix[4]arene. *International Journal of Quantum Chemistry*, 118(16):e25648:1–e25648:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patel:2012:RPI

[PM12] Vishesha Patel and Svetlana A. Malinovskaya. Realization of population inversion under nonadiabatic conditions induced by the coupling between vibrational modes via Raman fields. *International Journal of Quantum Chemistry*, 112(24):3739–3743, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2016:RCI

[PM16] M. Piris and N. H. March. Review: Chemical and ionization potentials: Relation via the Pauli potential and NOF theory. *International Journal of Quantum Chemistry*, 116 (11):805–818, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Prasad:2017:CAM

[PM17] Ajit Kumar Prasad and Phool Chand Mishra. Catalytic action of Mn-superoxide dismutase in scavenging superoxide radical anion by double hydrogen abstraction from dihydrolipoic acid: a theoretical study. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Preat:2012:PBD

[PMAP12] Julien Preat, Catherine Michaux, Jean-Marie André, and Eric A. Perpète. Pyrrolidine-based dye-sensitized solar cells: a time-dependent density functional theory investigation of the excited state electronic properties. *International Journal of Quantum Chemistry*, 112(9):2072–2084, May 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pop:2011:TCH

[PMC11] Raluca Pop, Mihai Medeleanu, and Carol Csunderlik. Theoretical considerations on the hydrolysis of 2-dichloromethylbenzimidazole. *International Journal of Quantum Chemistry*, 111(12):2868–2873, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petrovic:2019:TSN

[PMEP19] Ivana Petrović, Branislav Milovanović, Mihajlo Etinski, and Milena Petković. Theoretical scrutinization of nine benzoic acid dimers: Stability and energy decomposition analysis. *International Journal of Quantum Chemistry*, 119 (13):e25918:1–e25918:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pena:2012:UTE

[PMGMGR12] J. J. Peña, J. Morales, J. García-Martínez, and J. García-Ravelo. Unified treatment of exactly solvable quantum potentials with confluent hypergeometric eigenfunctions: Generalized potentials. *International Journal of Quantum Chemistry*, 112(24):3815–3821, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Paranthaman:2016:RMO

[PMH+16] Selvarengan Paranthaman, Jiwon Moon, Kiryong Hong, Jeongho Kim, Dong Eon Kim, Joonghan Kim, and Tae Kyu Kim. Reactivity of molecular oxygen with aluminum clusters: Density functional and ab initio molecular dynamics simulation study. *International Journal of Quantum Chemistry*, 116(7):547–554, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Polkosnik:2019:FQC

[PMHM19] Walter Polkosnik, Chérif F. Matta, Lulu Huang, and Lou Massa. Fast quantum crystallography. *International Journal of Quantum Chemistry*, 119(24):e25986:1–e25986:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palazzetti:2011:SHR

[PML+11] Federico Palazzetti, Elango Munusamy, Andrea Lombardi, Gaia Grossi, and Vincenzo Aquilanti. Spherical and hyperspherical representation of potential energy surfaces for intermolecular interactions. *International Journal of Quantum Chemistry*, 111(2):318–332, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PerezDeTudela:2011:TDE

[PMMGL+11] R. Pérez De Tudela, M. Márquez-Mijares, T. González-Lezana, O. Roncero, S. Miret-Artés, G. Delgado-Barrio, and P. Villarreal. Temperature dependence of the energetics and structure for the Ar dimer and trimer. *International Journal of Quantum Chemistry*, 111(2):472–479, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Punter:2019:APR

[PNC19] Alexander Punter, Paola Nava, and Yannick Carissan. Atomic pseudopotentials for reproducing π-orbital electron behavior in sp^2 carbon atoms. *International Journal of Quantum Chemistry*, 119(23):e25914:1–e25914:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Putz:2015:PBG

[PO15] Mihai V. Putz and Ottorino Ori. Predicting bondons by Goldstone mechanism with chemical topological indices. *International Journal of Quantum Chemistry*, 115(3):137–143, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pogliani:2012:MPA

[Pog12] Lionello Pogliani. Modeling of properties of amino acids with random, semirandom, and molecular connectivity descriptors. *International Journal of Quantum Chemistry*, 112(10):2267–2274, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pacheco-Ortin:2012:PDD

[POLV12] Sandy Pacheco-Ortín, Ricardo Gaitán Lozano, and Esther Agacino Valdés. Possible DNA damage by oxidation products of guanine: a density functional and electron propagator theoretical study. *International Journal of Quantum Chemistry*, 112(16):2840–2847, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

PonsViver:2019:PIL

[Pon19] Miquel Pons Viver. The practical implementation of Löwdin's method for spin projection. *International Journal of Quantum Chemistry*, 119(4):e25770:1–e25770:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Yos20].

Popelier:2015:PQC

[Pop15] Paul L. A. Popelier. Perspective: QCTFF: On the construction of a novel protein force field. *International Journal of Quantum Chemistry*, 115(16):1005–1011, August 15,

2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Popov:2019:SHC

[Pop19] Andrey Popov. Small helium clusters formation. *International Journal of Quantum Chemistry*, 119(24):e26045:1–e26045:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Panagiotides:2010:DPA

[PP10] Nicolas Panagiotides and Nicolas I. Papanicolaou. Diffusion of platinum adatoms and dimers on Pt(111) surface by molecular-dynamics simulation. *International Journal of Quantum Chemistry*, 110(1):202–209, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pu:2014:MPC

[PP14] Maoping Pu and Timofei Privalov. Multiple-pathways of carbon dioxide binding by a Lewis acid $[B(C_6F_5)_3]$ and a Lewis base $[P(tBu)_3]$: the energy landscape perspective. *International Journal of Quantum Chemistry*, 114(4):289–294, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pastorczak:2016:RME

[PP16] Ewa Pastorczak and Katarzyna Pernal. A road to a multiconfigurational ensemble density functional theory without ghost interactions. *International Journal of Quantum Chemistry*, 116(11):880–889, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2019:SMT

[PP19a] Yong Pan and Delin Pu. The structural, mechanical, and thermodynamic properties of B2-type TMZr (TM = Ru, Mo, Rh, Os, and Re) compounds from first-principles calculations. *International Journal of Quantum Chemistry*, 119(22):e26015:1–e26015:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pimienta:2019:HFT

[PP19b] Ian Pimienta and Konrad Patkowski. Heats of formation and thermal stability of substituted 1,1'-Azobis(tetrazole)

compounds with an extended nitrogen chain. *International Journal of Quantum Chemistry*, 119(4):e25794:1–e25794:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Padilha:2011:ICB

[PPDF11] José E. Padilha, Renato B. Pontes, Antônio J. R. Da Silva, and Adalberto Fazzio. IxV curves of boron and nitrogen doping zigzag graphene nanoribbons. *International Journal of Quantum Chemistry*, 111(7–8):1379–1386, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Punkvang:2013:CBB

[PPK+13] Auradee Punkvang, Pornpan Pungpo, Pharit Kamsri, Dararat Kasamsri, Apinya Srisupan, Patchreenart Saparpakorn, Supa Hannongbua, Peter Wolschann, Supakit Prueksaaroon, and Nipawan Pongprom. Computational biochemistry and biophysics: Molecular dynamics simulations of azanaphthoquinone annelated pyrrole derivatives as anticancer agent in DNA duplex. *International Journal of Quantum Chemistry*, 113(4):555–562, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palacios:2010:BKI

[PR10a] José Luis Palacios and José Miguel Renom. Bounds for the Kirchhoff index of regular graphs via the spectra of their random walks. *International Journal of Quantum Chemistry*, 110(9):1637–1641, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perdew:2010:FEL

[PR10b] John P. Perdew and Adrienn Ruzsinszky. Fourteen easy lessons in density functional theory. *International Journal of Quantum Chemistry*, 110(15):2801–2807, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palacios:2011:BKF

[PR11a] José Luis Palacios and José M. Renom. Broder and Karlin's formula for hitting times and the Kirchhoff Index. *International Journal of Quantum Chemistry*, 111(1):35–39,

January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palacios:2011:ALD

[PR11b] José Luis Palacios and José Miguel Renom. Another look at the degree-Kirchhoff index. *International Journal of Quantum Chemistry*, 111(14):3453–3455, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pereira:2017:BDF

[PRFR17] Andreia T. Pereira, António J. M. Ribeiro, Pedro A. Fernandes, and Maria J. Ramos. Benchmarking of density functionals for the kinetics and thermodynamics of the hydrolysis of glycosidic bonds catalyzed by glycosidases. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poltev:2010:CSM

[PRG+10] V. I. Poltev, E. Rodríguez, T. I. Grokhlina, A. Deriabina, and E. Gonzalez. Computational study of the molecular mechanisms of caffeine action: Caffeine complexes with adenosine receptors. *International Journal of Quantum Chemistry*, 110(3):681–688, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Poulain:2013:IPP

[PRPU+13] Enrique Poulain, Alberto Rubio-Ponce, Victor Hugo Uc, Virineya Bertin, and Oscar Olvera-Neria. Importance of Pd and Pt excited states in N_2 O capture and activation: a comparative study with Rh and Au atoms. *International Journal of Quantum Chemistry*, 113(13):1794–1802, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pacureanu:2010:DPP

[PS10a] Liliana Pacureanu and Zeno Simon. DFT plus PCM calculation for pairing specificity of Watson–Crick-type bases in aqueous solutions. *International Journal of Quantum Chemistry*, 110(6):1295–1305, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2010:DPC

[PS10b] Xiao-Yin Pan and Viraht Sahni. Density and physical current density functional theory. *International Journal of Quantum Chemistry*, 110(15):2833–2843, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [VUC13] and replies [PS13b, PS14].

Paine:2013:CST

[PS13a] S. W. Paine and A. Salam. Computational study of tautomerism and aromaticity in mono- and dithio-substituted tropolone. *International Journal of Quantum Chemistry*, 113(9):1245–1252, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2013:LER

[PS13b] Xiao-Yin Pan and Viraht Sahni. Letters to the Editor: Reply to the comment by Vignale et al. *International Journal of Quantum Chemistry*, 113(9):1424–1425, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [PS10b, VUC13, PS14].

Pan:2014:LEC

[PS14] Xiao-Yin Pan and Viraht Sahni. Letter to the editor: Comment on "Density and physical current density functional theory". *International Journal of Quantum Chemistry*, 114(3):233–236, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [PS10b, PS13b, VUC13].

Petraglia:2015:FCD

[PSC15] Riccardo Petraglia, Stephan N. Steinmann, and Clemence Corminboeuf. A fast charge-dependent atom-pairwise dispersion correction for DFTB3. *International Journal of Quantum Chemistry*, 115(18):1265–1272, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pooja:2017:QIE

[PSGK17] Pooja, Aarti Sharma, Rama Gupta, and Anil Kumar. Quantum information entropy of modified Hylleraas plus exponential Rosen–Morse potential and squeezed states.

International Journal of Quantum Chemistry, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Promkatkaew:2013:CBB

[PSK+13] Malinee Promkatkaew, Songwut Suramitr, Thitinun Karpkird, Masahiro Ehara, and Supa Hannongbua. Computational biochemistry and biophysics: Absorption and emission properties of various substituted cinnamic acids and cinnamates, based on TDDFT investigation. *International Journal of Quantum Chemistry*, 113(4):542–554, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2016:NIA

[PSK+16] Sudip Pan, Ranajit Saha, Anand Kumar, Ashutosh Gupta, Gabriel Merino, and Pratim K. Chattaraj. A noble interaction: an assessment of noble gas binding ability of metal oxides (metal = Cu, Ag, Au). *International Journal of Quantum Chemistry*, 116(13):1016–1024, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Petsis:2019:TSM

[PSKV19] George Petsis, Zoi Salta, Agnie Mylona Kosmas, and Oscar N. Ventura. Theoretical study of the microhydration of 1-chloro and 2-chloro ethanol as a clue for their relative propensity toward dehalogenation. *International Journal of Quantum Chemistry*, 119(17):e25931:1–e25931:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Perdew:2016:TRS

[PSMD16] John P. Perdew, Jianwei Sun, Richard M. Martin, and Bernard Delley. Tutorial reviews: Semilocal density functionals and constraint satisfaction. *International Journal of Quantum Chemistry*, 116(11):847–851, June 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Prates:2011:CBP

[PSPS11] Érica T. Prates, Paulo C. T. Souza, Mónica Pickholz, and Munir S. Skaf. CHARMM-based parameterization of

neutral articaine—A widely used local anesthetic. *International Journal of Quantum Chemistry*, 111(7–8):1339–1345, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pantos:2013:PBS

[PT13] Sotirios I. Pantos and Ekaterini Tiligada. Protein backbone structure determination using RDC: an inverse kinematics approach with fast and exact solutions. *International Journal of Quantum Chemistry*, 113(8):1095–1106, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pinheiro:2012:HMS

[PTD+12] Antonio Anderson Freitas Pinheiro, Alex Gutterres Taranto, Angelo Amâncio Duarte, Aristóteles Góes Neto, Braz Tavares da Hora Júnior, Gonçalo Amarante Guimarães Pereira, Manoelito Coelho dos Santos Júnior, and Sandra Aparecida de Assis. Homology modeling studies of beta(1,3)-D-glucan synthase of *Moniliophthora perniciosa*. *International Journal of Quantum Chemistry*, 112(20):3356–3363, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peach:2011:ECD

[PTH11] Michael J. G. Peach, David J. Tozer, and Nicholas C. Handy. Exchange and correlation in density functional theory and quantum chemistry. *International Journal of Quantum Chemistry*, 111(3):563–569, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2011:DSM

[PTS+11] Ya-Ru Pan, Yi-Zhen Tang, Jing-Yu Sun, Hao Sun, and Rong-Shun Wang. The DFT study on mechanisms for NCO with C_2 H_5 reaction. *International Journal of Quantum Chemistry*, 111(12):2922–2930, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Piris:2014:PNO

[PU14] Mario Piris and Jesus M. Ugalde. Perspective on natural orbital functional theory. *International Journal of Quan-*

tum Chemistry, 114(18):1169–1175, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pineda-Urbina:2018:FPT

[PUGSFM18] Kayim Pineda-Urbina, Zeferino Gómez-Sandoval, and Roberto Flores-Moreno. h function: a protonic take on the numerical Fukui function as a graphical descriptor for deprotonation. *International Journal of Quantum Chemistry*, 118(10):e25532:1–e25532:??, May 16, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Patoary:2011:EII

[PUH+11] M. A. R. Patoary, M. Alfaz Uddin, A. K. F. Haque, M. Shahjahan, A. K. Basak, and B. C. Saha. Electron impact ionization in K-, L-, and M-shells of atomic targets. *International Journal of Quantum Chemistry*, 111(5):923–936, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pulay:2011:PCM

[Pul11] Peter Pulay. A perspective on the CASPT2 method. *International Journal of Quantum Chemistry*, 111(13):3273–3279, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2011:ESH

[Pup11a] Vladimir I. Pupyshev. Electronic states of hydrogen atom in tetrahedral and similar polyhedral cavities. *International Journal of Quantum Chemistry*, 111(11):2510–2518, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pupyshev:2011:NFS

[Pup11b] Vladimir I. Pupyshev. Nikolai F. Stepanov: Half-a-century passion for quantum chemistry. *International Journal of Quantum Chemistry*, 111(11):2719–2725, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puzzarini:2010:TSC

[Puz10] Cristina Puzzarini. A theoretical study of the CH_2 N isomers: Molecular structure and energetics. *International Journal of Quantum Chemistry*, 110(13):2483–2494,

November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puzzarini:2016:PAM

[Puz16] Cristina Puzzarini. Perspective: Accurate molecular structures of small- and medium-sized molecules. *International Journal of Quantum Chemistry*, 116(21):1513–1519, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Puzzarini:2017:PAC

[Puz17] Cristina Puzzarini. Perspective: Astronomical complex organic molecules: Quantum chemistry meets rotational spectroscopy. *International Journal of Quantum Chemistry*, 117(2):129–138, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pidko:2010:MRC

[PvS10] Evgeny A. Pidko and Rutger A. van Santen. Molecular recognition in cation-exchanged zeolites. *International Journal of Quantum Chemistry*, 110(1):210–220, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palma:2011:TDS

[PVS11] A. Palma, M. Villa, and L. Sandoval. On the time-dependent solutions of the Schrödinger equation. I. The linear time-dependent potential. *International Journal of Quantum Chemistry*, 111(7–8):1646–1650, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Palma:2012:TDS

[PVS12] A. Palma, M. Villa, and L. Sandoval. On the time-dependent solutions of the Schrödinger's equation. II. The one-mode field perturbed harmonic oscillator. *International Journal of Quantum Chemistry*, 112(12):2441–2443, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Papas:2010:DWP

[PW10] Brian N. Papas and Jerry L. Whitten. Dissociation of water on a palladium nanoparticle. *International Jour-*

nal of Quantum Chemistry, 110(15):3072–3079, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pu:2012:MLU

[PWH+12] Shang-Zhi Pu, Ya-Nan Wang, Qiang He, Xue-Pin Liao, Wen-Hua Zhang, and Bi Shi. Molecular level understanding of the role of aldehyde in vegetable-aldehyde–collagen cross-linking reaction. *International Journal of Quantum Chemistry*, 112(16):2832–2839, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peng:2010:MHD

[PWL+10] Xinyu Peng, Xueye Wang, Liming Liu, Yanling Wang, and Yuanqiang Tan. Mechanisms for H_2 O decomposition on the Si(111)-7 $\times$ 7 surface: A DFT cluster model study. *International Journal of Quantum Chemistry*, 110(6):1197–1205, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Proud:2013:APE

[PWP13] Adam J. Proud, Michael P. Walker, and Jason K. Pearson. The analysis of polarization effects on the interelectronic separations in the atoms and molecules of the G1 test set. *International Journal of Quantum Chemistry*, 113(1):76–82, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pan:2018:RWK

[PWP+18] Jie Pan, Fei Wang, Yi-Qi Pan, Yu-Zhong Xie, Guang-Yan Sun, and Guang-De Jin. The reason why a kind of diketopyrrolopyrrole-analogue can act as acceptors: Theoretical study and characterization. *International Journal of Quantum Chemistry*, 118(24):e25782:1–e25782:??, December 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Philipp:2018:QCP

[PWY+18] Dean M. Philipp, Mark A. Watson, Haoyu S. Yu, Thomas B. Steinbrecher, and Art D. Bochevarov. Quantum chemical pK_a prediction for complex organic molecules. *International Journal of Quantum Chemistry*, 118(12):

e25561:1–e25561:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Pyykko:2011:BOR

[Pyy11] Pekka Pyykkö. Björn Olof Roos (1937–2010). *International Journal of Quantum Chemistry*, 111(13):3260, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Peng:2019:CIC

[PZ19] Suoping Peng and Shaohui Zheng. A computational investigation on core-expanded subphthalocyanines. *International Journal of Quantum Chemistry*, 119(15):e25942:1–e25942:??, August 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quapp:2015:ESP

[QB15] Wolfgang Quapp and Josep Maria Bofill. Embedding of the saddle point of index two on the PES of the ring opening of cyclobutene. *International Journal of Quantum Chemistry*, 115(23):1635–1649, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quapp:2018:TTM

[QBRA18] Wolfgang Quapp, Josep Maria Bofill, and Jordi Ribas-Ariño. Toward a theory of mechanochemistry: Simple models from the very beginnings. *International Journal of Quantum Chemistry*, 118(23):e25775:1–e25775:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Quintanar:2010:SEP

[QCB+10] Carlos Quintanar, Reyna Caballero, Jorge Barreto, Elizabeth Chavira, and Ernesto E. Marinero. Structural and electronic properties of cubic CeO_2: Unpaired electrons in CeO_2. *International Journal of Quantum Chemistry*, 110 (15):2949–2954, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2012:DSE

[QCW+12] Zhibo Qu, Xiaolan Chen, Donghui Wei, Diandian Ke, Lingbo Qu, Jinwei Yuan, Yunliang Bai, Fujun Wang, and

Yufen Zhao. A DFT study of the enantioselective reduction of oxime ethers promoted by chiral spiroborate esters. *International Journal of Quantum Chemistry*, 112(5):1449–1459, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qiang:2010:RVS

[QD10] Wen-Chao Qiang and Shi-Hai Dong. The rotation-vibration spectrum for Scarf II potential. *International Journal of Quantum Chemistry*, 110(13):2342–2346, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qi:2011:SSE

[QHS11] Qi Qi, Yongquan Ha, and Yueming Sun. Structural and solvent effects on the spectroscopic properties of 1, 8-naphthalimide derivatives: a density functional study. *International Journal of Quantum Chemistry*, 111(10):2234–2241, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qi:2013:ESC

[QJ13] Dongdong Qi and Jianzhuang Jiang. The electronic structures and charge transfer properties of tetra(naphthalenedione)porphyrins and tetra(naphthalene-dithione)porphyrins as dye-sensitized solar cell skeleton. *International Journal of Quantum Chemistry*, 113(24):2605–2610, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qian:2010:IIW

[QSLY10] Ping Qian, Wei Song, Linan Lu, and Zhongzhi Yang. Ab initio investigation of water clusters $(H_2\ O)_n$ $(n = 2--34)$. *International Journal of Quantum Chemistry*, 110(10): 1923–1937, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qin:2015:SNU

[QSX+15] Xinming Qin, Honghui Shang, Hongjun Xiang, Zhenyu Li, and Jinlong Yang. Software news & updates: HONPAS: a linear scaling open-source solution for large system simulations. *International Journal of Quantum Chemistry*, 115

(10):647–655, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2010:SAC

[QTCL10] Wenwen Qu, Hongwei Tan, Guangju Chen, and Ruozhuang Liu. The self-assembled of cyclic D, L-α-peptide systems: Insights into the structure and energetics. *International Journal of Quantum Chemistry*, 110(9):1648–1659, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qu:2013:QCS

[Qu13] Yuhui Qu. Quantum-chemical study of the spin transition complex [Fe(bt)$_2$ (NCS)$_2$] (bt = 2,2′-bithiazoline). *International Journal of Quantum Chemistry*, 113(7):943–948, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Qin:2013:LAP

[QZH13] Yufang Qin, Li Zheng, and Jifeng Huang. Locating apoptosis proteins by incorporating the signal peptide cleavage sites into the general form of Chou's pseudo amino acid composition. *International Journal of Quantum Chemistry*, 113(11):1660–1667, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roncaratti:2010:WHE

[RA10a] Luiz F. Roncaratti and Vincenzo Aquilanti. Whittaker–Hill equation, Ince polynomials, and molecular torsional modes. *International Journal of Quantum Chemistry*, 110(3):716–730, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Russo:2010:PPC

[RA10b] Nino Russo and Vincenzo Aquilanti. Preface: Papers collected on the occasion of the 34th Congress of Chemists of Latin Expression (XXXIV CHITEL). *International Journal of Quantum Chemistry*, 110(3):487–488, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rojas:2018:EFS

[RAFR18a] R. A. Rojas, N. Aquino, and A. Flores-Riveros. Erratum: Fine structure in the hydrogen atom boxed in a spherical impenetrable cavity. *International Journal of Quantum Chemistry*, 118(15), August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RAFR18b].

Rojas:2018:FSH

[RAFR18b] R. A. Rojas, N. Aquino, and A. Flores-Riveros. Fine structure in the hydrogen atom boxed in a spherical impenetrable cavity. *International Journal of Quantum Chemistry*, 118(14):e25584:1–e25584:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RAFR18a].

Rodriguez:2010:GST

[RAGM10] K. V. Rodriguez, L. U. Ancarani, G. Gasaneo, and D. M. Mitnik. Ground state for two-electron and electron-muon three-body atomic systems. *International Journal of Quantum Chemistry*, 110(10):1820–1832, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Russo:2010:MSO

[RAK10] Nino Russo, Victor Ya. Antonchenko, and Eugene S. Kryachko. Molecular self-organization in micro-, nano-, and macro-dimensions: From molecules to water, nanoparticles, DNA and proteins. *International Journal of Quantum Chemistry*, 110(1):1–4, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Radu:2018:BPT

[RALK18] Luana-Flavia Radu, Amr A. A. Attia, Alexandru Lupan, and R. Bruce King. Binuclear pentalene titanium carbonyls: Comparison with related cyclopentadienyltitanium carbonyls. *International Journal of Quantum Chemistry*, 118(22):e25762:1–e25762:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roch:2018:PAO

[RAMB18] Loïc M. Roch, Tyanko Aleksiev, Riccardo Murri, and Kim K. Baldridge. Performance analysis of open-source distributed file systems for practical large-scale molecular ab initio, density functional theory, and GW + BSE calculations. *International Journal of Quantum Chemistry*, 118 (1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randazzo:2018:TBM

[RAN18] Juan M. Randazzo and Antonio Aguilar-Navarro. Three-body molecular states of the LiH_2^+ system in the Born–Oppenheimer approximation. *International Journal of Quantum Chemistry*, 118(15):e25611:1–e25611:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2008:RSB

[RB08] Milan Randić and Alexandru T. Balaban. Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. *International Journal of Quantum Chemistry*, 108(5):865–897, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RB11a].

Randic:2011:ERS

[RB11a] Milan Randić and Alexandru T. Balaban. Erratum: Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. *International Journal of Quantum Chemistry*, 111(12):3252–3253, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RB08].

Roohi:2011:ISS

[RB11b] Hossein Roohi and Sotoodeh Bagheri. Influence of substitution on the strength and nature of CH$\cdots$N hydrogen bond in XCCH $\cdots$$NH_3$ complexes. *International Journal of Quantum Chemistry*, 111(5):961–969, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2018:LAA

[RB18] Milan Randić and Alexandru T. Balaban. Local aromaticity and aromatic sextet theory beyond Clar. *International Journal of Quantum Chemistry*, 118(17):e25657:1–e25657:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ragni:2010:ECA

[RBD+10] Mirco Ragni, Ana Carla Peixoto Bitencourt, Cristiane Da S. Ferreira, Vincenzo Aquilanti, Roger W. Anderson, and Robert G. Littlejohn. Exact computation and asymptotic approximations of $6j$ symbols: Illustration of their semiclassical limits. *International Journal of Quantum Chemistry*, 110(3):731–742, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramos-Berdullas:2018:TCT

[RBGGM18] Nicolás Ramos-Berdullas, Sara Gil-Guerrero, and Marcos Mandado. Transmission channels in the time–energy uncertainty relation approach to molecular conductance: Symmetry rules for the electron transport in molecules. *International Journal of Quantum Chemistry*, 118(20):e25651:1–e25651:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rybakov:2015:CZF

[RBLZ15] Andrey A. Rybakov, Ilya A. Bryukhanov, Alexander V. Larin, and Georgy M. Zhidomirov. Carbonates in zeolites: Formation, properties, reactivity. *International Journal of Quantum Chemistry*, 115(24):1709–1717, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rybakov:2019:ISL

[RBTL19] Andrey A. Rybakov, Ilya A. Bryukhanov, Dmitrii N. Trubnikov, and Alexander V. Larin. The influence of spatial limits on the modeling chemical reactivity: the example of CO_2 hydration in MeX zeolites (Me = K, Rb, Cs). *International Journal of Quantum Chemistry*, 119(5):e25820:1–e25820:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodriguez-Bautista:2018:EDD

[RBVAG18] Mariano Rodriguez-Bautista, Rubicelia Vargas, Norberto Aquino, and Jorge Garza. Electron-density delocalization in many-electron atoms confined by penetrable walls: a Hartree–Fock study. *International Journal of Quantum Chemistry*, 118(13):e25571:1–e25571:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2015:ICS

[RBZ15] Jie Ren, Fu-Quan Bai, and Hong-Xing Zhang. The induced current strengths and aromatic pathways of heteroporphyrins and their antiaromatic derivatives. *International Journal of Quantum Chemistry*, 115(15):983–988, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rizzo:2011:DBA

[RC11] Antonio Rizzo and Chiara Cappelli. David Bishop's approach to vibrational dynamic contributions to molecular properties: Application to Jones and magnetoelectric birefringences in diatomic molecules. *International Journal of Quantum Chemistry*, 111(4):760–771, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodriguez-Cantano:2014:PIM

[RCGLV+14] Rocío Rodríguez-Cantano, Tomás González-Lezana, Pablo Villarreal, David López-Durán, Franco A. Gianturco, and Gerardo Delgado-Barrio. Path integral Monte Carlo calculations of calcium-doped ^{4}He clusters. *International Journal of Quantum Chemistry*, 114(19):1318–1326, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rincon:2010:TSM

[RCM10] David A. Rincón, M. Natália D. S. Cordeiro, and Ricardo A. Mosquera. Theoretical study of morphine and heroin: Conformational study in gas phase and aqueous solution and electron distribution analysis. *International Journal of Quantum Chemistry*, 110(13):2472–2482, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramis:2019:DFT

[RCM+19] Rafael Ramis, Rodrigo Casasnovas, Laura Mariño, Juan Frau, Miquel Adrover, Bartolomé Vilanova, Nelaine Mora-Diez, and Joaquin Ortega-Castro. A density functional theory study of the free-radical scavenging activity of aminoguanidine. Comparison with its reactive carbonyl compound and metal scavenging activities. *International Journal of Quantum Chemistry*, 119(13):e25911:1–e25911:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Richter:2014:TLS

[RCP14] Falk Richter, Philippe Carbonniere, and Claude Pouchan. Toward linear scaling: Locality of potential energy surface coupling in valence coordinates. *International Journal of Quantum Chemistry*, 114(20):1401–1411, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rani:2014:FPS

[RD14] Babita Rani and Keya Dharamvir. A first principle study of adsorption of two proximate nitrogen atoms on graphene. *International Journal of Quantum Chemistry*, 114(23): 1619–1629, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ribeiro:2011:SES

[RdA11] André A. S. T. Ribeiro and Ricardo B. de Alencastro. Solvent effects in Spectroscopy and Reactivity of Molecular Liquids: Contributions from Sylvio Canuto. *International Journal of Quantum Chemistry*, 111(7–8):1252–1255, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rejmak:2018:FSA

[RDB18] Pawel Rejmak, Jerzy Datka, and Ewa Broclawik. Fine speciation of active sites in zeolites by a CO probe: Dynamics and IR frequencies. *International Journal of Quantum Chemistry*, 118(16):e25625:1–e25625:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rejmak:2019:ITT

[RDB19] Pawel Rejmak, Jerzy Datka, and Ewa Broclawik. Identity of two types of strong Brønsted acid sites in mazzite revealed by CO probe: IR study and periodic DFT modeling. *International Journal of Quantum Chemistry*, 119(9): e25873:1–e25873:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2011:QMS

[RDM+11] Tiago Rodrigues, Daniel J. V. A. Dos Santos, Rui Moreira, Francisca Lopes, and Rita C. Guedes. A quantum mechanical study of novel potential inhibitors of cytochrome bc_1 as antimalarial compounds. *International Journal of Quantum Chemistry*, 111(6):1196–1207, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2012:MOF

[RdPW+12] Marcelo O. Rodrigues, Marcos V. de Paula, Kaline A. Wanderley, Iane B. Vasconcelos, Severino Alves Jr., and Thereza A. Soares. Metal organic frameworks for drug delivery and environmental remediation: a molecular docking approach. *International Journal of Quantum Chemistry*, 112(20):3346–3355, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reiher:2015:PSI

[Rei15] Markus Reiher. Preface: Special issue on quantum information in chemistry. *International Journal of Quantum Chemistry*, 115(19):1273, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rodrigues:2010:PBI

[RF10] Pedro C. R. Rodrigues and Fernando M. S. Silva Fernandes. Phase behavior of ionic clusters down to nanoscale. a review of recent work. *International Journal of Quantum Chemistry*, 110(2):284–292, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Regueiro-Figueroa:2016:WER

[RFEGPP+16] Martín Regueiro-Figueroa, David Esteban-Gómez, Rosa Pujales-Paradela, Laura Caneda-Martínez, Andrés de Blas,

and Carlos Platas-Iglesias. Water exchange rates and mechanisms in tetrahedral $[Be(H_2\,O)_4]^{2+}$ and $[Li(H_2\,O)_4]^{+}$ complexes using DFT methods and cluster-continuum models. *International Journal of Quantum Chemistry*, 116(19): 1388–1396, October 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rossi-Fernandez:2019:NZD

[RFMC19] Ana C. Rossi-Fernández, Lorena A. Meier, and Norberto J. Castellani. Neutral and zwitterionic dopamine species adsorbed on silver surfaces: a DFT investigation of interaction mechanism. *International Journal of Quantum Chemistry*, 119(5):e25817:1–e25817:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2012:TSE

[RFN+12] Heidar Raissi, Farzaneh Farzad, Emad Saleh Nadim, Mehdi Yoosefian, Hossein Farsi, Alireza Nowroozi, and Danial Loghmaninejad. Theoretical study of the effects of substitution, solvation, and structure on the interaction between nitriles and methanol. *International Journal of Quantum Chemistry*, 112(5):1273–1284, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramanantoanina:2013:DFT

[RGPZD13] Harry Ramanantoanina, Maja Gruden-Pavlovic, Matija Zlatar, and Claude Daul. Density functional theory study of the multimode Jahn–Teller problem in the fullerene anion. *International Journal of Quantum Chemistry*, 113(6): 802–807, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roszak:2012:TSI

[RGR12] Rafał Roszak, Robert W. Góra, and Szczepan Roszak. The theoretical studies of interactions of the $OH^{-}(H_2\,O)_n$ clusters evolution toward the hydroxide anion hydration. *International Journal of Quantum Chemistry*, 112(18):3046–3051, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rohilla:2013:TES

[RGS+13] Mehak Rohilla, Neetu Goel, Tej Vir Singh, P. Venugopalan, N. V. Suresh Kumar, and K. Tewari. Theoretical and ex-

perimental studies on solubility and reactivity behavior of lysergol, elymoclavine, and dihydrolysergol. *International Journal of Quantum Chemistry*, 113(10):1427–1435, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ravi:2012:DSS

[RGST12] P. Ravi, Girish M. Gore, Arun K. Sikder, and Surya P. Tewari. A DFT study on the structure-property relationship of aminonitropyrazole-2-oxides. *International Journal of Quantum Chemistry*, 112(6):1667–1677, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ravi:2011:QCS

[RGTS11] P. Ravi, G. M. Gore, Surya P. Tewari, and A. K. Sikder. Quantum chemical studies on the structure and detonation properties of the fused polynitrodiazoles: New high energy density molecules. *International Journal of Quantum Chemistry*, 111(15):4352–4362, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rezaeian:2019:TSI

[RI19] Mojtaba Rezaeian and Mohammad Izadyar. Theoretical study on ionic liquids based on $DBUH^+$: Molecular engineering and hydrogen bond evaluation. *International Journal of Quantum Chemistry*, 119(17):e25966:1–e25966:??, September 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Riley:2010:ISC

[Ril10] Kevin E. Riley. Ab initio studies of the characteristics of hydrogen bonds involving aromatically bound hydroxyl and amino groups and the effects of aromatic fluorine substitution on these interactions. *International Journal of Quantum Chemistry*, 110(10):1833–1841, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:2011:QMD

[Rit11] Burke Ritchie. Quantum molecular dynamics. *International Journal of Quantum Chemistry*, 111(1):1–7, January

2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:2012:CDF

[Rit12a] Burke Ritchie. Calculation of a divergence-free lamb shift. *International Journal of Quantum Chemistry*, 112(14): 2632–2636, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:2012:GSC

[Rit12b] Burke Ritchie. General solution of the Coulomb–Dirac problem: calculation of a divergence-free Lamb shift. *International Journal of Quantum Chemistry*, 112(1):5–15, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivelino:2011:TSH

[Riv11] Roberto Rivelino. Theoretical studies on hydrogen bonding interactions: From small clusters to the liquid phase. *International Journal of Quantum Chemistry*, 111(7–8):1256–1269, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2010:IHBb

[RJA+10] H. Raissi, Abraham F. Jalbout, B. Abbasi, F. Fazli, F. Farzad, E. Nadim, and Aned de Leon. Intramolecular hydrogen bond in 3-imino-propenylamine isomers: AIM and NBO studies. *International Journal of Quantum Chemistry*, 110(4):893–901, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivera-Julio:2013:FPS

[RJLPGH+13] Jagger Rivera-Julio, William López-Pérez, Rafael González-Hernández, Gene E. Escorcia-Salas, and José Sierra-Ortega. First-principles study of vanadium adsorption and diffusion on the AlN(0001) surface. *International Journal of Quantum Chemistry*, 113(6):797–801, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2010:IHBa

[RJY+10] H. Raissi, A. F. Jalbout, M. Yoosefian, Mustapha Fazli, A. Nowroozi, M. Shahinin, and A. De Leon. Intramolecu-

lar hydrogen bonding in structural conformers of 2-amino methylene malonaldehyde: AIM and NBO studies. *International Journal of Quantum Chemistry*, 110(4):821–830, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rabone:2014:DII

[RK14] Jeremy Rabone and Attila Kovács. A DFT investigation of the interactions of Pd, Ag, Sn, and Cs with silicon carbide. *International Journal of Quantum Chemistry*, 114 (22):1534–1545, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryang:2019:CED

[RKCK19] Myong-Song Ryang, Chol-Jun Kang, Hyon-Chol Choe, and Nam-Hyok Kim. Correlation of electron density and bond length to band gap for binary oxides and halides. *International Journal of Quantum Chemistry*, 119(24):e26022:1–e26022:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez:2012:ESO

[RKM12] Jessica J. Ramirez, Dmitri S. Kilin, and David A. Micha. Electronic structure and optical absorbance of doped amorphous silicon slabs. *International Journal of Quantum Chemistry*, 112(1):300–313, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rampino:2012:BOU

[RL12] S. Rampino and A. Laganà. Bond order uniform grids for quantum reactive scattering. *International Journal of Quantum Chemistry*, 112(7):1818–1828, April 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2010:ATE

[RLER10] Jaime Fernández Rico, Rafael López, Ignacio Ema, and Guillermo Ramírez. Additivity and transferability of exchange energy. *International Journal of Quantum Chemistry*, 110(6):1137–1141, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez:2013:NAD

[RLER13a] Guillermo Ramírez, Rafael López, Ignacio Ema, and Jaime Fernández Rico. A note on atomic density. *International Journal of Quantum Chemistry*, 113(1):52–55, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2013:TRS

[RLER13b] Jaime Fernández Rico, Rafael López, Ignacio Ema, and Guillermo Ramírez. Translation of real solid spherical harmonics. *International Journal of Quantum Chemistry*, 113 (10):1544–1548, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rico:2014:NCC

[RLER14] Jaime Fernández Rico, Rafael López, Ignacio Ema, and Guillermo Ramírez. Nuclear cusp conditions and their fulfillment in molecular calculations with Slater basis sets. *International Journal of Quantum Chemistry*, 114(20):1393–1400, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rabanal-Leon:2019:RER

[RLTAT19] Walter A. Rabanal-León, William Tiznado, and Luis Alvarez-Thon. Relativistic effects on the ring current strengths of the substituted borazine: $B_3N_3H_6$ (X =H, F, Cl, Br, I, At). *International Journal of Quantum Chemistry*, 119(11):e25859:1–e25859:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raghunath:2013:ICK

[RLW+13] Putikam Raghunath, Yun-Min Lee, Shang-Ying Wu, Jong-Shinn Wu, and Ming-Chang Lin. Ab initio chemical kinetics for reactions of H atoms with SiH_x ($x = 1$–3) radicals and related unimolecular decomposition processes. *International Journal of Quantum Chemistry*, 113(12):1735–1746, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruzankin:2012:NSP

[RLZ12] Sergey Ph. Ruzankin, Igor Lyskov, and Igor L. Zilberberg. Net spin and polarization components of the spin density

for the single determinant in the basis of paired orbitals. *International Journal of Quantum Chemistry*, 112(18):3052–3058, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reyes:2019:PMO

[RMC19] Andrés Reyes, Félix Moncada, and Jorge Charry. The any particle molecular orbital approach: a short review of the theory and applications. *International Journal of Quantum Chemistry*, 119(2):e25705:1–e25705:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ray:2019:MPT

[RMG+19] Suvonil Sinha Ray, Shovan Manna, Anirban Ghosh, Rajat K. Chaudhuri, and Sudip Chattopadhyay. Multireference perturbation theory with improved virtual orbitals for radicals: More degeneracies, more problems. *International Journal of Quantum Chemistry*, 119(4):e25776:1–e25776:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rashev:2011:RRR

[RMJ11] Svetoslav Rashev, David C. Moule, and Richard H. Judge. The role of rotational relaxation in the intersystem crossing between a triplet and a singlet electronic state. *International Journal of Quantum Chemistry*, 111(2):279–287, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez-Montes:2016:TPE

[RMLPGGGH16] Luz Ramírez-Montes, William López-Pérez, Alvaro González-García, and Rafael González-Hernández. Theoretical prediction of the electronic and thermodynamic properties of YN–ZrN solid solutions. *International Journal of Quantum Chemistry*, 116(1):13–20, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rozhenko:2014:ICF

[RMP+14] Alexander B. Rozhenko, Sergiy S. Mykhaylychenko, Nadiya V. Pikun, Yuriy G. Shermolovich, and Jerzy Leszczynski. Intermediate carbene formation in the reaction of thioamides with phosphorus (III) derivatives: Quan-

tum chemical investigation. *International Journal of Quantum Chemistry*, 114(4):241–248, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Romanova:2011:SPD

[RMTG11] Julia Romanova, Galia Madjarova, Alia Tadjer, and Natalia Gospodinova. Solvent polarity and dopant effect on the electronic structure of the emeraldine salt. *International Journal of Quantum Chemistry*, 111(2):435–443, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryzhkov:2013:PAE

[RMY+13] Mickhail V. Ryzhkov, Alexei Mirmelstein, Sung-Woo Yu, Brandon W. Chung, and James G. Tobin. Probing actinide electronic structure through Pu cluster calculations. *International Journal of Quantum Chemistry*, 113(16):1957–1965, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roohi:2010:IBN

[RNB+10] Hossein Roohi, Alireza Nowroozi, Sadegh Bavafa, Fahemeh Akbary, and Fazlola Eshghi. Interaction between NH_2 NO and H_2 O_2: a quantum chemistry study. *International Journal of Quantum Chemistry*, 110(10):1972–1981, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rivalta:2014:PIS

[RNC+14] Ivan Rivalta, Artur Nenov, Giulio Cerullo, Shaul Mukamel, and Marco Garavelli. Perspectives: Ab initio simulations of two-dimensional electronic spectra: The SOS/QM/MM approach. *International Journal of Quantum Chemistry*, 114(2):85–93, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rey:2010:PDI

[RNdA+10] Nicolás A. Rey, Ademir Neves, Wagner B. de Almeida, Hélio F. Dos Santos, and Luiz Antônio S. Costa. A promiscuous dicopper(II) system promoting the hydrolysis of bis(2,4-dinitrophenyl)phosphate: Gaining mechanistic insight by means of structural and spectroscopic DFT

studies. *International Journal of Quantum Chemistry*, 110 (7):1432–1442, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roohi:2010:GPH

[RNE10] Hossein Roohi, Ali-Reza Nowroozi, and Fazlola Eshghi. The gas phase hydrogen-bonded dimers of HOCl: a high-level quantum chemical study. *International Journal of Quantum Chemistry*, 110(8):1489–1499, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2013:RMG

[RNP13] Milan Randić, Marjana Novič, and Dejan Plavšić. Review: Milestones in graphical bioinformatics. *International Journal of Quantum Chemistry*, 113(22):2413–2446, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2012:ECP

[RNV+12] Milan Randić, Marjana Novič, Marjan Vračko, Damir Vukičević, and Dejan Plavšić. π-electron currents in polycyclic conjugated hydrocarbons: Coronene and its isomers having five and seven member rings. *International Journal of Quantum Chemistry*, 112(4):972–985, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Romanowski:2010:ALP

[Rom10] Zbigniew Romanowski. Application of Lobatto polynomials in atomic physics. *International Journal of Quantum Chemistry*, 110(10):1793–1802, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2013:SSE

[Roy13] Amlan K. Roy. Studies on some exponential-screened Coulomb potentials. *International Journal of Quantum Chemistry*, 113(10):1503–1510, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2014:RVS

[Roy14] Amlan K. Roy. Ro-vibrational studies of diatomic molecules in a shifted Deng–Fan oscillator potential. *Inter-*

national Journal of Quantum Chemistry, 114(6):383–391, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2015:SCC

[Roy15] Amlan K. Roy. Spherical confinement of Coulombic systems inside an impenetrable box: H atom and the Hulthén potential. *International Journal of Quantum Chemistry*, 115(15):937–947, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Roy:2016:CPS

[Roy16] Amlan K. Roy. Critical parameters and spherical confinement of H atom in screened Coulomb potential. *International Journal of Quantum Chemistry*, 116(12):953–960, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Radhakrishnan:2011:EMF

[RP11a] N. Radhakrishnan and A. John Peter. Effect of magnetic field on diamagnetic susceptibility of two interacting electrons in a quantum dot. *International Journal of Quantum Chemistry*, 111(5):1101–1107, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Radhakrishnan:2011:LEE

[RP11b] N. Radhakrishnan and A. John Peter. Laser effects in excitons in a quantum wire. *International Journal of Quantum Chemistry*, 111(3):661–668, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rhee:2016:PIM

[RP16] Young Min Rhee and Jae Woo Park. Perspectives: Interpolation for molecular dynamics simulations: from ions in gas phase to proteins in solution. *International Journal of Quantum Chemistry*, 116(8):573–577, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ragni:2011:AVM

[RPBB11] Mirco Ragni, Frederico V. Prudente, Ana C. P. Bitencourt, and Patricia R. P. Barreto. Analysis of vibrational modes

of the P_4 molecule through hyperspherical variants of the local orthogonal coordinates: The limit of dissociation in dimers. *International Journal of Quantum Chemistry*, 111 (7–8):1719–1733, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rasanen:2010:SLD

[RPVM10] E. Räsänen, S. Pittalis, J. G. Vilhena, and M. A. L. Marques. Semi-local density functional for the exchange-correlation energy of electrons in two dimensions. *International Journal of Quantum Chemistry*, 110(12):2308–2314, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramachandran:2011:EIA

[RR11] C. N. Ramachandran and Eli Ruckenstein. Encapsulation of the interstellar abundant H_3^+ in a C_{60} fullerene. *International Journal of Quantum Chemistry*, 111(14):3695–3700, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rusakov:2019:LRR

[RR19] Yuriy Yu. Rusakov and Irina L. Rusakova. Long-range relativistic heavy atom effect on^1 H NMR chemical shifts of selenium- and tellurium-containing compounds. *International Journal of Quantum Chemistry*, 119(3):e25809:1–e25809:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rupp:2012:FPS

[RRB12] Caroline Jaskulski Rupp, Jussane Rossato, and Rogério José Baierle. First-principles study of oxidized BC_2 N nanotubes. *International Journal of Quantum Chemistry*, 112 (20):3312–3319, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruiz:2011:CIC

[RRCO11] M. Belén Ruiz, Miguel Rojas, Guillermo Chicón, and Peter Otto. Configuration interaction calculations on the ^{2}P ground state of boron atom and C^+ using Slater orbitals. *International Journal of Quantum Chemistry*, 111(9):1921–1930, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rusakov:2016:HEN

[RRK16] Yu. Yu. Rusakov, Irina L. Rusakova, and Leonid B. Krivdin. On the HALA effect in the NMR carbon shielding constants of the compounds containing heavy *p*-elements. *International Journal of Quantum Chemistry*, 116(19): 1404–1412, October 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rastogi:2019:ISE

[RRRV19] Anugya Rastogi, Priyanka Rajpoot, Rupali Rastogi, and Udai P. Verma. Ab-initio study of electronic, optical, thermal, and transport properties of Cr_4 AlB_6. *International Journal of Quantum Chemistry*, 119(11):e25897:1–e25897:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramasami:2010:SMI

[RRVJ10] K. Ramasami, M. Ramalingam, P. Venuvanalingam, and M. Jaccob. Singlet methylene insertion into polar O — H and N — H bonds of water and ammonia — Ab initio and DFT study. *International Journal of Quantum Chemistry*, 110(7):1310–1316, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rolik:2009:MMP

[RS09] Zoltán Rolik and Ágnes Szabados. Multipartitioning Møller–Plesset perturbation theory: Size-extensivity at third order and symmetry conservation. *International Journal of Quantum Chemistry*, 109(11):2554–2563, ???? 2009. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [RS11a].

Rolik:2011:EMM

[RS11a] Zoltán Rolik and Ágnes Szabados. Erratum: Multipartitioning Møller–Plesset perturbation theory: Size-extensivity at third order and symmetry conservation. *International Journal of Quantum Chemistry*, 111(14):3992, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [RS09].

Roychoudhury:2011:API

[RS11b] Mihir Roychoudhury and Rakesh Kumar Srivastav. Analysis of pair interaction in a bipolar mesogen 4-(4-hydroxylbutyloxy)-4′-cyano-biphenyl: a comparative study based on semiempirical and DFT methods. *International Journal of Quantum Chemistry*, 111(15):4113–4123, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez-Solis:2012:ESA

[RS12a] A. Ramírez-Solís. The electronic spectrum of $AgBr_2$: Ab initio benchmark calculations on the $^2\Pi_u$ and $^2\Sigma_u^+$ charge transfer states including spin-orbit effects. *International Journal of Quantum Chemistry*, 112(21):3535–3542, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez-Solis:2012:MSA

[RS12b] A. Ramírez-Solís. The molecular structure of $AgBr_2$ and $AgBr_2^+$. A benchmark CASSCF, CASPT2, and averaged coupled pair functional study. *International Journal of Quantum Chemistry*, 112(22):3559–3563, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryabinkin:2013:ERB

[RS13] Ilya G. Ryabinkin and Viktor N. Staroverov. Exact relations between the electron density and external potential for systems of interacting and noninteracting electrons. *International Journal of Quantum Chemistry*, 113(11):1626–1632, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruette:2010:MAS

[RSCS10] Fernando Ruette, Morella Sánchez, Olga Castellano, and Humberto Soscún. Methodologies to analyze surface bonding properties using parametric and density functional methods. *International Journal of Quantum Chemistry*, 110(3):743–754, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rampino:2010:MBP

[RSL10] Sergio Rampino, Dimitris Skouteris, and Antonio Laganà. Microscopic branching processes: The O + O_2 reaction and its relaxed potential representations. *International Journal of Quantum Chemistry*, 110(2):358–367, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Robb:2011:F

[RSL11] Mike Robb, Per Siegbahn, and Roland Lindh. Foreword. *International Journal of Quantum Chemistry*, 111 (13):3255, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez-Solis:2012:NVE

[RSM12] Alejandro Ramírez-Solís and Laurent Maron. Nonharmonic vibrational effects in HgClOH: an MP2 Born–Oppenheimer molecular dynamics study. *International Journal of Quantum Chemistry*, 112(21):3484–3489, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ramirez-Solis:2012:NES

[RSN12] Alejandro Ramírez-Solís and Octavio Novaro. Nonadditive effects on the stability of Be_3: a benchmark CASSCF + averaged quadratic coupled cluster study of the equilateral and linear symmetrical configurations. *International Journal of Quantum Chemistry*, 112(17):2952–2956, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reyes:2010:P

[RSV10] Andrés Reyes and José Luis Sanz-Vicario. Preface. *International Journal of Quantum Chemistry*, 110(13):2331, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rahimi:2019:STN

[RTG+19] Ali Mehdizadeh Rahimi, Amirhossein Molavi Tabrizi, Spencer Goossens, Matthew G. Knepley, and Jaydeep P. Bardhan. Solvation thermodynamics of neutral and

charged solutes using the solvation-layer interface condition continuum dielectric model. *International Journal of Quantum Chemistry*, 119(1):e25771:1–e25771:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ryzhkov:2010:FRC

[RTT10] M. V. Ryzhkov, A. Yu. Teterin, and Yu. A. Teterin. Fully relativistic calculations of ThF_4. *International Journal of Quantum Chemistry*, 110(14):2697–2704, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruangpornvisuti:2010:DID

[Rua10] Vithaya Ruangpornvisuti. A DFT investigation of dissociation of nitrous acid, transformation of its monomeric isomers, their dimeric isomers, and dimerization. *International Journal of Quantum Chemistry*, 110(5):1019–1029, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rudbeck:2012:BSD

[Rud12] Maria Rudbeck. Basis set dependence of phosphate frequencies in density functional theory calculations. *International Journal of Quantum Chemistry*, 112(11):2435–2439, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rupp:2015:PSI

[Rup15a] Matthias Rupp. Preface: Special issue on machine learning and quantum mechanics. *International Journal of Quantum Chemistry*, 115(16):1003–1004, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rupp:2015:TRM

[Rup15b] Matthias Rupp. Tutorial reviews: Machine learning for quantum mechanics in a nutshell. *International Journal of Quantum Chemistry*, 115(16):1058–1073, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ruscic:2014:PUQ

[Rus14] Branko Ruscic. Perspectives: Uncertainty quantification in thermochemistry, benchmarking electronic structure computations, and Active Thermochemical Tables. *International Journal of Quantum Chemistry*, 114(17):1097–1101, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Randic:2012:ECL

[RVNP12] Milan Randić, Damir Vukičević, Marjana Novič, and Dejan Plavšić. π-electron currents in larger fully aromatic benzenoids. *International Journal of Quantum Chemistry*, 112 (12):2456–2462, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rossikhin:2014:ACD

[RVO+14] Vladimir Rossikhin, Eugene Voronkov, Sergiy Okovytyy, Tetiana Sergeieva, Karina Kapusta, and Jerzy Leszczynski. Accurate calculations of dynamic first hyperpolarizability: Construction of physically justified Slater-type basis sets. *International Journal of Quantum Chemistry*, 114 (11):689–695, June 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rowland:2011:CIW

[RW11] Brad A. Rowland and Robert E. Wyatt. Computational investigation of wave packet scattering in the complex plane: Numerical analytic continuation techniques. *International Journal of Quantum Chemistry*, 111(1):60–75, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ritchie:2012:APS

[RW12] Burke Ritchie and Charles A. Weatherford. Algebra of physical space and the geometric spacetime solution of Dirac's equation. *International Journal of Quantum Chemistry*, 112(24):3722–3728, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Reina:2019:BMM

[RWW+19] Miguel Reina, William T. Wallace, Richard B. Wyrwas, Robert L. Whetten, and Ana Martínez. Binding of mul-

tiple SO_2 molecules to small gold cluster anions (Au_N^-, Au_NOH^-, $N = 1$–8). *International Journal of Quantum Chemistry*, 119(19):e25987:1–e25987:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2012:SER

[RY12] Heidar Raissi and Mehdi Yoosefian. Substituent effect on the reaction mechanism of proton transfer in formamide. *International Journal of Quantum Chemistry*, 112(11): 2378–2381, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Raissi:2012:CSI

[RYM12] Heidar Raissi, Mehdi Yoosefian, and Fariba Mollania. Comprehensive study of the interaction between hydrogen halides and methanol derivatives. *International Journal of Quantum Chemistry*, 112(16):2782–2786, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2015:DSD

[RYW+15] Jun Ren, Jinzhou Yang, Wei Wang, Hailong Guo, Zhijun Zuo, Jianying Lin, and Zhong Li. A DFT study of DMC formation on Rh-doped Cu/AC surfaces. *International Journal of Quantum Chemistry*, 115(13):853–858, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rahman:2017:GFA

[RZ17] Faiz Ur Rahman and Rui-Qin Zhang. A Green's function approach to the nonrelativistic radial wave equation of hydrogen atom. *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ren:2013:EMP

[RZC13] Juan Ren, Hong Zhang, and Xinlu Cheng. Electronic and magnetic properties of all 3*d* transition-metal-doped ZnO monolayers. *International Journal of Quantum Chemistry*, 113(19):2243–2250, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rebollar-Zepeda:2012:FPC

[RZG12] Aida Mariana Rebollar-Zepeda and Annia Galano. First principles calculations of pK_a values of amines in aqueous solution: Application to neurotransmitters. *International Journal of Quantum Chemistry*, 112(21):3449–3460, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Rahman:2018:SNS

[RZSZ18] Faiz Ur Rahman, Rundong Zhao, Yanoar Pribadi Sarwono, and Rui-Qin Zhang. A scheme of numerical solution for three-dimensional isoelectronic series of hydrogen atom using one-dimensional basis functions. *International Journal of Quantum Chemistry*, 118(19):e25694:1–e25694:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarkar:2011:FGH

[SA11a] Pranab Sarkar and Basir Ahamed. The Fourier grid Hamiltonian method for calculating vibrational energy levels of triatomic molecules. *International Journal of Quantum Chemistry*, 111(10):2268–2274, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serrano-Andres:2011:OSU

[SA11b] Luis Serrano-Andrés. Organic spectroscopy under Björn O. Roos. *International Journal of Quantum Chemistry*, 111(13):3284–3290, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahu:2018:DCI

[SA18] Pooja Sahu and Sk. Musharaf Ali. Dispersion corrected interaction of polar and nonpolar fluids confined within carbon nanotubes: Density functional theoretical analysis using Grimme's D3 scheme. *International Journal of Quantum Chemistry*, 118(14):e25578:1–e25578:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santiago:2012:AAC

[SÁBA+12] R. D. Santiago, O. Álvarez-Bajo, J. M. Arias, J. Gómez-Camacho, and R. Lemus. An algebraic approach to the

collinear collision $N_2 + N_2$ in the semiclassical approximation. *International Journal of Quantum Chemistry*, 112(1): 16–27, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sierraalta:2018:NTI

[SACA18] Anibal Sierraalta, Rafael Añez, David S. Coll, and Paola Alejos. New theoretical insight on the acid sites distribution, their local structures and acid strength of the SAPO-11 molecular sieve. *International Journal of Quantum Chemistry*, 118(11):e25541:1–e25541:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salin:2013:QCI

[SAG13] Alexey V. Salin, Roza M. Aminova, and Vladimir I. Galkin. Quantum chemical investigation on the reaction mechanism of tertiary phosphines with unsaturated carboxylic acids: an insight into kinetic data. *International Journal of Quantum Chemistry*, 113(8):1086–1094, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shalabi:2012:SQM

[SAHA12] Ahmad S. Shalabi, Safaa Abdel Aal, Wael S. Abdel Halim, and Noha Abdullah. Spin quenching of Mn in complexes and CO binding with Mn deposited on MgO and CaO supports: DFT calculations. *International Journal of Quantum Chemistry*, 112(15):2743–2751, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Siddiqui:2016:IIB

[SAHAA16] Shamoon Ahmad Siddiqui, Ali Al-Hajry, and M. S. Al-Assiri. Ab initio investigation of 2,2′-bis(4-trifluoromethylphenyl)-5,5′-bithiazole for the design of efficient organic field-effect transistors. *International Journal of Quantum Chemistry*, 116(5):339–345, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shalabi:2011:SQT

[SAHG11] A. S. Shalabi, S. Abdel Aal, W. S. Abdel Halim, and M. S. Ghonaim. Spin quenching of transition metals deposited on

MgO insulator and CdO semiconductor density functional calculations. *International Journal of Quantum Chemistry*, 111(10):2444–2453, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Septelean:2019:ICP

[SALK19] Raluca Anamaria Septelean, Amr A. A. Attia, Alexandru Lupan, and R. Bruce King. The isocloso capped pentagonal bipyramid versus the closo bisdisphenoid in hypoelectronic eight-vertex metallaboranes having 16 skeletal electrons. *International Journal of Quantum Chemistry*, 119 (9):e25880:1–e25880:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saavedra:2012:MCI

[SAS+12] Edgardo J. Saavedra, Sebastian A. Andujar, Fernando D. Suvire, Miguel A. Zamora, Monica L. Freile, and Ricardo D. Enriz. Multistep conformational interconversion mechanism of cyclododecane. A simple and fast analysis using potential energy curves. *International Journal of Quantum Chemistry*, 112(11):2382–2391, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Satpati:2011:PPP

[Sat11a] Priyadarshi Satpati. Possibility of proton passage through all metal aromatic Al_4^{2-} ring in HAl_4^-. *International Journal of Quantum Chemistry*, 111(14):3816–3820, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Satpati:2011:SCC

[Sat11b] Priyadarshi Satpati. Stable complex C_2 H_4 Al_4 Li_3^- and its similarity with bicyclo[2.2.0]hex-2-ene: A DFT study. *International Journal of Quantum Chemistry*, 111(15):4241–4246, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sauer:2011:DMB

[Sau11] Stephan P. A. Sauer. David M. Bishop: Esteemed colleague and dear friend. *International Journal of Quantum Chemistry*, 111(4):723–724, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santoro:2010:CAS

[SB10a] Fabrizio Santoro and Vincenzo Barone. Computational approach to the study of the lineshape of absorption and electronic circular dichroism spectra. *International Journal of Quantum Chemistry*, 110(2):476–486, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Siegbahn:2010:BDU

[SB10b] Per E. M. Siegbahn and Margareta R. A. Blomberg. Bond-dissociation using hybrid DFT. *International Journal of Quantum Chemistry*, 110(2):317–322, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shchegoleva:2016:RPE

[SB16] Lyudmila N. Shchegoleva and Irina V. Beregovaya. Reviews: Potential energy surface as a key to understanding the structure and properties of short-living radical ions of cyclic organic molecules. *International Journal of Quantum Chemistry*, 116(3):161–173, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2018:BHP

[SB18] Bapan Saha and Pradip Kr. Bhattacharyya. B-$H_b \leftarrow :X$ (X = N, O, P, S, F, Cl, Br) interactions: a density functional study. *International Journal of Quantum Chemistry*, 118(16):e25654:1–e25654:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahin:2016:CCI

[ŞBAT16] Sevgi Şahin, Erdi A. Bleda, Zikri Altun, and Carl Trindle. Computational characterization of isomeric C_4H_2O systems: Thermochemistry, vibrational frequencies, and optical spectra for butatrienone, ethynyl ketene, butadiynol, and triafulvenone. *International Journal of Quantum Chemistry*, 116(6):444–451, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soltani:2016:EMP

[SBB16] Abdelhamid Soltani, Abdel-Ghani Boudjahem, and Mohammed Bettahar. Electronic and magnetic properties of small Rh_nCa (n = 1–9) clusters: a DFT study. *International Journal of Quantum Chemistry*, 116(5):346–356, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stroppa:2016:TRA

[SBD+16] Alessandro Stroppa, Paolo Barone, Domenico Di Sante, Mario Cuoco, Silvia Picozzi, and Myung-Hwan Whangbo. Tutorial review: Analogies between Jahn–Teller and Rashba spin physics. *International Journal of Quantum Chemistry*, 116(20):1442–1450, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sandberg:2011:SAS

[SBEH11] Thomas Sandberg, Yury Brusentsev, Patrik Eklund, and Matti Hotokka. Structural analysis of sterically hindered 1,4-diols from the naturally occurring lignan hydroxymatairesinol a quantum chemical study. *International Journal of Quantum Chemistry*, 111(15):4309–4317, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Spackman:2018:QCE

[SBKJ18] Peter R. Spackman, Björn Bohman, Amir Karton, and Dylan Jayatilaka. Quantum chemical electron impact mass spectrum prediction for de novo structure elucidation: Assessment against experimental reference data and comparison to competitive fragmentation modeling. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szymczak:2011:IAS

[SBL11] Jaroslaw J. Szymczak, Mario Barbatti, and Hans Lischka. Influence of the active space on CASSCF nonadiabatic dynamics simulations. *International Journal of Quantum Chemistry*, 111(13):3307–3315, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2016:RVC

[SBM16] Jayanta K. Saha, Sukhamoy Bhattacharyya, and Tapan K. Mukherjee. Ritz variational calculation for the singly excited states of compressed two-electron atoms. *International Journal of Quantum Chemistry*, 116(23):1802–1813, December 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2011:RST

[SBMM11] Jayanta K. Saha, S. Bhattacharyya, T. K. Mukherjee, and P. K. Mukherjee. $^1S^e$ resonance states of two electron atoms by stabilization method. *International Journal of Quantum Chemistry*, 111(7–8):1819–1823, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Surducan:2018:HFI

[SBSD18] Mihai Surducan, Adrian M. V. Brânzanic, and Radu Silaghi-Dumitrescu. Heme Fe — SO^{2-} intermediates in sulfite reduction: Contrasts with Fe — OO^{2-} species from oxygen-oxygen bond activating systems. *International Journal of Quantum Chemistry*, 118(19):e25697:1–e25697:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2010:BSA

[SC10a] Elena F. Sheka and Leonid A. Chernozatonskii. Broken symmetry approach and chemical susceptibility of carbon nanotubes. *International Journal of Quantum Chemistry*, 110(8):1466–1480, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2010:CRM

[SC10b] Elena F. Sheka and Leonid A. Chernozatonskii. Chemical reactivity and magnetism of graphene. *International Journal of Quantum Chemistry*, 110(10):1938–1946, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stashans:2011:NIR

[SC11] Arvids Stashans and Gaston Chamba. A new insight on the role of Mg in calcite. *International Journal of Quantum*

Chemistry, 111(10):2436–2443, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saracoglu:2012:EQC

[SC12a] Hanife Saraçoğlu and Alaaddin Cukurovali. Experimental and quantum chemical calculational studies on N-[4-(3-Methyl-3-phenyl-cyclobutyl)-thiazol-2-yl]-N′-pyridin-3ylmethylene-hydrazine. *International Journal of Quantum Chemistry*, 112(16):2775–2781, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saracoglu:2012:ETA

[SC12b] Hanífe Saraçoğlu and Alaaddin Cukurovali. An experimental and theoretical approach to the molecular structure of 3-[4-(3-Methyl-3-phenyl-cyclobutyl)-thiazol-2-yl]-hydrazono-1,3-dihydro- indol-2-one. *International Journal of Quantum Chemistry*, 112(6):1566–1578, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sutradhar:2018:HBB

[SC18] Dipankar Sutradhar and Asit. K. Chandra. Halogen bonding between substituted chlorobenzene and trimethylamine: Decisive role of σ-hole and C Cl bond breaking energy. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sousa:2014:RET

[SCB+14] Sérgio F. Sousa, Nuno M. F. S. A. Cerqueira, Natércia F. Brás, Pedro A. Fernandes, and Maria J. Ramos. Reviews: Enzymatic "tricks": Carboxylate shift and sulfur shift. *International Journal of Quantum Chemistry*, 114(19):1253–1256, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Swann:2017:EPQ

[SCBP17] Ellen T. Swann, Michelle L. Coote, Amanda S. Barnard, and Manolo C. Per. Efficient protocol for quantum Monte Carlo calculations of hydrogen abstraction barriers: Application to methanol. *International Journal of Quantum*

Chemistry, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soriano-correa:2010:IED

[ScBsR+10] Catalina Soriano-correa, Carolina Barrientos-salcedo, Angélica Raya, Consuelo Rubio Póo, and Rodolfo O. Esquivel. The influence of electron donor and electron acceptor groups on the electronic structure of the anti-inflammatory tripeptide Cys-Asn-Ser. *International Journal of Quantum Chemistry*, 110(13):2398–2410, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheiner:2010:BR

[Sch10a] Steve Scheiner. Book review. *International Journal of Quantum Chemistry*, 110(14):2719–2720, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheiner:2010:ECH

[Sch10b] Steve Scheiner. Effect of CH$\cdots$O hydrogen bond length on the geometric and spectroscopic features of the peptide unit of proteins. *International Journal of Quantum Chemistry*, 110(15):2775–2783, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheiner:2012:EDM

[Sch12a] Steve Scheiner. Evaluation of DFT methods to study reactions of benzene with OH radical. *International Journal of Quantum Chemistry*, 112(8):1879–1886, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheiner:2012:I

[Sch12b] Steve Scheiner. Introduction. *International Journal of Quantum Chemistry*, 112(8):1859, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheiner:2013:RDC

[Sch13] Steve Scheiner. Reviews: Detailed comparison of the pnicogen bond with chalcogen, halogen, and hydrogen bonds. *International Journal of Quantum Chemistry*, 113(11):1609–

1620, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scheiner:2015:IBC

[Sch15] Steve Scheiner. The interplay between charge transfer, rehybridization, and atomic charges in the internal geometry of subunits in noncovalent interactions. *International Journal of Quantum Chemistry*, 115(1):28–33, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stetina:2019:XRA

[SCL19] Torin F. Stetina, Aurora E. Clark, and Xiaosong Li. X-ray absorption signatures of hydrogen-bond structure in water–alcohol solutions. *International Journal of Quantum Chemistry*, 119(1):e25802:1–e25802:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanchez-Castellanos:2012:PES

[SCLCPB12] M. Sánchez-Castellanos, R. Lemus, M. Carvajal, and F. Pérez-Bernal. The potential energy surface of CO_2 from an algebraic approach. *International Journal of Quantum Chemistry*, 112(21):3498–3507, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suwannakham:2015:PDT

[SCS15] Parichart Suwannakham, Sermsiri Chaiwongwattana, and Kritsana Sagarik. Proton dissociation and transfer in hydrated phosphoric acid clusters. *International Journal of Quantum Chemistry*, 115(8):486–501, April 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2010:OEH

[SCTW10] Lili Sun, Yingfei Chang, Shuwei Tang, and Rongshun Wang. Orientation of endohedral H_2, CO, and LiH inside heptagon-containing C_{58} and C_{58} H_{18}. *International Journal of Quantum Chemistry*, 110(5):1080–1085, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2012:EFS

[SCZG12] Yan Sun, Feng Chen, Lin Zhuo, and Bing Cong Gou. Energies, fine structures, and radiative lifetimes for the multi-excited quartet states of B-like oxygen. *International Journal of Quantum Chemistry*, 112(4):1114–1121, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sutradhar:2016:TSI

[SCZH16] Dipankar Sutradhar, Asit K. Chandra, and Thérèse Zeegers-Huyskens. Theoretical study of the interaction of fluorinated dimethyl ethers and the ClF and HF molecules. Comparison between halogen and hydrogen bonds. *International Journal of Quantum Chemistry*, 116(9):670–680, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shojaie:2012:VMA

[SD12] Fahimeh Shojaie and Maryam Dehestani. Vibrational mode analysis for the multichannel reaction of CH_3Cl + OH. *International Journal of Quantum Chemistry*, 112(12):2450–2455, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saikia:2013:CEN

[SD13a] Nabanita Saikia and Ramesh C. Deka. A comparison of the effect of nanotube chirality and electronic properties on the π–π interaction of single-wall carbon nanotubes with pyrazinamide antitubercular drug. *International Journal of Quantum Chemistry*, 113(9):1272–1284, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serrano:2013:PQR

[SD13b] Fernando Adan Serrano and Shi-Hai Dong. Proper quantization rule approach to three-dimensional quantum dots. *International Journal of Quantum Chemistry*, 113(20):2282–2286, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sulston:2013:TGF

[SD13c] Kenneth W. Sulston and Sydney G. Davison. Tensorial green-function theory of atomic-wire T-junction transmission. *International Journal of Quantum Chemistry*, 113 (10):1498–1502, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Samanta:2016:CQM

[SD16a] Pabitra Narayan Samanta and Kalyan Kumar Das. Comparative QM/MM studies of H_2 adsorption on lithium doped single walled armchair and zigzag nanotubes: SiCNT, GeCNT, and SnCNT. *International Journal of Quantum Chemistry*, 116(20):1467–1476, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Samanta:2016:QMS

[SD16b] Pabitra Narayan Samanta and Kalyan Kumar Das. QM/MM study of the interaction between zigzag SnC nanotube and small toxic gas molecules. *International Journal of Quantum Chemistry*, 116(6):411–420, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2015:SIE

[SDL+15] Guo-Hua Sun, Shi-Hai Dong, Kristina D. Launey, Tomas Dytrych, and Jerry P. Draayer. Shannon information entropy for a hyperbolic double-well potential. *International Journal of Quantum Chemistry*, 115(14):891–899, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silaghi-Dumitrescu:2012:SCS

[SDM12] Radu Silaghi-Dumitrescu and Sergei V. Makarov. Siroheme-containing sulfite reductase: a density functional investigation of the mechanism. *International Journal of Quantum Chemistry*, 112(3):900–908, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salvadori:2016:SNU

[SDP+16] Andrea Salvadori, Gianluca Del Frate, Marco Pagliai, Giordano Mancini, and Vincenzo Barone. Software news &

updates: Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data. *International Journal of Quantum Chemistry*, 116(22):1731–1746, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shibl:2013:MAE

[SDR+13] Mohamed F. Shibl, Li Dang, Rajesh K. Raju, Michael B. Hall, and Edward N. Brothers. A mechanism for the addition of ethylene to nickel bis-dithiolene. *International Journal of Quantum Chemistry*, 113(11):1621–1625, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadhukhan:2019:CSQ

[SDS19] Anjan Sadhukhan, Sayantan Dutta, and Jayanta K. Saha. Critical stability and quantum phase transition of screened two-electron system. *International Journal of Quantum Chemistry*, 119(24):e26042:1–e26042:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See corrigendum [SDS20].

Sadhukhan:2020:CCS

[SDS20] Anjan Sadhukhan, Sayantan Dutta, and Jayanta K. Saha. Corrigendum: Critical stability and quantum phase transition of screened two-electron system. *International Journal of Quantum Chemistry*, 120(3):e26084:1–e26084:??, February 5, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [SDS19].

Staykov:2016:ODP

[SDY16] Aleksandar Staykov, Durgesh Derekar, and Keisuke Yamamura. Oxygen dissociation on palladium and gold core/shell nanoparticles. *International Journal of Quantum Chemistry*, 116(20):1486–1492, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silvi:2011:I

[SE11] B. Silvi and L. A. Eriksson. Introduction. *International Journal of Quantum Chemistry*, 111(6):1127, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serdaroglu:2011:DIC

[Ser11a] Goncagül Serdaroğlu. DFT and Ab initio computational study on the reactivity sites of the GABA and its agonists, such as CACA, TACA, DABA, and muscimol: In the gas phase and dielectric media. *International Journal of Quantum Chemistry*, 111(14):3938–3948, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Serdaroglu:2011:DSD

[Ser11b] Goncagül Serdaroğlu. A DFT study of determination of the reactive sites of the acetylcholine and its agonists: In the gas phase and dielectric medium. *International Journal of Quantum Chemistry*, 111(10):2464–2475, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Safi:2013:PMT

[SF13] Zaki S. Safi and Gernot Frenking. Protonation of 5-methylhydantoin and its thio derivatives in the gas phase: a theoretical study. *International Journal of Quantum Chemistry*, 113(7):908–915, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schleder:2019:ONC

[SFA19] Gabriel R. Schleder, Adalberto Fazzio, and Jeverson T. Arantes. Oxidation of Ni_{13} clusters. *International Journal of Quantum Chemistry*, 119(9):e25874:1–e25874:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sala:2016:RKE

[SFC16] Fabio Della Sala, Eduardo Fabiano, and Lucian A. Constantin. Reviews: Kinetic-energy-density dependent semilocal exchange-correlation functionals. *International Journal of Quantum Chemistry*, 116(22):1641–1694, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sala:2010:REE

[SFL+10] Fabio Della Sala, Eduardo Fabiano, Savio Laricchia, Stefania D'Agostino, and Manuel Piacenza. The role of exact-

exchange in the theoretical description of organic-metal interfaces. *International Journal of Quantum Chemistry*, 110 (12):2162–2171, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

San-Fabiin:2013:PUG

[SFM13] E. San-Fabiín and F. Moscardó. Polarized-unpolarized ground state of small polycyclic aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 113(6):815–819, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Staykov:2018:STS

[SFNC+18] Aleksandar Staykov, Elias Paiva Ferreira-Neto, Jean Mina Ybarrena Santa Cruz, Sajjad Ullah, and Ubirajara Pereira Rodrigues-Filho. The stability of titania–silica interface. *International Journal of Quantum Chemistry*, 118 (4), February 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salter:2012:RST

[SFW12] E. Alan Salter, David C. Forbes, and Andrzej Wierzbicki. Relative stabilities of transition states determine diastereocontrol in sulfur ylide additions onto chiral N-sulfinyl imines. *International Journal of Quantum Chemistry*, 112 (2):509–518, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2012:WTQ

[SFY12] Jun Song, Hong-Yi Fan, and Hong-Chun Yuan. Wavelet transform of quantum chemical states. *International Journal of Quantum Chemistry*, 112(11):2343–2347, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Simoes:2014:RPL

[SG14] Ana Simões and Kostas Gavroglu. Reviews: P.-O. Löwdin and the International Journal of Quantum Chemistry: a kaleidoscopic agenda for quantum chemistry. *International Journal of Quantum Chemistry*, 114(2):116–127, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sen:2019:PSD

[SG19] Anik Sen and Axel Groß. Promising sensitizers for dye sensitized solar cells: a comparison of Ru(II) with other earth's scarce and abundant metal polypyridine complexes. *International Journal of Quantum Chemistry*, 119(16): e25963:1–e25963:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salehzadeh:2011:PMP

[SGB11] Sadegh Salehzadeh, Yasin Gholiee, and Mehdi Bayat. Prediction of microscopic protonation constants of polybasic molecules via computational methods: a complete microequilibrium analysis of spermine. *International Journal of Quantum Chemistry*, 111(14):3608–3615, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Site:2013:EEF

[SGC13] Luigi Delle Site, Luca M. Ghiringhelli, and David M. Ceperley. Electronic energy functionals: Levy–Lieb principle within the ground state path integral quantum Monte Carlo. *International Journal of Quantum Chemistry*, 113 (2):155–160, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scordino:2010:DLC

[SGG+10] Agata Scordino, Rosaria Grasso, Marisa Gulino, Luca Lanzanò, Francesco Musumeci, Giuseppe Privitera, Maurizio Tedesco, Antonio Triglia, and Larissa Brizhik. Delayed luminescence from collagen as arising from soliton and small polaron states. *International Journal of Quantum Chemistry*, 110(1):221–229, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shepard:2010:ERA

[SGH10] Ron Shepard, Gergely Gidofalvi, and Paul D. Hovland. An efficient recursive algorithm to compute wave function optimization gradients for the graphically contracted function method. *International Journal of Quantum Chemistry*, 110 (15):2938–2948, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabin:2010:BR

[SGJ10] John R. Sabin, Frederick Gregory, and Naja Jeppesen. Book reviews. *International Journal of Quantum Chemistry*, 110(4):960–961, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senthilkumar:2012:HBC

[SGKG12] Lakshmipathi Senthilkumar, Tapan K. Ghanty, Ponmalai Kolandaivel, and Swapan K. Ghosh. Hydrogen-bonded complexes of nicotine with simple alcohols. *International Journal of Quantum Chemistry*, 112(16):2787–2793, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salazar:2016:SSS

[SGL+16] Edison X. Salazar, Pedro F. Guarderas, Eduardo V. Ludeña, Mauricio H. Cornejo, and Valentin V. Karasiev. Study of some simple approximations to the non-interacting kinetic energy functional. *International Journal of Quantum Chemistry*, 116(17):1313–1321, September 05, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2019:MSI

[SGL19] Xiaoli Sun, Caiyun Geng, and Jilai Li. Mechanistic study on iron(II)-mediated direct arylation of benzene with chlorobenzene. *International Journal of Quantum Chemistry*, 119(13):e25912:1–e25912:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santiago:2018:REI

[SH18a] Régis T. Santiago and Roberto L. A. Haiduke. Relativistic effects on inversion barriers of pyramidal group 15 hydrides. *International Journal of Quantum Chemistry*, 118 (15):e25585:1–e25585:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santoro:2018:MSR

[SH18b] Stefano Santoro and Fahmi Himo. Mechanism and selectivity of rhodium-catalyzed C — H bond arylation of indoles. *International Journal of Quantum Chemistry*, 118

(9):e25526:1–e25526:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahraeian:2019:MSC

[SH19] Taghi Sahraeian and M. R. Hadizadeh. Momentum space calculations of the binding energies of argon dimer. *International Journal of Quantum Chemistry*, 119(3):e25807:1–e25807:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shahbazian:2011:LEM

[Sha11a] Shant Shahbazian. Letter to the Editor: The mathematical soundness and the physical content of the subsystem variational procedure of the QTAIM. *International Journal of Quantum Chemistry*, 111(15):4497–4500, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shavitt:2011:PBR

[Sha11b] Isaiah Shavitt. Perspective: Björn Roos and direct configuration interaction. *International Journal of Quantum Chemistry*, 111(13):3263–3266, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shahbazian:2018:RFQ

[Sha18] Shant Shahbazian. Revisiting the foundations of the quantum theory of atoms in molecules: Some open problems. *International Journal of Quantum Chemistry*, 118(16): e25637:1–e25637:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shibl:2010:DSC

[SHE10] Mohamed F. Shibl, Salem A. Hameed, and Shabaan A. K. Elroby. A DFT study of the complexation behavior of hemispherands toward alkali metal cations. *International Journal of Quantum Chemistry*, 110(14):2645–2652, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2012:CSG

[She12] Elena F. Sheka. Computational strategy for graphene: Insight from odd electrons correlation. *International Journal*

of Quantum Chemistry, 112(18):3076–3090, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2013:CMN

[She13] E. F. Sheka. Computational meso- and nano-science: Why sp^2-like nanosilicons should not form: Insight from quantum chemistry. *International Journal of Quantum Chemistry*, 113(4):612–618, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheka:2014:UPC

[She14] Elena F. Sheka. The uniqueness of physical and chemical natures of graphene: Their coherence and conflicts. *International Journal of Quantum Chemistry*, 114(16):1079–1095, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shigemitsu:2013:CBB

[Shi13] Yasuhiro Shigemitsu. Computational biochemistry and biophysics: Quantum chemical study on molecular-level affinity of DJ-1 binding compounds. *International Journal of Quantum Chemistry*, 113(4):574–579, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shil:2018:EDM

[Shi18] Suranjan Shil. Effect of deprotonation on the magnetic exchange coupling constant of fluorene-based verdazyl diradical: a computational study. *International Journal of Quantum Chemistry*, 118(11):e25543:1–e25543:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shigeta:2015:RQC

[SHKS15] Yasuteru Shigeta, Ryuhei Harada, Megumi Kayanuma, and Mitsuo Shoji. Reviews: Quantal cumulant dynamics for real-time simulations of quantum many-body systems. *International Journal of Quantum Chemistry*, 115(5):300–308, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2013:RBA

[SHL+13] Hongwei Shi, Xiangui Huang, Guixia Liu, Kunqian Yu, Congying Xu, Weihua Li, Bubing Zeng, and Yun Tang. The role of benzoic acid in proline-catalyzed asymmetric Michael addition: a density functional theory study. *International Journal of Quantum Chemistry*, 113(9):1339–1348, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sylvester-Hvid:2011:ISC

[SHMR11] Kristian O. Sylvester-Hvid, Kurt V. Mikkelsen, and Mark A. Ratner. The iterative self-consistent reaction-field method: The refractive index of pure water. *International Journal of Quantum Chemistry*, 111(4):904–913, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2013:FMS

[SHS+13] Mitsuo Shoji, Kyohei Hanaoka, Akimasa Sato, Daiki Kondo, Moon Young Yang, Katsumasa Kamiya, and Kenji Shiraishi. Frontiers in molecular simulations: Calculation of the electron transfer coupling matrix element in diabatic reactions. *International Journal of Quantum Chemistry*, 113(3):342–347, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2013:EBE

[SHW+13] Ming-Xing Song, Zhao-Min Hao, Zhi-Jian Wu, Shu-Yan Song, Liang Zhou, Rui-Ping Deng, and Hong-Jie Zhang. Efficient blue-emitting Ir(III) complexes with phenyl-methyl-benzimidazolyl and picolinate ligands: a DFT and time-dependent DFT study. *International Journal of Quantum Chemistry*, 113(11):1641–1649, June 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shigeta:2013:FMS

[SIB+13] Yasuteru Shigeta, Tomoya Inui, Takeshi Baba, Katsuki Okuno, Hiroyuki Kuwabara, Ryohei Kishi, and Masayoshi Nakano. Frontiers in molecular simulations: Quantal cumulant mechanics and dynamics for multidimensional quantum many-body clusters. *International Journal of Quan-*

tum Chemistry, 113(3):348–355, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sicilia:2016:PCM

[Sic16] Emilia Sicilia. Perspective: Computation modeling as a tool for the exploration of complex multistep reaction cycles in homogeneous catalysis. Some selected examples in the framework of the use of hydrogen as a fuel of the future. *International Journal of Quantum Chemistry*, 116(21):1507–1512, November 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sikorska:2018:MFS

[Sik18] Celina Sikorska. $Mg_3 F_7$: a superhalogen with potential for new nanomaterials design. *International Journal of Quantum Chemistry*, 118(21):e25728:1–e25728:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silverstone:2014:CBE

[Sil14] Harris J. Silverstone. Convergence of the bipolar expansion for the Coulomb potential. *International Journal of Quantum Chemistry*, 114(16):1073–1078, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saitow:2014:IDO

[SIM14] Masaaki Saitow, Tomonori Ida, and Yuji Mochizuki. Improved description of the orbital relaxation effect by practical use of the self-energy. *International Journal of Quantum Chemistry*, 114(9):577–586, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shoji:2008:TCB

[SIS+08] Mitsuo Shoji, Hiroshi Isobe, Toru Saito, Hirotaka Yabushita, Kenichi Koizumi, Yasutaka Kitagawa, Shusuke Yamanaka, Takashi Kawakami, Mitsutaka Okumura, Masayuki Hagiwara, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes. VII. Hybrid-density functional theory studies on the electronic structures of P450. *International Journal of Quantum Chemistry*, 108 (4):631–650, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saito:2012:MDSb

[SIT+12] Hiroaki Saito, Masashi Iwayama, Hiroyuki Takagi, Megumi Nishimura, Takeshi Miyakawa, Kazutomo Kawaguchi, Masako Takasu, Taku Mizukami, and Hidemi Nagao. Molecular dynamics study of gramicidin A in lipid bilayer: Structure and lateral pressure profile. *International Journal of Quantum Chemistry*, 112(24):3834–3839, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Site:2015:SEM

[Sit15] Luigi Delle Site. Shannon entropy and many-electron correlations: Theoretical concepts, numerical results, and Collins conjecture. *International Journal of Quantum Chemistry*, 115(19):1396–1404, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sjoqvist:2015:RGP

[Sjö15] Erik Sjöqvist. Reviews: Geometric phases in quantum information. *International Journal of Quantum Chemistry*, 115(19):1311–1326, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2013:CEW

[SJW13] Chang-Liang Sun, Xiao-Nan Jiang, and Chang-Sheng Wang. Cooperative enhancement of water binding to antiparallel β-sheet models: Analysis by ab initio calculations. *International Journal of Quantum Chemistry*, 113 (10):1453–1460, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2018:HBC

[SJZ+18] Yulei Shi, Wanrun Jiang, Zhiyuan Zhang, Danhui Li, Huajie Song, and Zhigang Wang. Hydrogen bonding cooperation in glycine-(water)$_n$ clusters studied by density functional theory calculations. *International Journal of Quantum Chemistry*, 118(12):e25556:1–e25556:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2012:CEC

[SJZL12] Zhiqiang Shi, Ningning Ji, Rengao Zhao, and Zhifeng Li. Combined experimental and computational modeling studies on 3,5-dimethyl-pyrazole-1-carbodithioic acid benzyl ester. *International Journal of Quantum Chemistry*, 112(2): 373–381, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugimori:2010:TSN

[SK10] Kimikazu Sugimori and Hiroyuki Kawabe. Theoretical study of NMR chemical shift induced by H/D isotope effect. *International Journal of Quantum Chemistry*, 110 (15):2989–2995, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2011:IEB

[SK11] R. K. Singh and Mohd. Adil Khan. Interaction energy-based drug–receptor interaction study of metal–bicyclam complexes. *International Journal of Quantum Chemistry*, 111(15):4174–4185, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seybold:2012:TEA

[SK12a] Paul G. Seybold and W. C. Kreye. Theoretical estimation of the acidities of alcohols and azoles in gas phase, DMSO, and water. *International Journal of Quantum Chemistry*, 112(24):3769–3776, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Su:2012:TSG

[SK12b] Yan Su and Li-Hua Kang. Theoretical studies of ground and excited electronic states in a series of heteroleptic iridium complexes using density functional theory. *International Journal of Quantum Chemistry*, 112(11):2422–2428, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Salta:2014:CSR

[SK14] Zoi Salta and Agnie M. Kosmas. Computational study of the reaction of the methylsulfonyl radical, $CH_3S(O)_2$, with NO_2. *International Journal of Quantum Chemistry*,

114(21):1430–1437, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sellier:2017:HAB

[SK17a] Jean Michel Sellier and Kristina G. Kapanova. On the hydrogen atom beyond the Born–Oppenheimer approximation. *International Journal of Quantum Chemistry*, 117 (21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sellier:2017:SES

[SK17b] Jean Michel Sellier and Kristina G. Kapanova. A study of entangled systems in the many-body signed particle formulation of quantum mechanics. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sliwa:2018:OFE

[ŚKB18] Pawel Śliwa, Rafal Kurczab, and Andrzej J. Bojarski. ONIOM and FMO-EDA study of metabotropic glutamate receptor 1: Quantum insights into the allosteric binding site. *International Journal of Quantum Chemistry*, 118(15):e25617:1–e25617:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scivetti:2011:TSW

[SKG11] Iván Scivetti, Jorge Kohanoff, and Nikitas I. Gidopoulos. On the treatment of singularities of the Watson Hamiltonian for nonlinear molecules. *International Journal of Quantum Chemistry*, 111(2):307–317, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saparpakorn:2013:CBB

[SKHN13] Patchreenart Saparpakorn, Masato Kobayashi, Supa Hannongbua, and Hiromi Nakai. Computational biochemistry and biophysics: Divide-and-conquer-based quantum chemical study for interaction between HIV-1 reverse transcriptase and MK-4965 inhibitor. *International Journal of Quantum Chemistry*, 113(4):510–517, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szarek:2010:FFA

[SKL10] Paweł Szarek, Ludwik Komorowski, and Józef Lipiński. Fukui functions for atoms and ions: Polarizability justified approach. *International Journal of Quantum Chemistry*, 110(12):2315–2319, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sellier:2019:MLS

[SKLC19] Jean Michel Sellier, Kristina G. Kapanova, Jacob Leygonie, and Gaetan Marceau Caron. Machine learning and signed particles, an alternative and efficient way to simulate quantum systems. *International Journal of Quantum Chemistry*, 119(23):e26017:1–e26017:??, December 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2011:HAA

[SKM11] P. K. Shukla, N. Kumar, and P. C. Mishra. Hydrogen atom abstraction reactions of the sugar moiety of 2′-deoxyguanosine with an OH radical: a quantum chemical study. *International Journal of Quantum Chemistry*, 111 (9):2160–2169, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skouteris:2016:PTD

[Sko16] Dimitrios Skouteris. Perspective: Time-dependent calculations on systems of chemical interest: Dynamical and kinetic approaches. *International Journal of Quantum Chemistry*, 116(22):1618–1622, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shankar:2010:RMC

[SKS10] R. Shankar, P. Kolandaivel, and K. Senthilkumar. Reaction mechanism of cysteine proteases model compound HSH with diketone inhibitor $PhCOCOCH_{3-n}X_n$, (X = F, Cl, $n = 0, 1, 2$). *International Journal of Quantum Chemistry*, 110(9):1660–1674, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shankar:2011:TSD

[SKS11] R. Shankar, P. Kolandaivel, and K. Senthilkumar. A theoretical study on decomposition and rearrangement reaction

mechanism of trichloroacetyl chloride (CCl_3 COCl). *International Journal of Quantum Chemistry*, 111(14):3482–3496, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Scarborough:2015:ASB

[SKTI15] David L. A. Scarborough, Rika Kobayashi, Christopher D. Thompson, and Ekaterina I. Izgorodina. Active space and basis set effects in CASPT2 models of the 1,3-butadiene-ethene cycloaddition and the 1,3-butadiene dimerization. *International Journal of Quantum Chemistry*, 115(15):989–1001, August 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Spiriti:2012:DAE

[SKV12] Justin Spiriti, Hiqmet Kamberaj, and Arjan Van Der Vaart. Development and application of enhanced sampling techniques to simulate the long-time scale dynamics of biomolecular systems. *International Journal of Quantum Chemistry*, 112(1):33–43, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sumimoto:2013:FDF

[SKY+13] Michinori Sumimoto, Yukio Kawashima, Daisuke Yokogawa, Kenji Hori, and Hitoshi Fujimoto. Frontiers in density functional theory: Influences of dispersion and long-range corrections on molecular structures of three types of lithium phthalocyanine dimer. *International Journal of Quantum Chemistry*, 113(3):272–276, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2010:GWS

[SL10] Manoj K. Shukla and Jerzy Leszczynski. Guanine in water solution: Comprehensive study of hydration cage versus continuum solvation model. *International Journal of Quantum Chemistry*, 110(15):3027–3039, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Siegbahn:2011:BRM

[SL11] Per Siegbahn and Roland Lindh. Björn O. Roos: 1937–2010. Mentor, colleague, innovator. *International Journal*

of Quantum Chemistry, 111(13):3256–3259, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Skouteris:2013:EMT

[SL13] Dimitrios Skouteris and Antonio Laganà. Electronuclear multiconfiguration time-dependent Hartree calculations on the confined H atom with mobile electron and nucleus. *International Journal of Quantum Chemistry*, 113(9):1333–1338, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2012:IDT

[SLA12] José Rogério Araújo Silva, Jerônimo Lameira, and Cláudio Nahum Alves. Insights for design of *Trypanosoma cruzi* GAPDH inhibitors: a QM/MM MD study of 1,3-bisphospo-D-glyceric acid analogs. *International Journal of Quantum Chemistry*, 112(20):3398–3402, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sciortino:2018:APV

[SLC+18] Giuseppe Sciortino, Norbert Lihi, Tamás Czine, Jean-Didier Maréchal, Agustí Lledós, and Eugenio Garribba. Accurate prediction of vertical electronic transitions of Ni(II) coordination compounds via time dependent density functional theory. *International Journal of Quantum Chemistry*, 118(16):e25655:1–e25655:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sagar:2011:EPD

[SLG11] Robin P. Sagar, Humberto G. Laguna, and Nicolais L. Guevara. Electron pair density information measures in atomic systems. *International Journal of Quantum Chemistry*, 111 (14):3497–3504, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2010:HMM

[SLS+10] José Rogério Araújo Silva, Jerônimo Lameira, Priscila P. B. Santana, Artur Silva, Maria Paula Cruz Schneider, and Cláudio Nahum Alves. Homology modeling and molecular dynamics simulation of an alpha methyl coenzyme M

reductase from methanogenic archea. *International Journal of Quantum Chemistry*, 110(11):2067–2075, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2011:SIH

[SLS+11] De-Heng Shi, Hui Liu, Jin-Feng Sun, Yu-Fang Liu, and Zun-Lue Zhu. Spectroscopic investigations on HBr^+ ($X\,^2\Pi$) ion using CCSD(T) theory in combination with cc-pV5Z basis set. *International Journal of Quantum Chemistry*, 111(1):52–59, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2012:SCMb

[SLS+12] De-Heng Shi, Wen-Tao Li, Jin-Feng Sun, Zun-Lue Zhu, and Yu-Fang Liu. Spectroscopic constants and molecular properties of the $X^2\ \Pi$ and $a^4\ \Sigma^-$ electronic states of the SiF radical. *International Journal of Quantum Chemistry*, 112(14):2615–2622, July 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shang:2014:TSE

[SLS+14] Xiao-Hong Shang, Yu-Qi Liu, Juan-Juan Su, Godefroid Gahungu, Xiao-Chun Qu, and Zhi-Jian Wu. Theoretical study on the electronic structures and optical properties of blue-green and blue phosphorescent iridium(III) complexes with tetraphenylimidodiphosphinate ligand. *International Journal of Quantum Chemistry*, 114(3):183–191, February 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2015:TMS

[SLS+15] Chuanzhi Sun, Mingshu Liu, Haitao Sun, Fang Hang, Nan Sun, and Dezhan Chen. Theoretical mechanism for selective catalysis of ruthenium complex catalyzed hydroboration of terminal alkynes to Z-vinylboronates. *International Journal of Quantum Chemistry*, 115(2):59–67, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stamm:2019:HMC

[SLS+19] Benjamin Stamm, Louis Lagardère, Giovanni Scalmani, Paolo Gatto, Eric Cancès, Jean-Philip Piquemal, Yvon

Maday, Benedetta Mennucci, and Filippo Lipparini. How to make continuum solvation incredibly fast in a few simple steps: a practical guide to the domain decomposition paradigm for the conductor-like screening model. *International Journal of Quantum Chemistry*, 119(1):e25669:1–e25669:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2013:TSS

[SLSZ13] De-Heng Shi, Wen-Tao Li, Jin-Feng Sun, and Zun-Lue Zhu. Theoretical study of spectroscopic and molecular properties of several low-lying electronic states of CO molecule. *International Journal of Quantum Chemistry*, 113(7):934–942, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2011:SIB

[SLZ+11a] De-Heng Shi, Hui Liu, Jin-Ping Zhang, Jin-Feng Sun, Yu-Fang Liu, and Zun-Lue Zhu. Spectroscopic investigations on $BH^+(X^2\Sigma^+)$ ion using MRCI method and correlation-consistent sextuple basis set augmented with diffuse functions. *International Journal of Quantum Chemistry*, 111 (10):2171–2179, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2011:MID

[SLZ+11b] De-Heng Shi, Hui Liu, Xiao-Niu Zhang, Jin-Feng Sun, Yu-Fang Liu, and Zun-Lue Zhu. MRCI investigations on dissociation energy and molecular constants of $BCl(X^1\Sigma^+)$ radical. *International Journal of Quantum Chemistry*, 111 (12):2825–2834, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2011:SIA

[SLZ+11c] De-Heng Shi, Hui Liu, Xiao-Niu Zhang, Jin-Feng Sun, Yu-Fang Liu, and Zun-Lue Zhu. Spectroscopic investigations on $AlH(X^1\Sigma^+)$ radical using multireference configuration interaction theory in combination with correlation-consistent quintuple basis set augmented with diffuse functions. *International Journal of Quantum Chemistry*, 111 (3):554–562, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2012:DIB

[SLZ+12] Wei Song, Wen-Cai Lu, Qing-Jun Zang, C. Z. Wang, and K. M. Ho. Double icosahedron-based motif of Ni_n ($n = 20$–30). *International Journal of Quantum Chemistry*, 112(6): 1717–1724, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2012:TSI

[SLZH12] Jian-Chao Song, Hui-Ling Liu, Zhong-Jun Zhou, and Xu-Ri Huang. Theoretical study on the ion–molecule reaction of NH^+ with CH_2 O. *International Journal of Quantum Chemistry*, 112(6):1654–1666, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2010:MMC

[SM10a] Richard H. Squire and Norman H. March. Microscopic model of cuprate superconductivity. *International Journal of Quantum Chemistry*, 110(15):2808–2822, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stevenson:2010:DCA

[SM10b] William H. Stevenson III and Michael J. McQuaid. Dissociation constants of 2-azidoethanamines in aqueous solution. *International Journal of Quantum Chemistry*, 110(7): 1376–1393, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2012:IEU

[SM12] Raman K. Singh and Manoj K. Mishra. Investigation of ethynylpyridines using the electron propagator theory. *International Journal of Quantum Chemistry*, 112(2):426–439, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2013:BPP

[SM13] Pradeep Kumar Shukla and P. C. Mishra. Base pairing patterns of DNA base lesion spiroiminodihydantoin: A DFT study. *International Journal of Quantum Chemistry*, 113 (24):2600–2604, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Speranza:2014:CDH

[SM14a] Giorgio Speranza and Luca Minati. Charge distribution in homonuclear bonds: a semiempirical modeling. *International Journal of Quantum Chemistry*, 114(8):493–500, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2014:HOS

[SM14b] A. K. Srivastava and N. Misra. The highest oxidation state of Au revealed by interactions with successive Cl ligands and superhalogen properties of $AuCl_n$ (n = 1–6) species. *International Journal of Quantum Chemistry*, 114 (22):1513–1517, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2014:IIS

[SM14c] Ambrish Kumar Srivastava and Neeraj Misra. Ab initio investigations on the stabilities of AuO_n^{q-} (q = 0 to 3; n = 1 to 4) species: Superhalogen behavior of AuO_n ($n \geq 2$) and their interactions with an alkali metal. *International Journal of Quantum Chemistry*, 114(8):521–524, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2014:TIS

[SM14d] Ambrish Kumar Srivastava and Neeraj Misra. Theoretical investigations on the superhalogen properties and interaction of PdO_n (n = 1–5) species. *International Journal of Quantum Chemistry*, 114(5):328–332, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2016:SBL

[SM16] Ambrish Kumar Srivastava and Neeraj Misra. Structures and basicity of Li_NOH (N = 1–5) species. *International Journal of Quantum Chemistry*, 116(7):524–528, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2017:CBA

[SM17] Ambrish Kumar Srivastava and Neeraj Misra. Competition between alkalide characteristics and nonlinear optical

properties in OLi_3MLi_3O (M = Li, Na, and K) complexes. *International Journal of Quantum Chemistry*, 117(3):208–212, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senami:2019:EEC

[SM19] Masato Senami and Shunji Matsunaga. The effect of electric current on chemical bonding of hydrogen adsorption on an aluminum nanowire. *International Journal of Quantum Chemistry*, 119(22):e26004:1–e26004:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solimannejad:2011:GOC

[SMA11] Mohammad Solimannejad, Shokofeh Massahi, and Ibon Alkorta. Glyoxal oligomers: a computational study. *International Journal of Quantum Chemistry*, 111(12):3057–3069, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2018:HNA

[SMC18] Ranajit Saha, Bijoya Mandal, and Pratim K. Chattaraj. $HNgBeF_3$ (Ng = Ar–Rn): Superhalogen-supported noble gas insertion compounds. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sen:2015:EFH

[SMEH15] Anik Sen, Pavlin D. Mitev, Anders Eriksson, and Kersti Hermansson. From electric fields to H_2O dipoles and OH dynamics — towards a data-base of crystalline water molecules from DFT calculations. *International Journal of Quantum Chemistry*, 115(18):??, September 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). This article will be published in an upcoming issue of the *International Journal of Quantum Chemistry*.

Sen:2016:HBE

[SMEH16] Anik Sen, Pavlin D. Mitev, Anders Eriksson, and Kersti Hermansson. H-bond and electric field correlations for water in highly hydrated crystals. *International Journal of Quantum Chemistry*, 116(2):67–80, January 15, 2016. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stanchev:2013:DSP

[SMGZ13] Stancho Stanchev, Javor Mitkov, Maya Georgieva, and Alexander Zlatkov. DFT study of the physicochemical characteristics and spectral behavior of new 8-substituted 1,3,7-trimethylxanthines. *International Journal of Quantum Chemistry*, 113(9):1384–1393, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanchez-Marquez:2019:NIC

[SMGZF19] Jesús Sánchez-Márquez, Víctor García, David Zorrilla, and Manuel Fernández. New insights in conceptual DFT: New model for the calculation of local reactivity indices based on the Sanderson's principle. *International Journal of Quantum Chemistry*, 119(7):e25844:1–e25844:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saito:2012:MDSa

[SMK+12] Hiroaki Saito, Taku Mizukami, Shuhei Kawamoto, Takeshi Miyakawa, Masashi Iwayama, Masako Takasu, and Hidemi Nagao. Molecular dynamics studies of lipid bilayer with gramicidin A: Effects of gramicidin A on membrane structure and hydrophobic match. *International Journal of Quantum Chemistry*, 112(1):161–170, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2013:TRC

[SMMT13] Richard H. Squire, Norman H. March, Rebecca A. Minnick, and Richard Turschmann. Tutorial review: Comparison of various types of coherence and emergent coherent systems. *International Journal of Quantum Chemistry*, 113 (19):2181–2199, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanchez-Moreno:2011:EFL

[SMOD11] P. Sánchez-Moreno, J. J. Omiste, and J. S. Dehesa. Entropic functionals of Laguerre polynomials and complexity properties of the half-line Coulomb potential. *International*

Journal of Quantum Chemistry, 111(10):2283–2294, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shields:2010:DTH

[SMP10] Zenaida P. Shields, Jane S. Murray, and Peter Politzer. Directional tendencies of halogen and hydrogen bonds. *International Journal of Quantum Chemistry*, 110(15):2823–2832, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Squire:2014:TRC

[SMR14] Richard H. Squire, Norman H. March, and Angel Rubio. Are there really Cooper pairs and persistent currents in aromatic molecules? *International Journal of Quantum Chemistry*, 114(7):437–440, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarrami:2018:CIS

[SMRK18] Farzaneh Sarrami, Felix A. Mackenzie-Rae, and Amir Karton. A computational investigation of the sulphuric acid-catalysed 1,4-hydrogen transfer in higher Criegee intermediates. *International Journal of Quantum Chemistry*, 118 (15):e25599:1–e25599:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santos:2011:ASY

[SMV11] Leandro C. Santos, M. Graças R. Martins, and J. David M. Vianna. Analytical solutions for Yukawa potential applied to atomic systems embedded in Debye plasmas. *International Journal of Quantum Chemistry*, 111(7–8):1671–1679, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sulatha:2011:ICG

[SN11] M. S. Sulatha and U. Natarajan. Ab initio calculations of the geometry and polarizabilities of bisphenyls having aliphatic substituents. *International Journal of Quantum Chemistry*, 111(5):1092–1100, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Senior:2012:DPS

[SN12] Samir A. Senior and Ahmed M. Nassar. Determination of pKa for substituted benzoic acids in mixed solvent using density functional theory and QSPR. *International Journal of Quantum Chemistry*, 112(3):683–694, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Seino:2015:PLS

[SN15] Junji Seino and Hiromi Nakai. Perspectives: Large-scale two-component relativistic quantum-chemical theory: Combination of the infinite-order Douglas–Kroll–Hess method with the local unitary transformation scheme and the divide-and-conquer method. *International Journal of Quantum Chemistry*, 115(5):253–257, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanchez:2010:IQP

[SOF+10] M. Sánchez, M. Oldenhof, J. A. Freitez, K. C. Mundim, and F. Ruette. An improvement of quantum parametric methods by using SGSA parameterization technique and new elementary parametric functionals. *International Journal of Quantum Chemistry*, 110(3):755–764, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Singh:2010:TFA

[SOM10] Raman K. Singh, J. V. Ortiz, and Manoj K. Mishra. Tautomeric forms of adenine: Vertical ionization energies and Dyson orbitals. *International Journal of Quantum Chemistry*, 110(10):1901–1915, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stemmle:2019:QEC

[SP19] Christian Stemmle and Beate Paulus. Quantification of electron correlation effects: Quantum Information Theory vs Method of Increments. *International Journal of Quantum Chemistry*, 119(21):e26007:1–e26007:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sendiuk:2018:ISD

[SPD+18] Volodymyr A. Sendiuk, Elena L. Pavlenko, Oksana P. Dmytrenko, Mykola P. Kulish, Oleksandr O. Viniychuk, Yaroslav O. Prostota, and Olexiy D. Kachkovsky. Interaction of solitons on 2-dimensional branched π-electron surface of graphene ribbons. *International Journal of Quantum Chemistry*, 118(2):??, January 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sladek:2014:SEI

[SPIL14] Vladimir Sladek, Kraiwan Punyain, Michal Ilčin, and Vladimír Lukeš. Substitution effect on the intermolecular halogen and hydrogen bonds of the σ-bonded fluorinated pyridine$\cdots$XY/HX complexes (XY = F_2, Cl_2, ClF; HX = HF, HCl). *International Journal of Quantum Chemistry*, 114(13):869–878, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szalay:2015:TRT

[SPM+15] Szilárd Szalay, Max Pfeffer, Valentin Murg, Gergely Barcza, Frank Verstraete, Reinhold Schneider, and Örs Legeza. Tutorial reviews: Tensor product methods and entanglement optimization for ab initio quantum chemistry. *International Journal of Quantum Chemistry*, 115(19):1342–1391, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sauer:2011:CRV

[SPO+11] S. P. A. Sauer, I. Paidarová, J. Oddershede, K. L. Bak, and J. F. Ogilvie. Calculated rotational and vibrational g factors of LiH $X\,^1\Sigma^+$ and evaluation of parameters in radial functions from rotational and vibration-rotational spectra. *International Journal of Quantum Chemistry*, 111 (4):736–752, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sagarik:2015:DPE

[SPPT15] Kritsana Sagarik, Pannipa Panajapo, Mayuree Phonyiem, and Jittima Thisuwan. Dynamics of proton exchange in a model phosphonic acid-functionalized polymer. *International Journal of Quantum Chemistry*, 115(17):1161–1174,

September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sardar:2011:CTD

[SPSA11] Subhankar Sardar, Amit Kumar Paul, Rahul Sharma, and Satrajit Adhikari. A "classical" trajectory driven nuclear dynamics by a parallelized quantum-classical approach to a realistic model Hamiltonian of benzene radical cation. *International Journal of Quantum Chemistry*, 111(12):2741–2759, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Soo:2010:ADC

[SQ10] Tsz-Yan Soo and Changyong Qin. Adsorption and dissociation of carbon trioxide on Ag(100). *International Journal of Quantum Chemistry*, 110(4):946–952, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2011:CIP

[SR11a] Pedro J. Silva and Maria João Ramos. Computational insights into the photochemical step of the reaction catalyzed by protochlorophylide oxidoreductase. *International Journal of Quantum Chemistry*, 111(7–8):1472–1479, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2011:DFF

[SR11b] Chang-Ik Song and Young Min Rhee. Development of force field parameters for oxyluciferin on its electronic ground and excited states. *International Journal of Quantum Chemistry*, 111(15):4091–4105, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sahoo:2012:FSS

[SR12] Shaon Sahoo and S. Ramasesha. Full spin and spatial symmetry adapted technique for correlated electronic Hamiltonians: Application to an icosahedral cluster. *International Journal of Quantum Chemistry*, 112(4):1041–1054, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Siddiqui:2013:QCS

[SR13] Shamoon Ahmad Siddiqui and Tabish Rasheed. Quantum chemical study of IrF_n ($n = 1$–7) clusters: an investigation of superhalogen properties. *International Journal of Quantum Chemistry*, 113(7):959–965, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sinha:2018:RMM

[SR18] Sourab Sinha and Abhijeet Raj. Reaction mechanism and modeling study for the oxidation by SO_2 of *o*-xylene and *p*-xylene in Claus process. *International Journal of Quantum Chemistry*, 118(14):e25583:1–e25583:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanchez:2019:CAE

[SR19] Morella Sánchez and Fernando Ruette. Calculations of adsorption energies, coadsorptions, and diffusion barriers of H atoms, and the H_2 formation on a nanographene surface (coronene). *International Journal of Quantum Chemistry*, 119(10):e25893:1–e25893:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stephen:2011:PWB

[SRA+11] A. David Stephen, M. Revathi, S. N. Asthana, Rajesh B. Pawar, and P. Kumaradhas. Probing the weakest bond and the cleavage of *p*-chlorobenzaldehyde diperoxide energetic molecule via quantum chemical calculations and theoretical charge density analysis. *International Journal of Quantum Chemistry*, 111(14):3741–3754, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shahbazi-Raz:2016:TCP

[SRASZ16] Farsheed Shahbazi-Raz, Maryam Adineh, Nasser Safari, and Mansour Zahedi. Theoretical calculation and prediction for experimental design to obtain spin crossover complexes. *International Journal of Quantum Chemistry*, 116 (15):1179–1186, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2018:SDE

[Sri18] Ambrish Kumar Srivastava. Single- and double-electron reductions of CO_2 by using superalkalis: an ab initio study. *International Journal of Quantum Chemistry*, 118 (15):e25598:1–e25598:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2019:CAE

[Sri19] Ambrish Kumar Srivastava. CO_2-activation and enhanced capture by C_6Li_6: a density functional approach. *International Journal of Quantum Chemistry*, 119(20):e25904:1–e25904:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Snyder:2015:NGD

[SRMB15] John C. Snyder, Matthias Rupp, Klaus-Robert Müller, and Kieron Burke. Nonlinear gradient denoising: Finding accurate extrema from inaccurate functional derivatives. *International Journal of Quantum Chemistry*, 115(16):1102–1114, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Steinmann:2019:RPE

[SRN+19] Casper Steinmann, Peter Reinholdt, Morten Steen Nørby, Jacob Kongsted, and Jógvan Magnus Haugaard Olsen. Response properties of embedded molecules through the polarizable embedding model. *International Journal of Quantum Chemistry*, 119(1):e25717:1–e25717:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadhukhan:2016:DEM

[SRPD16] M. Sadhukhan, Amlan K. Roy, P. K. Panigrahi, and B. M. Deb. Dynamics of electronic motion in hydrogen atom under parallel strong oscillating magnetic field and intense laser fields. *International Journal of Quantum Chemistry*, 116(5):377–387, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2017:FGM

[SRS+17] Rishabh Shukla, Debmalya Ray, Kanchan Sarkar, Mayank Kumar Dixit, and Shankar Prasad Bhattacharyya. Flying onto

global minima on potential energy surfaces: a swarm intelligence guided route to molecular electronic structure. *International Journal of Quantum Chemistry*, 117(5):??, March 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadlej-Sosnowska:2010:TED

[SS10] N. Sadlej-Sosnowska. Transfer of electron density as a result of hydrogen bond formation — a case of charged complexes. *International Journal of Quantum Chemistry*, 110 (7):1354–1359, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solimannejad:2011:UHB

[SS11] Mohammad Solimannejad and Steve Scheiner. Unconventional H-bonds: SH$\cdots$N interaction. *International Journal of Quantum Chemistry*, 111(12):3196–3200, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stefanska:2012:EMD

[SS12] Patrycja Stefańska and Radosław Szmytkowski. Electric and magnetic dipole shielding constants for the ground state of the relativistic hydrogen-like atom: Application of the Sturmian expansion of the generalized Dirac–Coulomb Green function. *International Journal of Quantum Chemistry*, 112(5):1363–1372, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suzuki:2013:DFT

[SS13] Hidenori Suzuki and Chikatoshi Satoko. Density functional theory study on magnetic interactions in the V^{3+} dimer complexes. *International Journal of Quantum Chemistry*, 113(6):745–752, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sandhiya:2018:EMR

[SS18a] Lakshmanan Sandhiya and Kittusamy Senthilkumar. Exploring the mechanisms for the radical induced damage of 6-thioguanine. *International Journal of Quantum Chemistry*, 118(11):e25544:1–e25544:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shukla:2018:CAN

[SS18b] Madhulata Shukla and Indrajit Sinha. Catalytic activation of nitrobenzene on PVP passivated silver cluster: a DFT investigation. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sabzyan:2019:BIC

[SS19a] Hassan Sabzyan and Hossein Shirani. Bistability of an iron–cobalt binuclear complex. *International Journal of Quantum Chemistry*, 119(7):e25856:1–e25856:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slamet:2019:SKE

[SS19b] Marlina Slamet and Viraht Sahni. Study of the kinetic energy densities of electrons as applied to quantum dots in a magnetic field. *International Journal of Quantum Chemistry*, 119(5):e25818:1–e25818:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sinha:2018:TSP

[SSA18] Nidhi Sinha, Suvam Singh, and Bobby Antony. Theoretical study of positron scattering by group 14 tetra hydrides: a quantum mechanical approach. *International Journal of Quantum Chemistry*, 118(18):e25679:1–e25679:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shandilya:2013:TDW

[SSAM13] Bhavesh K. Shandilya, Manabendra Sarma, Satrajit Adhikari, and Manoj K. Mishra. Time dependent wave packet treatment of $^2\Pi_g$ N_2^- and $^3\Sigma^-$ NO^- shape resonances using two-dimensional surfaces for electron-N_2 and NO interactions. *International Journal of Quantum Chemistry*, 113 (2):130–138, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sarkar:2012:CVA

[SSB12a] Kanchan Sarkar, Rahul Sharma, and S. P. Bhattacharyya. A constrained variational approach to the designing of

low transport band gap materials: a multiobjective random mutation hill climbing method. *International Journal of Quantum Chemistry*, 112(6):1547–1558, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szaleniec:2012:QCM

[SSB+12b] Maciej Szaleniec, Aleksander Salwiński, Tomasz Borowski, Johann Heider, and Małgorzata Witko. Quantum chemical modeling studies of ethylbenzene dehydrogenase activity. *International Journal of Quantum Chemistry*, 112(8):1990–1999, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saha:2019:NBH

[SSB19] Bapan Saha, Himakshi Sharma, and Pradip Kr. Bhattacharyya. Nonclassical B-$H_b \cdots \pi$ interaction in diborane$\cdots$localized-π sandwiches: a DFT-D3 study. *International Journal of Quantum Chemistry*, 119(20):e25998:1–e25998:??, October 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2017:GPA

[SSdS17] Jing Sun, Sui So, and Gabriel da Silva. The gas phase aldose-ketone isomerization mechanism: Direct interconversion of the model hydroxycarbonyls 2-hydroxypropanal and hydroxyacetone. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saito:2010:TCB

[SSI+10] Toru Saito, Mitsuo Shoji, Hiroshi Isobe, Shusuke Yamanaka, Yasutaka Kitagawa, Satoru Yamada, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes. XIV. Correspondence between magnetic coupling mode and radical coupling mechanism in hydroxylations with methane monooxygenase and related species. *International Journal of Quantum Chemistry*, 110(15):2955–2981, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santhanamoorthi:2011:LRC

[SSK11] N. Santhanamoorthi, K. Senthilkumar, and P. Kolandaivel. Long-range charge transfer in donor-peptide bridge-acceptor model systems — a theoretical study. *International Journal of Quantum Chemistry*, 111(14):3904–3914, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saito:2012:TCB

[SSK+12] Toru Saito, Mitsuo Shoji, Keita Kanda, Hiroshi Isobe, Shusuke Yamanaka, Yasutaka Kitagawa, Satoru Yamada, Takashi Kawakami, Mitsutaka Okumura, and Kizashi Yamaguchi. Theory of chemical bonds in metalloenzymes. XVII. Symmetry breaking in manganese cluster structures and chameleonic mechanisms for the O — O bond formation of water splitting reaction. *International Journal of Quantum Chemistry*, 112(1):121–135, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saranya:2012:CTO

[SSKS12] Govindarajan Saranya, Nachimuthu Santhanamoorthi, Ponmalai Kolandaivel, and Kittusamy Senthilkumar. Charge transport and optical properties of discotic liquid crystalline molecules THDDP and substituted THDP. *International Journal of Quantum Chemistry*, 112(3):713–723, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Silva:2014:PPR

[SSP14] Carlos M. Silva, Poliana L. Silva, and Josefredo R. Pliego. Prediction of the pH-rate profile for dimethyl sulfide oxidation by hydrogen peroxide: the role of elusive $H_3\ O_2^+$ Ion. *International Journal of Quantum Chemistry*, 114(8):501–507, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sadhu:2017:SSS

[SSP+17a] Biswajit Sadhu, Mahesh Sundararajan, Anilkumar Pillai, Rajvir Singh, and Tusar Bandyopadhyay. Selective separation of strontium by multitopic ion-pair receptor: a DFT exploration. *International Journal of Quantum Chemistry*,

117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sririrak:2017:CDF

[SSP+17b] Jitnapa Sririrak, Darunee Sertphon, Wasinee Phonsri, Phimphaka Harding, and David J. Harding. Comparison of density functionals for the study of the high spin low spin gap in Fe(III) spin crossover complexes. *International Journal of Quantum Chemistry*, 117(9):??, May 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srikanth:2015:MDC

[SSS15] Malladi Srikanth, Garikapati Narahari Sastry, and Yarasi Soujanya. Molecular design of corrole-based D-π-A sensitizers for dye-sensitized solar cell applications. *International Journal of Quantum Chemistry*, 115(12):745–752, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sidir:2011:TSE

[SSTÖ11] Yadİgar Gülseven Sidir, İsa Sidir, Erol Taşal, and Cemİl Öğretir. A theoretical study on electronic structure and structure–activity properties of novel drug precursor 6-acylbenzothiazolon derivatives. *International Journal of Quantum Chemistry*, 111(14):3616–3629, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

South:2016:DEE

[SSW16] Christopher South, George Schoendorff, and Angela K. Wilson. Dissociation energy and electronic structure of the low valent lanthanide compound NdF^+. *International Journal of Quantum Chemistry*, 116(10):791–794, May 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sathya:2015:SBV

[ST15] Rajendran Sathya and Subbiah Thamotharan. In silico based virtual screening and mixed mode QM/MM calculation identifies caffeine scaffold for designing potential inhibitors for tyrosyl tRNA synthetase of *Mycobacterium tuberculosis*. *International Journal of Quantum Chemistry*,

115(3):187–195, February 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stanek:2010:WFR

[Sta10] Jerzy Stanek. The Wigner function of the rotating Kratzer oscillator mapped onto the Morse oscillator. *International Journal of Quantum Chemistry*, 110(9):1615–1621, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2012:IRC

[STL12] Chongfu Song, Zhimei Tian, and Quanxin Li. Ab initio and RRKM calculations for the reaction channels of $O(^1D)$ + CH_3CHF_2. *International Journal of Quantum Chemistry*, 112(5):1353–1362, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Suzuki:2017:MLA

[STM17] Teppei Suzuki, Ryo Tamura, and Tsuyoshi Miyazaki. Machine learning for atomic forces in a crystalline solid: Transferability to various temperatures. *International Journal of Quantum Chemistry*, 117(1):33–39, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Srivastava:2018:ABS

[STM18] Ambrish Kumar Srivastava, Sugriva Nath Tiwari, and Neeraj Misra. Alkalized borazine: a simple recipe to design closed-shell superalkalis. *International Journal of Quantum Chemistry*, 118(6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Stopkowicz:2018:PCC

[Sto18] Stella Stopkowicz. Perspective: Coupled cluster theory for atoms and molecules in strong magnetic fields. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sugimoto:2019:MQS

[STU19] Hideya Sugimoto, Masanori Tachikawa, and Taro Udagawa. Multicomponent QM study on the reaction of HOSO

+ NO_2 with H_2O: Nuclear quantum effect on structure and reaction energy profile. *International Journal of Quantum Chemistry*, 119(10):e25895:1–e25895:??, May 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Slanina:2011:CSM

[SUL+11] Zdeněk Slanina, Filip Uhlík, Shyi-Long Lee, Ludwik Adamowicz, Takeshi Akasaka, and Shigeru Nagase. Computed stabilities in metallofullerene series: Al@C_{82}, Sc@C_{82}, Y@C_{82}, and La@C_{82}. *International Journal of Quantum Chemistry*, 111(11):2712–2718, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sutcliffe:2012:SDC

[Sut12] Brian Sutcliffe. Some difficulties in considering rotation motion within the Born–Oppenheimer approximation for polyatomic molecules. *International Journal of Quantum Chemistry*, 112(17):2894–2903, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Swart:2011:ARM

[SV11] Marcel Swart and Piet Th. Van Duijnen. Atomic radii in molecules for use in a polarizable force field. *International Journal of Quantum Chemistry*, 111(7–8):1763–1772, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sanz-Vicario:2010:MFP

[SVPTM+10] J. L. Sanz-Vicario, J. F. Pérez-Torres, F. Morales, E. Plésiat, and F. Martín. Molecular frame photoelectron angular distributions for H_2 ionization by single and trains of attosecond XUV laser pulses. *International Journal of Quantum Chemistry*, 110(13):2462–2471, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Santillan-Vargas:2012:DFT

[SVRGV12] Hilda Santillán-Vargas, José-Zeferino Ramírez, Jorge Garza, and Rubicelia Vargas. Density-functional-theory

study of α-cyclodextrin inclusion complexes. *International Journal of Quantum Chemistry*, 112(22):3587–3593, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Schwarz:2010:SSP

[SW10] W. H. Eugen Schwarz and Shu-Guang Wang. Some solved problems of the periodic system of chemical elements. *International Journal of Quantum Chemistry*, 110(8):1455–1465, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2012:CIW

[SW12] Chang-Liang Sun and Chang-Sheng Wang. Cooperative influence of water binding to peptides by NH $\cdots$OH$_2$ and C O $\cdots$HOH hydrogen bonds: Study by Ab Initio calculations. *International Journal of Quantum Chemistry*, 112 (10):2336–2341, May 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Swart:2013:SSB

[Swa13] Marcel Swart. Spin states of (bio)inorganic systems: Successes and pitfalls. *International Journal of Quantum Chemistry*, 113(1):2–7, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2012:MCI

[SWS12] Jin-Feng Sun, Jie-Min Wang, and De-Heng Shi. Multireference configuration interaction study on spectroscopic parameters and molecular constants of PO and PO$^+$. *International Journal of Quantum Chemistry*, 112(3):672–682, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2014:DSM

[SWS+14] Chuanzhi Sun, Kui Wang, Haitao Sun, Nan Sun, and Dezhan Chen. A DFT study on a mutipathways, one product reaction: Initially divergent radical reactions reconverge to form a single product. *International Journal of Quantum Chemistry*, 114(12):769–781, June 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Su:2015:PTC

[SX15] Neil Qiang Su and Xin Xu. Perspectives: Toward the construction of parameter-free doubly hybrid density functionals. *International Journal of Quantum Chemistry*, 115(10): 589–595, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheng:2018:VCB

[SXH18] Xiaowei Sheng, Xian Xu, and Shizhong Huang. On the validity of complete basis set extrapolation formula optimized for the equilibrium distance applied to the potential energy surface for the correlation energy of the helium dimer. *International Journal of Quantum Chemistry*, 118 (12):e25552:1–e25552:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2012:SCMa

[SXS+12] De-Heng Shi, Wei Xing, Jin-Feng Sun, Zun-Lue Zhu, and Yu-Fang Liu. Spectroscopic constants and molecular properties of $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, and $B'3\Sigma_u^-$ electronic states of the N_2 molecule. *International Journal of Quantum Chemistry*, 112(5):1323–1342, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Samanta:2010:OPW

[SY10] Kousik Samanta and Danny L. Yeager. Obtaining positions and widths of scattering resonances from a complex multiconfigurational self-consistent field state using the M_1 method. *International Journal of Quantum Chemistry*, 110 (4):798–812, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Saito:2012:PMW

[SYK+12] T. Saito, S. Yamanaka, K. Kanda, H. Isobe, Y. Takano, Y. Shigeta, Y. Umena, K. Kawakami, J.-R. Shen, N. Kamiya, M. Okumura, M. Shoji, Y. Yoshioka, and K. Yamaguchi. Possible mechanisms of water splitting reaction based on proton and electron release pathways revealed for $CaMn_4O_5$ cluster of PSII refined to 1.9Å X-ray resolution. *International Journal of Quantum Chemistry*, 112(1):253–276, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shan:2018:ASC

[SYL+18] Shimin Shan, Shuang Yin, Yi Lian, Haifeng Xu, and Bing Yan. Accurate spectroscopic constants of the lowest three electronic states in halonitrenes with multireference configuration interaction. *International Journal of Quantum Chemistry*, 118(16):e25649:1–e25649:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2010:IMM

[SYQ+10] Shi-Ling Sun, Guo-Chun Yang, Chun-Sheng Qin, Yong-Qing Qiu, Li-Kai Yan, Zhong-Min Su, and Rong-Shun Wang. The influence of M...M attraction on nonlinear optical properties of $(XMPH_3)_2$ (X = F, Cl; and M = Au, Ag and Cu): a theoretical study. *International Journal of Quantum Chemistry*, 110(4):865–873, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Staykov:2014:EHG

[SYS14] Aleksandar Staykov, Junichiro Yamabe, and Brian P. Somerday. Effect of hydrogen gas impurities on the hydrogen dissociation on iron surface. *International Journal of Quantum Chemistry*, 114(10):626–635, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sutay:2016:PHS

[SYY16] Berkay Sütay, Mine Yurtsever, and Ersin Yurtsever. A post-HF study on the halogen bonding interaction of pyrene with diatomic halogen molecules. *International Journal of Quantum Chemistry*, 116(9):702–709, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Solkan:2011:PHF

[SZ11] V. N. Solkan and G. M. Zhidomirov. Post-Hartree–Fock (MP2 and MP4) study on decomposition of nitrous oxide on the nonframework AlO(+) site in ZSM-5 zeolite. *International Journal of Quantum Chemistry*, 111(11):2639–2648, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2015:RDP

[SZ15] Zhigang Sun and Dong H. Zhang. Reviews: Development of the potential energy surface and current stage of the quantum dynamics studies of the F + H_2 /HD reaction. *International Journal of Quantum Chemistry*, 115(11):689–699, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szalay:2013:PCC

[Sza13] Péter G. Szalay. Perspectives: Can coupled-cluster methods be used to describe excited states of the building blocks of DNA? *International Journal of Quantum Chemistry*, 113(14):1821–1827, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Szczepanik:2018:SAP

[Szc18] Dariusz W. Szczepanik. A simple alternative to the pseudo-π method. *International Journal of Quantum Chemistry*, 118(19):e25696:1–e25696:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2014:GVF

[SZL+14] Erping Sun, Junfeng Zhang, Rui Li, Qixiang Sun, Changli Wei, Haifeng Xu, and Bing Yan. Geometries, vibrational frequencies, and excitation energies of a series of fluorine-substituted carbenes, FCX (X = H, F, Cl, Br, and I): a high-level multireference configuration interaction study. *International Journal of Quantum Chemistry*, 114(1):66–73, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2015:TSD

[SZL+15] Shengmin Sun, Kun Zhang, Yang Lu, Ping Liu, and Hui Zhang. Theoretical study on the degradation mechanism of methamidophos and chloramine phosphorus with OH radicals. *International Journal of Quantum Chemistry*, 115(17):1187–1193, September 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Shi:2010:SIH

[SZS+10] De-Heng Shi, Jin-Ping Zhang, Jin-Feng Sun, Hui Liu, Yu-Fang Liu, Zun-Lue Zhu, and Zheng-He Zhu. Spectroscopic

investigations on the HCl($X\,^2\Pi$) ion using coupled-cluster theory in combination with the correlation-consistent quintuple basis set augmented with diffuse functions. *International Journal of Quantum Chemistry*, 110(8):1481–1488, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sun:2017:QRD

[SZY17] Zhao-Peng Sun, Wen-Kai Zhao, and Chuan-Lu Yang. Quantum reaction dynamics of C(^{1}D) + HDCH(CD) + D(H) on the ground state potential energy surface. *International Journal of Quantum Chemistry*, 117(21):??, November 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2012:CCS

[SZZ+12] Ming-Xing Song, Zeng-Xia Zhao, Wei Zhang, Fu-Quan Bai, Hong-Xing Zhang, and Chia-Chung Sun. A CASSCF/CASPT2 study on the low-lying electronic states of the CH_3SS and its cation. *International Journal of Quantum Chemistry*, 112(6):1537–1546, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Sheng:2019:AAF

[SZZ+19] Xiaowei Sheng, Hongjuan Zhu, Zixuan Zhang, Danyang Zhang, Jingyang Lu, and Jianping Xiao. An accurate analytical formula for the van der Waals potentials of homonuclear rare-gas dimers with one adjustable parameter. *International Journal of Quantum Chemistry*, 119(3):e25800:1–e25800:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Song:2011:TSS

[SZZZ11] Xiudan Song, Yongfang Zhao, Pingxia Zhang, and Guohua Zhang. Theoretical study on structures and vibrational spectra of $M^+(H_2O)Ar$ (M = Cu, Ag, Au). *International Journal of Quantum Chemistry*, 111(9):2109–2116, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2010:CAE

[TÁ10] A. L. Tchougréeff and J. G. Ángyán. Classes of admissible exchange-correlation density functionals for pure spin and

angular momentum states. *International Journal of Quantum Chemistry*, 110(2):454–475, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talman:2011:MEO

[Tal11] James D. Talman. Multipole expansions of orbital products about an intermediate center. *International Journal of Quantum Chemistry*, 111(10):2221–2227, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tanak:2012:DFC

[Tan12] Hasan Tanak. Density functional computational studies on 2-[(2,4-Dimethylphenyl)iminomethyl]-3,5-dimethoxyphenol. *International Journal of Quantum Chemistry*, 112(11): 2392–2402, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2013:HSC

[Tan13] Qian-Lin Tang. H_2S splitting on Cu(110): Insight from combined periodic density functional theory calculations and microkinetic simulation. *International Journal of Quantum Chemistry*, 113(16):1992–2001, August 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tapia:2015:QMP

[Tap15] Orlando Tapia. Quantum-matter photonic framework perspective of chemical processes: Entanglement shifts in HCN/CNH isomerization. *International Journal of Quantum Chemistry*, 115(20):1490–1500, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tasinato:2014:WSP

[Tas14] Nicola Tasinato. What are the spectroscopic properties of HFC-32? Answers from DFT. *International Journal of Quantum Chemistry*, 114(21):1472–1485, November 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tavakol:2011:KTS

[Tav11] Hossein Tavakol. Kinetic and thermodynamic study of inter- and intramolecular proton transfer in N'-acetyl formohydrazide tautomers. *International Journal of Quantum Chemistry*, 111(14):3717–3724, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tavakol:2012:DMS

[Tav12] Hossein Tavakol. DFT and MP2 study of isomery scheme in Formazan and intermolecular and intramolecular proton transfer between its tautomers. *International Journal of Quantum Chemistry*, 112(4):1215–1224, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tanak:2011:CEC

[TAY11] Hasan Tanak, Ayşen Ağar, and Metin Yavuz. Combined experimental and computational modeling studies on 4-[(2-hydroxy-3-methylbenzylidene) amino]-1,5-dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one. *International Journal of Quantum Chemistry*, 111(9):2123–2136, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taylor:2012:BR

[Tay12] Charles A. Taylor. Book review. *International Journal of Quantum Chemistry*, 112(11):2440, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trout:2015:RMS

[TB15] Colin J. Trout and Kenneth R. Brown. Reviews: Magic state distillation and gate compilation in quantum algorithms for quantum chemistry. *International Journal of Quantum Chemistry*, 115(19):1296–1304, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trindle:2013:SEC

[TBA13] Carl Trindle, Erdi A. Bleda, and Zikri Altun. Structure and energetics of cyclopropane carboxaldehyde. *International Journal of Quantum Chemistry*, 113(8):1155–1161, April

15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tecmer:2019:MES

[TBB+19] Paweł Tecmer, Katharina Boguslawski, Mateusz Borkowski, Piotr S. Zuchowski, and Dariusz Kedziera. Modeling the electronic structures of the ground and excited states of the ytterbium atom and the ytterbium dimer: a modern quantum chemistry perspective. *International Journal of Quantum Chemistry*, 119(18):e25983:1–e25983:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trouillas:2011:TUP

[TBHL11] Patrick Trouillas, Jacqueline Bergès, and Chantal Houée-Lévin. Toward understanding the protein oxidation processes: ·OH addition on tyrosine, phenylalanine, or methionine? *International Journal of Quantum Chemistry*, 111 (6):1143–1151, May 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teillet-Billy:2010:IAG

[TBRIS10] D. Teillet-Billy, N. Rougeau, V. V. Ivanovskaya, and V. Sidis. Interaction of atoms with graphenic-type surfaces for the chemistry of the interstellar medium: New properties of H dimers on the surface. *International Journal of Quantum Chemistry*, 110(12):2231–2236, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [TBRIS12].

Teillet-Billy:2011:EIA

[TBRIS11] D. Teillet-Billy, N. Rougeau, V. V. Ivanovskaya, and V. Sidis. Erratum: Interaction of atoms with graphenic-type surfaces for the chemistry of the interstellar medium: New properties of H dimers on the surface. *International Journal of Quantum Chemistry*, 111(15):4504, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [TBRIS10].

Teillet-Billy:2012:EIA

[TBRIS12] D. Teillet-Billy, N. Rougeau, V. V. Ivanovskaya, and V. Sidis. Erratum: Interaction of Atoms With Graphenic-Type Surfaces for the Chemistry of the Interstellar

Medium: New Properties of H Dimers on the Surface. *International Journal of Quantum Chemistry*, 112(6):1758, March 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [TBRIS10].

Tkachenko:2010:PAP

[TBST10] M. Y. Tkachenko, O. P. Boryskina, A. V. Shestopalova, and M. Y. Tolstorukov. ProtNA-ASA: Protein-nucleic acid structural database with information on accessible surface area. *International Journal of Quantum Chemistry*, 110(1): 230–232, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torrens:2010:CNS

[TC10] Francisco Torrens and Gloria Castellano. Cluster nature of the solvent features of single-wall carbon nanohorns. *International Journal of Quantum Chemistry*, 110(3):563–570, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Turbiner:2012:CCS

[TC12] A. V. Turbiner and H. Medel Cobaxin. Critical charges of simple Coulomb molecular systems: One-two electron case. *International Journal of Quantum Chemistry*, 112 (11):2411–2421, June 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tognetti:2010:APS

[TCA10] Vincent Tognetti, Pietro Cortona, and Carlo Adamo. Assessing the performances of some recently proposed density functionals for the description of bond dissociations involving organic radicals. *International Journal of Quantum Chemistry*, 110(12):2320–2329, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trejo:2010:CSP

[TCCI10] A. Trejo, M. Calvino, and M. Cruz-Irisson. Chemical surface passivation of 3C-SiC nanocrystals: a first-principle study. *International Journal of Quantum Chemistry*, 110 (13):2455–2461, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsinberg:2013:SCT

[TCG13] Michael B. Tsinberg, Rohith Chindam, and Jonathan D. Gough. Structural and charge-transfer properties of indolylfulgides. *International Journal of Quantum Chemistry*, 113(15):1949–1955, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Talukder:2017:SAB

[TCG17] Srijeeta Talukder, Pinaki Chaudhury, and Subhasree Ghosh. Simulated annealing-based optimal control over tunneling process through SDWP and Eckart barrier: a momentum basis representation. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2011:I

[Tch11] Andrei L. Tchougréeff. Introduction. *International Journal of Quantum Chemistry*, 111(11):2477, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2013:EVF

[Tch13] Andrei L. Tchougréeff. Editorial: The 13th V. A. Fock meeting on quantum and computational chemistry. *International Journal of Quantum Chemistry*, 113(14):1813, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2016:RSS

[Tch16] Andrei L. Tchougréeff. Reviews: Several stories from theoretical chemistry with some Russian flavor and implications for theorems of chemistry, vagueness of its concepts, fuzziness of its definitions, iconicity of its language, and peculiarities of its nomenclature. *International Journal of Quantum Chemistry*, 116(3):137–160, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Topol:2012:MAK

[TCM+12] Igor Topol, Jack Collins, Vladimir Mironov, Alexander Savitsky, and Alexander Nemukhin. Modeling absorption of the kindling fluorescent protein with the neutral form

of the chromophore. *International Journal of Quantum Chemistry*, 112(17):2947–2951, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsironis:2010:EAC

[TCS10] G. P. Tsironis, A. Ciudad, and J. M. Sancho. Electrostatic analysis of charge interactions in proteins. *International Journal of Quantum Chemistry*, 110(1):233–241, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2012:SEE

[TCSD12] Xiao-Yu Tang, Zhong-Hua Cui, Chang-Bin Shao, and Yi-Hong Ding. Structural and energetic exploration of a boron-rich sulfide cluster B_6S. *International Journal of Quantum Chemistry*, 112(5):1299–1306, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2011:CES

[TD11] Andrei L. Tchougréeff and Richard Dronskowski. Crystal and electronic structure of the room temperature organometallic ferrimagnet $V(TCNE)_2$. Analysis of numerical DoS and magnetic properties as related to orbital and spin-Hamiltonian models. *International Journal of Quantum Chemistry*, 111(11):2490–2509, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tripathi:2019:BAS

[TD19] Divya Tripathi and Achintya Kumar Dutta. Bound anionic states of DNA and RNA nucleobases: An EOM-CCSD investigation. *International Journal of Quantum Chemistry*, 119(9):e25875:1–e25875:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tezsevin:2017:DFT

[TDOD17] Ilker Tezsevin, Cansu Demirtas, Isik Onal, and Cerag Dilek. Density functional theory study of interactions between carbon dioxide and functionalized polyhedral oligomeric silsesquioxanes. *International Journal of Quan-*

tum Chemistry, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tognetti:2010:CMQ

[TFA10] Vincent Tognetti, Guillaume Fayet, and Carlo Adamo. Can molecular quantum descriptors predict the butene selectivity in nickel(II) catalyzed ethylene dimerization? A QSPR study. *International Journal of Quantum Chemistry*, 110 (3):540–548, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torres:2011:TSS

[TFB11] M. B. Torres, E. M. Fernández, and L. C. Balbás. Theoretical study of the structural and electronic properties of aggregates, wires, and bulk phases formed from M@Si_{16} superatoms (M = Sc^-, Ti, V^+). *International Journal of Quantum Chemistry*, 111(2):444–462, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tabacchi:2014:POP

[TFBG14] Gloria Tabacchi, Ettore Fois, Davide Barreca, and Alberto Gasparotto. Perspectives: Opening the Pandora's jar of molecule-to-material conversion in chemical vapor deposition: Insights from theory. *International Journal of Quantum Chemistry*, 114(1):1–7, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tlahuice-Flores:2019:BPS

[TFMC19] Alfredo Tlahuice-Flores and Alvaro Muñoz-Castro. Bonding and properties of superatoms. Analogs to atoms and molecules and related concepts from superatomic clusters. *International Journal of Quantum Chemistry*, 119(2): e25756:1–e25756:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tarakeshwar:2011:QCE

[TFSRM11] Pilarisetty Tarakeshwar, Daniel Finkelstein-Shapiro, Tijana Rajh, and Vladimiro Mujica. Quantum confinement effects on the surface enhanced Raman spectra of hybrid systems molecule-TiO_2 nanoparticles. *International Journal of Quantum Chemistry*, 111(7–8):1659–1670, June/July

2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2015:DFS

[TFZ+15] Changke Tian, Aiping Fu, Chengyan Zhao, Hongliang Li, Zonghua Wang, and Yunbo Duan. Density functional study of organocatalytic Mannich-type reactions: Insight into reverse diastereoselectivities arising from catalysts with different scaffolds. *International Journal of Quantum Chemistry*, 115(6):398–405, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsipis:2013:PES

[TG13] Athanassios Tsipis and Dimitrios Gkarmpounis. Probing the electronic structure, magnetotropicity, and absorption spectra of benzene trapped by lanthanide monoxides, $C_6 H_6 \cdots LnO$, using DFT methods. *International Journal of Quantum Chemistry*, 113(5):694–708, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Theophilou:2016:SEP

[TG16] Andreas K. Theophilou and Vitaly N. Glushkov. Subspace effective potential theory for configuration interaction. *International Journal of Quantum Chemistry*, 116(6):469–475, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsyshevsky:2011:TSE

[TGA+11] Roman V. Tsyshevsky, Guzel G. Garifzianova, Ilia V. Aristov, Alexander G. Shamov, and Grigorii M. Khrapkovskii. Theoretical study of ethene hydrogenation reaction on Ir_4 tetrahedral cluster. *International Journal of Quantum Chemistry*, 111(11):2663–2670, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tolle:2019:CCP

[TGRP19] Johannes Tölle, André Severo Pereira Gomes, Pablo Ramos, and Michele Pavanello. Charged-cell periodic DFT simulations via an impurity model based on density embedding: Application to the ionization potential of liquid water. *International Journal of Quantum Chemistry*, 119(1):

e25801:1–e25801:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Terrabuio:2012:EPP

[TH12] Luiz Alberto Terrabuio and Roberto L. A. Haiduke. Electrostatic potentials and polarization effects in proton-molecule interactions by means of multipoles from the quantum theory of atoms in molecules. *International Journal of Quantum Chemistry*, 112(19):3198–3204, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tew:2013:FWF

[TH13] David P. Tew and Christof Hättig. Frontiers in wave function theory: Pair natural orbitals in explicitly correlated second-order Møller–Plesset theory. *International Journal of Quantum Chemistry*, 113(3):224–229, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tan:2015:PCD

[THL+15] Bisheng Tan, Ming Huang, Xinping Long, Jinshan Li, Xiaodong Yuan, and Ruijuan Xu. From planes to cluster: the design of polynitrogen molecules. *International Journal of Quantum Chemistry*, 115(2):84–89, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Touil:2013:CSC

[THSR13] M'hamed Touil, Najat Hajjaji, Dage Sundholm, and Hassan Rabaâ. Computational studies of the corrosion-inhibition efficiency of iron by triazole surfactants. *International Journal of Quantum Chemistry*, 113(9):1365–1371, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torabi:2014:IIG

[THVP14] Susan Torabi, Lukas Hammerschmidt, Elena Voloshina, and Beate Paulus. Ab initio investigation of ground-state properties of group-12 fluorides. *International Journal of Quantum Chemistry*, 114(14):943–951, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toprek:2013:SPD

[TIKL13] Dragan Toprek, Zoran Ivić, Darko Kapor, and Sreten Lekić. Stationary polarons in discrete molecular chains. *International Journal of Quantum Chemistry*, 113(10):1522–1533, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahashi:2011:QMS

[TIKN11] Hideaki Takahashi, Yuichi Iwata, Ryohei Kishi, and Masayoshi Nakano. The QM/MM-ER studies for the origin of the antioxidative properties of MCI-186 in aqueous solutions. *International Journal of Quantum Chemistry*, 111 (7–8):1748–1762, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tanaka:2013:CCR

[TIN13] Nobuaki Tanaka, Shigeo Itoh, and Hiromasa Nishikiori. Computations of chemical reactions and dynamics: Density functional theory studies on the addition and abstraction reactions of OH radicals with terephthalate dianions. *International Journal of Quantum Chemistry*, 113(4):418–422, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Todde:2017:EEF

[TJS17] Guido Todde, Sanjiv K. Jha, and Gopinath Subramanian. The effect of external forces on the initial dissociation of RDX (1,3,5-trinitro-1,3,5-triazine): a mechanochemical study. *International Journal of Quantum Chemistry*, 117 (20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tachikawa:2016:DIM

[TK16a] Hiroto Tachikawa and Hiroshi Kawabata. Direct ab-initio molecular dynamics study on the radiation effects on catalytic triad composed of Ser-His-Glu residues. *International Journal of Quantum Chemistry*, 116(2):123–129, January 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tehrani:2016:RFM

[TK16b] Zahra Aliakbar Tehrani and Kwang S. Kim. Reviews: Functional molecules and materials by π-interaction based quantum theoretical design. *International Journal of Quantum Chemistry*, 116(8):622–633, April 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tarumi:2013:FWF

[TKN13] Moto Tarumi, Masato Kobayashi, and Hiromi Nakai. Frontiers in wave function theory: Accelerating convergence in the antisymmetric product of strongly orthogonal geminals method. *International Journal of Quantum Chemistry*, 113 (3):239–244, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Taubert:2011:APC

[TKS11] Stefan Taubert, Ville R. I. Kaila, and Dage Sundholm. Aromatic pathways in conjugated rings connected by single bonds. *International Journal of Quantum Chemistry*, 111 (4):848–857, March 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tulyabaev:2017:TRD

[TKSK17] Arthur R. Tulyabaev, Ilya I. Kiryanov, Ilnaz S. Samigullin, and Leonard M. Khalilov. Are there reliable DFT approaches for ^{13}C NMR chemical shift predictions of fullerene C_{60} derivatives? *International Journal of Quantum Chemistry*, 117(1):7–14, January 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2015:CBH

[TL15] WenKai Tian and QingZhong Li. Competition between halogen bond and hydrogen bond in complexes of superalkali Li_3S and halogenated acetylene XCCH (X = F, Cl, Br, and I). *International Journal of Quantum Chemistry*, 115(2):99–105, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torres:2017:SFS

[TLC+17] F. J. Torres, E. V. Ludeña, Y. Carrillo, L. Rincón, P. Iza, and D. Zambrano. Stability of finite subspaces in density

functional theory: Application to simple atoms. *International Journal of Quantum Chemistry*, 117(16):??, August 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teramae:2013:CCR

[TM13] Hiroyuki Teramae and Yasuko Y. Maruo. Computations of chemical reactions and dynamics: Theoretical study on the reaction mechanism of formation of 3,5-diacetyl-1,4-dihydrolutidine. *International Journal of Quantum Chemistry*, 113(4):393–396, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tantardini:2019:DMP

[TM19] Christian Tantardini and Adam A. L. Michalchuk. Dess–Martin periodinane: the reactivity of a λ^5-iodane catalyst explained by topological analysis. *International Journal of Quantum Chemistry*, 119(6):e25838:1–e25838:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tao:2013:BAW

[TMC+13] Jia-Yuan Tao, Wei-Hua Mu, Gregory Adam Chass, Ting-Hua Tang, and De-Cai Fang. Balancing the atomic waistline: Isodensity-based SCRF radii for main-group elements and transition metals. *International Journal of Quantum Chemistry*, 113(7):975–984, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teixeira:2018:ERC

[TMC18] Filipe Teixeira, André Melo, and M. Natália D. S. Cordeiro. Exploring rare chemical phenomena using fractional nuclear charges: the cis- effect in N_2 F_2. *International Journal of Quantum Chemistry*, 118(17):e25662:1–e25662:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Teixeira:2014:CDM

[TMM+14] Filipe Teixeira, Ricardo Mosquera, André Melo, Cristina Freire, and Maria Natália D. S. Cordeiro. Charge distribution in Mn(salen) complexes. *International Journal of Quantum Chemistry*, 114(8):525–533, April 15, 2014. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tashakor:2016:FDI

[TNN16] Saeedeh Tashakor, Mohammad R. Noorbala, and Mansoor Namazian. F_2 dimer: Improved intermolecular potential energy surface using ab initio calculations. *International Journal of Quantum Chemistry*, 116(20):1477–1485, October 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takahashi:2018:ESO

[TNT18] Lauren Takahashi, Tessui Nakagawa, and Keisuke Takahashi. Electronic structure of octagonal boron nitride nanotubes. *International Journal of Quantum Chemistry*, 118 (11):e25542:1–e25542:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tobola:2019:EBS

[Tob19] Robert Tobola. Employing broken symmetry effects from unrestricted coupled cluster wave function to determine dynamic and non-dynamic electron correlation during triple bond breaking in the N_2 molecule. *International Journal of Quantum Chemistry*, 119(8):e25865:1–e25865:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tokmachev:2016:PPG

[Tok16] Andrey M. Tokmachev. Perspectives: Perspectives of geminal methods for large molecular systems. *International Journal of Quantum Chemistry*, 116(4):265–269, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takano:2012:DFS

[TOSN12] Yu Takano, Orio Okuyama, Yasuteru Shigeta, and Haruki Nakamura. Density functional studies of the structural variety of the Cu_2S_2 core of the Cu_A site. *International Journal of Quantum Chemistry*, 112(24):3756–3762, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toutounji:2011:NAE

[Tou11a] Mohamad Toutounji. A new approach to the exact and approximate anharmonic vibrational partition function of diatomic and polyatomic molecules utilizing Morse and Rosen–Morse oscillators. *International Journal of Quantum Chemistry*, 111(9):1885–1892, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toutounji:2011:WHW

[Tou11b] Mohamad Toutounji. What happens when translational energy levels are quantized? *International Journal of Quantum Chemistry*, 111(14):3475–3481, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Toutounji:2013:LEC

[Tou13] Mohamad Toutounji. Letters to the Editor: Comment on "Statistical physics of a mesoscopic fermion system inside a rectangular box" by Radu Lungu. *International Journal of Quantum Chemistry*, 113(8):1243, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Lun13b] and response [Lun13a].

Tsukerblat:2012:SAA

[TPCJ+12] Boris Tsukerblat, Andrew Palii, Juan M. Clemente-Juan, Alejandro Gaita-Ariño, and Eugenio Coronado. A symmetry adapted approach to the dynamic Jahn–Teller problem: Application to mixed-valence polyoxometalate clusters with Keggin structure. *International Journal of Quantum Chemistry*, 112(17):2957–2964, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Turra:2012:NSB

[TPdMB12] Kely Medeiros Turra, Kerly Fernanda Mesquita Pasqualoto, and Silvia Berlanga de Moraes Barros. A novel set of β-N-biaryl ether sulfonamide hydroxamates as potential MMPs inhibitors: Molecular dynamics simulations and molecular properties evaluation. *International Journal of Quantum Chemistry*, 112(20):3374–3389, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tzeli:2013:TSF

[TPT+13] Demeter Tzeli, Ioannis D. Petsalakis, Giannoula Theodorakopoulos, Dariush Ajami, and Julius Rebek Jr. Theoretical study of free and encapsulated carboxylic acid and amide dimers. *International Journal of Quantum Chemistry*, 113(5):734–739, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tzeli:2019:TSP

[TPT19] Demeter Tzeli, Ioannis D. Petsalakis, and Giannoula Theodorakopoulos. Theoretical study of the photophysical processes of a styryl-bodipy derivative eliciting an AND molecular logic gate response. *International Journal of Quantum Chemistry*, 119(16):e25958:1–e25958:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tratnik:2019:CWS

[Tra19] Niko Tratnik. Computing weighted Szeged and PI indices from quotient graphs. *International Journal of Quantum Chemistry*, 119(21):e26006:1–e26006:??, November 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Trindade:2014:FGS

[Tri14] Marco A. S. Trindade. Factor groups, semidirect product and quantum chemistry. *International Journal of Quantum Chemistry*, 114(22):1528–1533, November 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Torres:2019:RIC

[TRZ+19] Fernando J. Torres, Luis Rincón, Cesar Zambrano, José R. Mora, and Miguel Méndez. A review on the information content of the pair density as a tool for the description of the electronic properties in molecular systems. *International Journal of Quantum Chemistry*, 119(2):e25763:1–e25763:??, January 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tenorio:2012:DAE

[TSBSM12] Francisco J. Tenorio, Roberto Sato-Berrú, José M. Saniger, and Ana Martínez. Is the donor–acceptor electronegativity a good indicator for the surface enhanced Raman scattering (SERS)? *International Journal of Quantum Chemistry*, 112(21):3516–3524, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tolosa:2017:TTS

[TSH17] Santiago Tolosa, Jorge Antonio Sansón, and Antonio Hidalgo. Theoretical thermodynamic study of the adenine–thymine tautomeric equilibrium: Electronic structure calculations and steered molecular dynamic simulations. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takano:2012:ESC

[TSKN12] Yu Takano, Yasuteru Shigeta, Kenichi Koizumi, and Haruki Nakamura. Electronic structures of the Cu_2S_2 core of the Cu_A site in cytochrome c oxidase and nitrous oxide reductase. *International Journal of Quantum Chemistry*, 112(1):208–218, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2011:ISP

[TSL11] Zhimei Tian, Chongfu Song, and Quanxin Li. Ab initio study of the potential energy surface and product branching ratios for the reaction of O(^{1} D) with CH_3 CH_2 Br. *International Journal of Quantum Chemistry*, 111(3):631–643, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tranter:2015:BKT

[TSS+15] Andrew Tranter, Sarah Sofia, Jake Seeley, Michael Kaicher, Jarrod McClean, Ryan Babbush, Peter V. Coveney, Florian Mintert, Frank Wilhelm, and Peter J. Love. The Bravyi–Kitaev transformation: Properties and applications. *International Journal of Quantum Chemistry*, 115(19):1431–1441, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsuneda:2015:RCR

[Tsu15] Takao Tsuneda. Reviews: Chemical reaction analyses based on orbitals and orbital energies. *International Journal of Quantum Chemistry*, 115(5):270–282, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2016:REH

[TSvL+16] Andrei L. Tchougréeff, Alexander V. Soudackov, Jan van Leusen, Paul Kögerler, Klaus-Dieter Becker, and Richard Dronskowski. Reviews: Effective Hamiltonian crystal field: Present status and applications to iron compounds. *International Journal of Quantum Chemistry*, 116(4):282–294, February 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tezcan:2010:CSA

[TT10] Habíbe Tezcan and Nesrín Tokay. A computational study of the absorption spectra of 1-substituted phenyl-3,5-diphenylformazans. *International Journal of Quantum Chemistry*, 110(12):2140–2146, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tchougreeff:2013:RRT

[TTD13] Andrei L. Tchougréeff, Andrei M. Tokmachev, and Richard Dronskowski. Reviews: Resonance theory of catalytic action of transition-metal complexes: Isomerization of quadricyclane to norbornadiene catalyzed by metal porphyrins. *International Journal of Quantum Chemistry*, 113 (14):1833–1846, July 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tsoneva:2016:NCD

[TTM16] Yana Tsoneva, Alia Tadjer, and Tzonka Mineva. NMR characterization of dilauroyl phosphatidylcholine in adsorbed monolayers at fluid interfaces studied by multiscale computations. *International Journal of Quantum Chemistry*, 116(19):1419–1426, October 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tassi:2013:HFC

[TTT13] M. Tassi, Iris Theophilou, and S. Thanos. Hartree–Fock calculation for excited states. *International Journal of Quantum Chemistry*, 113(5):690–693, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Thirumuruganandham:2010:LFV

[TU10] Saravana Prakash Thirumuruganandham and Herbert M. Urbassek. Low-frequency vibrational modes in blue opsin: a computational study. *International Journal of Quantum Chemistry*, 110(2):278–283, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tugsuz:2013:DSS

[Tug13] Tugba Tugsuz. A DFT study on the standard electrode potentials of 2-substituted imidazoles. *International Journal of Quantum Chemistry*, 113(5):715–722, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tarade:2013:RAH

[TV13] Tena Tarade and Valerije Vrček. Reactivity of amines with hypochlorous acid: Computational study of steric, electronic, and medium effects. *International Journal of Quantum Chemistry*, 113(7):881–890, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2010:AMM

[TW10] Fu-Yang Tian and Yuan-Xu Wang. Adjusting magnetic moments of Sc_{13} and Y_{13} clusters by doping different X atom (X = Na, Mg, Al, Si, P). *International Journal of Quantum Chemistry*, 110(8):1573–1582, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tan:2014:PRH

[TWHZ14] Rongri Tan, Dongqi Wang, Lin Hu, and Feng-Shou Zhang. Probing the reactivity of hydroxyl radicals toward isolated thymine using theoretical calculations. *International Journal of Quantum Chemistry*, 114(6):367–374, March 15,

2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tyminska:2015:MCB

[TWR15] Nina Tymińska, Marta Włoch, and A. Timothy Royappa. Mind the correct basis set: a case study for predicting gas phase acidities of small compounds using calculations from first principles. *International Journal of Quantum Chemistry*, 115(1):42–49, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2019:NGQ

[TXK+19] Tian Tian, Tianlv Xu, Steven R. Kirk, Michael Filatov, and Samantha Jenkins. Next-generation quantum theory of atoms in molecules for the ground and excited state of the ring-opening of cyclohexadiene. *International Journal of Quantum Chemistry*, 119(8):e25862:1–e25862:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2010:TSMb

[TXL10] Chun Liang Tian, Yue Hua Xu, and Xiu Hui Lu. Theoretical studies on the mechanism of formation of a heteropolycyclic germanic compound between dimethyl-germylidene and ethylene. *International Journal of Quantum Chemistry*, 110(9):1675–1681, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tennyson:2017:SNU

[TY17] Jonathan Tennyson and Sergei N. Yurchenko. Software news & updates: The ExoMol project: Software for computing large molecular line lists. *International Journal of Quantum Chemistry*, 117(2):92–103, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tian:2010:TSMa

[TYL10] Chun Liang Tian, Hai Bin Yu, and Xiu Hui Lu. Theoretical study of mechanism of forming a silapolycyclic compound between methylenesilylene and acetone. *International Journal of Quantum Chemistry*, 110(7):1344–1353, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Takano:2013:CBB

[TYN13] Yu Takano, Kizashi Yamaguchi, and Haruki Nakamura. Computational biochemistry and biophysics: Theoretical studies of electrostatic effect of protein environment on electronic structures and chemical indices of the active site of oxygenated and deoxygenated hemerythrin. *International Journal of Quantum Chemistry*, 113(4):497–503, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2011:FPI

[TZ11] Shanshan Tang and Jingping Zhang. First principles investigation on the key factors of broad absorption spectra and electronic properties for oligothiophene and its derivatives for solar cells. *International Journal of Quantum Chemistry*, 111(9):2089–2098, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Tang:2019:EZA

[TZD+19] Jianling Tang, Cairong Zhang, Ning Du, Yanyan Zhao, and Hongshan Chen. Enhanced Zintl anions by carbon doping in Al — Na clusters and new magic structure Al_6 Na_4 C. *International Journal of Quantum Chemistry*, 119(9): e25871:1–e25871:??, May 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ullah:2019:ADA

[UDS19a] Saif Ullah, Pablo A. Denis, and Fernando Sato. Adsorption and diffusion of alkali-atoms (Li, Na, and K) on BeN dual doped graphene. *International Journal of Quantum Chemistry*, 119(11):e25900:1–e25900:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ullah:2019:MBA

[UDS19b] Saif Ullah, Pablo A. Denis, and Fernando Sato. Monolayer boron-arsenide as a perfect anode for alkali-based batteries with large storage capacities and fast mobilities. *International Journal of Quantum Chemistry*, 119(18):e25975:1–e25975:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uribe:2010:NCH

[UDVD10] Emilbus A. Uribe, Martha C. Daza, José L. Villaveces, and Silvia A. Delgado. On the nature of copper–hydrogen bonding: AIM and NBO analysis of CuH_n $(1 \leq n \leq 6)$ complexes. *International Journal of Quantum Chemistry*, 110 (3):524–531, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ugandi:2018:UBS

[UGWL18] Mihkel Ugandi, Ignacio Fdez. Galván, Per-Olof Widmark, and Roland Lindh. Uncontracted basis sets for ab initio calculations of muonic atoms and molecules. *International Journal of Quantum Chemistry*, 118(21):e25755:1–e25755:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uppuladinne:2013:QCS

[UJSJ13] Mallikarjunachari V. N. Uppuladinne, Vinod Jani, Uddhavesh B. Sonavane, and Rajendra R. Joshi. Quantum chemical studies of novel 2′–4′ conformationally restricted antisense monomers. *International Journal of Quantum Chemistry*, 113(23):2523–2533, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ueno:2011:TSG

[UKF+11] Leonardo T. Ueno, Valéria O. Kiohara, Luiz F. A. Ferrão, Luiz R. Marim, Orlando Roberto-Neto, and Francisco B. C. Machado. Theoretical study of the Ge_mSi_n $(m + n = 3)$ clusters. *International Journal of Quantum Chemistry*, 111 (7–8):1562–1569, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uzunova:2013:DFS

[UMS13] Ellie L. Uzunova, Hans Mikosch, and Georgi St. Nikolov. Density functional study of copper-exchanged zeolites and related microporous materials: Adsorption of nitrosyls. *International Journal of Quantum Chemistry*, 113(5):723–728, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Uhlik:2013:SCE

[USL+13] Filip Uhlík, Zdeněk Slanina, Shyi-Long Lee, Ludwik Adamowicz, and Shigeru Nagase. Stability calculations for Eu@C_{74} isomers. *International Journal of Quantum Chemistry*, 113(5):729–733, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ueno:2013:FMS

[UTTn13] Seiji Ueno, Yoshitaka Tanimura, and Seiichiro Ten-no. Frontiers in molecular simulations: Molecular dynamics simulation for infrared spectroscopy with intramolecular forces from electronic properties of on-the-fly quantum chemical calculations. *International Journal of Quantum Chemistry*, 113(3):330–335, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ulian:2018:ESH

[UV18a] Gianfranco Ulian and Giovanni Valdrè. Equation of state of hexagonal hydroxylapatite ($P6_3$) as obtained from density functional theory simulations. *International Journal of Quantum Chemistry*, 118(12):e25553:1–e25553:??, June 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ulian:2018:SOE

[UV18b] Gianfranco Ulian and Giovanni Valdrè. Second-order elastic constants of hexagonal hydroxylapatite ($P6_3$) from ab initio quantum mechanics: Comparison between DFT functionals and basis sets. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ueda:2013:FMS

[UYN+13] Koki Ueda, Shusuke Yamanaka, Kazuto Nakata, Masahiro Ehara, Mitsutaka Okumura, Kizashi Yamaguchi, and Haruki Nakamura. Frontiers in molecular simulations: Linear response function approach for the boundary problem of QM/MM methods. *International Journal of Quantum Chemistry*, 113(3):336–341, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valle:2013:TRV

[Val13] Mario Valle. Tutorial review: Visualization: a cognition amplifier. *International Journal of Quantum Chemistry*, 113(17):2040–2052, September 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valadbeigi:2017:DNO

[Val17] Younes Valadbeigi. Design of neutral organic superacids using fulvene derivatives with di-enol substituent. *International Journal of Quantum Chemistry*, 117(3):190–196, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varandas:2011:HFP

[Var11] A. J. C. Varandas. Helium-fullerene pair interactions: an ab initio study by perturbation theory and coupled cluster methods. *International Journal of Quantum Chemistry*, 111(2):416–429, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varandas:2014:ROH

[Var14] António J. C. Varandas. Reviews: Odd-hydrogen: an account on electronic structure, kinetics, and role of water in mediating reactions with atmospheric ozone. Just a catalyst or far beyond? *International Journal of Quantum Chemistry*, 114(20):1327–1349, October 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2012:IDE

[VAT12] Carmela Valdemoro, Diego R. Alcoba, and Luis M. Tel. Ionization and double-excitations within the framework of the G-particle-hole hypervirial equation method. *International Journal of Quantum Chemistry*, 112(17):2965–2970, September 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valdemoro:2011:STQ

[VATPR11] C. Valdemoro, D. R. Alcoba, L. M. Tel, and E. Pérez-Romero. Some theoretical questions about the G-particle-hole hypervirial equation. *International Journal of Quantum Chemistry*, 111(2):245–255, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velarde:2012:EPO

[VBC+12a] M. G. Velarde, L. Brizhik, A. P. Chetverikov, L. Cruzeiro, W. Ebeling, and G. Röpke. Electron pairing in one-dimensional anharmonic crystal lattices. *International Journal of Quantum Chemistry*, 112(2):551–565, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velarde:2012:QLI

[VBC+12b] M. G. Velarde, L. Brizhik, A. P. Chetverikov, L. Cruzeiro, W. Ebeling, and G. Röpke. Quartic lattice interactions, soliton-like excitations, and electron pairing in one-dimensional anharmonic crystals. *International Journal of Quantum Chemistry*, 112(13):2591–2598, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vo:2018:QCB

[VBJK18] Minh Nguyen Vo, Vyacheslav S. Bryantsev, J. Karl Johnson, and John A. Keith. Quantum chemistry benchmarking of binding and selectivity for lanthanide extractants. *International Journal of Quantum Chemistry*, 118(7), April 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vovusha:2015:ESS

[VBO+15] Hakkim Vovusha, Debapriya Banerjee, Nassima Oumata, Biplab Sanyal, and Suparna Sanyal. Electronic structure and spectroscopic properties of 6-aminophenanthridine and its derivatives: Insights from density functional theory. *International Journal of Quantum Chemistry*, 115(13):846–852, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valiev:2013:IBR

[VC13] Rashid R. Valiev and Victor N. Cherepanov. The influence of benzene rings on aromatic pathways in the porphyrins. *International Journal of Quantum Chemistry*, 113 (23):2563–2567, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Villaseca:2013:LAP

[VDG13] S. Alarcón Villaseca, J.-M. Dubois, and É. Gaudry. Lead adsorption on the pseudo-10-fold surface of the $Al_{13}Co_4$ complex metallic alloy: a first principle study. *International Journal of Quantum Chemistry*, 113(6):840–846, March 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Venkataramanan:2012:MDD

[Ven12] Natarajan Sathiyamoorthy Venkataramanan. Microsolvation of DMSO: Density functional study on the structure and polaraizabilities. *International Journal of Quantum Chemistry*, 112(13):2599–2606, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valadbeigi:2013:DCQ

[VF13a] Younes Valadbeigi and Hossein Farrokhpour. DFT, CBS-Q, W1BD and G4MP2 calculation of the proton and electron affinities, gas phase basicities and ionization energies of saturated and unsaturated carboxylic acids (C_1–C_4). *International Journal of Quantum Chemistry*, 113(12):1717–1721, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valadbeigi:2013:TSK

[VF13b] Younes Valadbeigi and Hossein Farrokhpour. Theoretical study on keto–enol tautomerism and isomerization in pyruvic acid. *International Journal of Quantum Chemistry*, 113(21):2372–2378, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vallejo:2017:IES

[VFCSC17] Emmanuel Vallejo, Miguel Fuentes-Cabrera, Bobby G. Sumpter, and Eduardo Rangel Cortes. Isomeric effects on the self-assembly of a plausible prebiotic nucleoside analogue: a theoretical study. *International Journal of Quantum Chemistry*, 117(3):213–221, February 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Villar:2019:CSF

[VGGPdL19] Pedro Villar, Lucía Guillade, Adán B. González-Pérez, and Angel R. de Lera. Computational studies on the forma-

tion of aza-oxypentadienyl intermediates from alkylidene oxaziridines and keteneimine oxides and their conversion to 1,5-dihydropyrrolones. *International Journal of Quantum Chemistry*, 119(4):e25796:1–e25796:??, February 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Voychuk:2010:MFP

[VGS10] Sergei I. Voychuk, Elena N. Gromozova, and Mikhail G. Sadovskiy. The model of fungal population dynamics affected by nystatin. *International Journal of Quantum Chemistry*, 110(1):242–251, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vega-Hissi:2015:MII

[VHTEG15] Esteban Gabriel Vega-Hissi, Rodrigo Tosso, Ricardo Daniel Enriz, and Lucas Joel Gutierrez. Molecular insight into the interaction mechanisms of amino-2H-imidazole derivatives with BACE1 protease: A QM/MM and QTAIM study. *International Journal of Quantum Chemistry*, 115(6):389–397, March 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Viegas:2017:AMC

[Vie17] Luís P. Viegas. Assessment of model chemistries for hydrofluoropolyethers: a DFT/M08-HX benchmark study. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vikas:2011:AQF

[Vik11a] Vikas. Attosecond quantum fluid dynamics of H_2 molecule in a strong time-dependent magnetic field. *International Journal of Quantum Chemistry*, 111(10):2324–2331, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vikas:2011:EPE

[Vik11b] Vikas. Effective potential energy curves of H_2 molecule evolving in a strong time-dependent magnetic field. *International Journal of Quantum Chemistry*, 111(12):3135–3150, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vikas:2013:CDF

[Vik13] Vikas. Current-density functional study of the HeH^+ molecular ion under a strong ultrashort magnetic field. *International Journal of Quantum Chemistry*, 113(2):139–147, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Villard:2019:TSM

[VKF+19] Arnaud Villard, Sarah Khanniche, Camille Fortin, Laurent Cantrel, Ivan Cernusák, and Florent Louis. A theoretical study of the microhydration processes of iodine nitrogen oxides. *International Journal of Quantum Chemistry*, 119(3): e25792:1–e25792:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vonLilienfeld:2013:TRF

[vL13] O. Anatole von Lilienfeld. Tutorial reviews: First principles view on chemical compound space: Gaining rigorous atomistic control of molecular properties. *International Journal of Quantum Chemistry*, 113(12):1676–1689, June 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vila:2012:CHR

[VLFG12] Henrique Vieira Rivera Vila, Luciano Almeida Leal, A. L. A. Fonseca, and Ricardo Gargano. Calculation of the H_2^+ rovibrational energies and spectroscopic constants in the $2p\pi$, $3d\sigma$, $4d\sigma$, $4f\pi$, $4f\sigma$, $5g\sigma$, and $6i\sigma$ electronic states. *International Journal of Quantum Chemistry*, 112 (3):829–833, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vazquez-Lima:2012:ASF

[VLG12] Hugo Vázquez-Lima and Patricia Guadarrama. Analysis of structural factors related to spectroscopic data and redox potentials of CuT1 models through DFT tools. *International Journal of Quantum Chemistry*, 112(5):1431–1438, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vitkovskaya:2011:MVM

[VLK+11] Nadezhda M. Vitkovskaya, Elena Yu. Larionova, Vladimir B. Kobychev, Natalia V. Kaempf, and Boris A. Trofimov. Methanol vinylation mechanism in the KOH/DMSO/CH_3 OH/C_2 H_2 system. *International Journal of Quantum Chemistry*, 111(11):2519–2524, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velasco:2010:TSR

[VLM+10] A. M. Velasco, C. Lavín, I. Martin, M. V. Vega, J. Pitarch-Ruiz, and J. Sánchez-Marín. A theoretical study of the rotational structure of the $\epsilon(0,0)$ band of NO. *International Journal of Quantum Chemistry*, 110(3):505–512, March 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

vonLilienfeld:2015:FSA

[vLRRK15] O. Anatole von Lilienfeld, Raghunathan Ramakrishnan, Matthias Rupp, and Aaron Knoll. Fourier series of atomic radial distribution functions: a molecular fingerprint for machine learning models of quantum chemical properties. *International Journal of Quantum Chemistry*, 115 (16):1084–1093, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vasini:2011:EVT

[VMC11] Enrique Julio Vasini, María Virginia Mirífico, and José Alberto Caram. On experimental versus theoretically calculated properties of thiadiazole derivatives. *International Journal of Quantum Chemistry*, 111(9):1879–1884, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Veryazov:2011:HSA

[VMR11] Valera Veryazov, Per Åke Malmqvist, and Björn O. Roos. How to select active space for multiconfigurational quantum chemistry? *International Journal of Quantum Chemistry*, 111(13):3329–3338, November 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vyas:2011:CDC

[VO11] Nidhi Vyas and Animesh K. Ojha. Calculation of dissociation constants and chemical hardness of some biologically important molecules: a theoretical study. *International Journal of Quantum Chemistry*, 111(14):3961–3970, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vyas:2012:ITS

[VO12] Nidhi Vyas and Animesh K. Ojha. Investigation on transition states of [Alanine + M^{2+}] (M = Ca, Cu, and Zn) complexes: a quantum chemical study. *International Journal of Quantum Chemistry*, 112(5):1526–1536, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valencia-Ortega:2018:TPD

[VOAH18] Gabriel Valencia-Ortega and Luis-Antonio Arias-Hernandez. Thermodynamic properties of diatomic molecule systems under SO(2,1)-anharmonic Eckart potential. *International Journal of Quantum Chemistry*, 118(15):e25589:1–e25589:??, July 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vitkovskaya:2018:TCH

[VOK+18] Nadezhda M. Vitkovskaya, Vladimir B. Orel, Vladimir B. Kobychev, Elena Yu. Schmidt, and Boris A. Trofimov. Two classes of heterocycles-6,8-dioxabicyclo[3.2.1]octanes and cyclopentenols from the same reagents: a quantum-chemical comparison of mechanism. *International Journal of Quantum Chemistry*, 118(18):e25689:1–e25689:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Velilla:2011:BSC

[VPA11] Luis Velilla, Miguel Paniagua, and Alfredo Aguado. Basis set convergence of potential energy surfaces: Ground electronic state of H_2 and H. *International Journal of Quantum Chemistry*, 111(2):387–399, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valenzano:2010:IQM

[VPFD10] L. Valenzano, F. Pascale, M. Ferrero, and R. Dovesi. Ab initio quantum-mechanical prediction of the IR and Raman spectra of Ca_3 Cr_2 Si_3 O_{12} Uvarovite garnet. *International Journal of Quantum Chemistry*, 110(2):416–421, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valencia:2012:RMH

[VPGC12] Diego Valencia, Laura Peña, and Isidoro García-Cruz. Reaction mechanism of hydrogenation and direct desulfurization routes of dibenzothiophene-like compounds: a density functional theory study. *International Journal of Quantum Chemistry*, 112(22):3599–3605, November 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vyas:2019:RMS

[VPOG19] Nidhi Vyas, Bhawana Pandey, Animesh Ojha, and Abhinav Grover. Revisiting mechanistic studies on dinitrogen reduction to ammonia by an iron dinitrogen complex as nitrogenase mimic. *International Journal of Quantum Chemistry*, 119(24):e26025:1–e26025:??, December 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Voronkov:2012:NPA

[VRO+12] E. Voronkov, V. Rossikhin, S. Okovytyy, A. Shatckih, V. Bolshakov, and J. Leszczynski. Novel physically adapted STO##-3G basis sets. Efficiency for prediction of second-order electric and magnetic properties of aromatic hydrocarbons. *International Journal of Quantum Chemistry*, 112 (12):2444–2449, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vorontsov:2019:SCS

[VS19] Alexander V. Vorontsov and Panagiotis G. Smirniotis. Semiempirical computational study of oxygen vacancies in a decahedral anatase nanoparticle. *International Journal of Quantum Chemistry*, 119(5):e25806:1–e25806:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vu:2015:UKR

[VSL+15] Kevin Vu, John C. Snyder, Li Li, Matthias Rupp, Brandon F. Chen, Tarek Khelif, Klaus-Robert Müller, and Kieron Burke. Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. *International Journal of Quantum Chemistry*, 115 (16):1115–1128, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Venkataramanan:2013:TSE

[VSMK13] Natarajan Sathiyamoorthy Venkataramanan, Ambigapathy Suvitha, Hiroshi Mizuseki, and Yoshiyuki Kawazoe. A theoretical study of the effects of transition metal dopants on the adsorption and dissociation of hydrogen on nickel clusters. *International Journal of Quantum Chemistry*, 113 (15):1940–1948, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Venkataramanan:2015:CSI

[VSMK15] Natarajan Sathiyamoorthy Venkataramanan, Ambigapathy Suvitha, Hiroshi Mizuseki, and Yoshiyuki Kawazoe. Computational study on the interactions of mustard gas with cucurbituril macrocycles. *International Journal of Quantum Chemistry*, 115(21):1515–1525, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Venkataramanan:2011:ESS

[VSN+11] Natarajan Sathiyamoorthy Venkataramanan, Ambigapathy Suvitha, Hitoshi Nejo, Hiroshi Mizuseki, and Yoshiyuki Kawazoe. Electronic structures and spectra of symmetric meso-substituted porphyrin: DFT and TDDFT–PCM investigations. *International Journal of Quantum Chemistry*, 111(10):2340–2351, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vijay:2011:IBS

[VSS11] Dolly Vijay, Hidehiro Sakurai, and G. Narahari Sastry. The impact of basis set superposition error on the structure of π π dimers. *International Journal of Quantum Chemistry*, 111(9):1893–1901, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vignale:2013:LEC

[VUC13] Giovanni Vignale, Carsten A. Ullrich, and Klaus Capelle. Letters to the Editor: Comment on "Density and physical current density functional theory" by Xiao-Yin Pan and Viraht Sahni. *International Journal of Quantum Chemistry*, 113(9):1422–1423, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [PS10b, PS13b, PS14].

Vidal:2012:CSA

[VV12] Luciano N. Vidal and Pedro A. M. Vazquez. CCSD study of anharmonic Raman cross sections of fundamental, overtone, and combination transitions. *International Journal of Quantum Chemistry*, 112(19):3205–3215, October 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See comment [CK13] and reply [VV13].

Vidal:2013:LER

[VV13] Luciano N. Vidal and Pedro A. M. Vazquez. Letters to the editor: Reply to the comment on "CCSD study of anharmonic Raman cross sections of fundamental, overtone, and combination transitions". *International Journal of Quantum Chemistry*, 113(24):2637–2639, December 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [CK13, VV12].

Valadbeigi:2018:SPO

[VV18] Younes Valadbeigi and Robert Vianello. Superacidity of — $p(oh)_3$ and — $so(oh)_2$ derivatives of cyclopentadiene and vinylcyclopentadiene in the gas phase: a computational DFT analysis. *International Journal of Quantum Chemistry*, 118(21):e25754:1–e25754:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vazquez-Villavicencio:2012:FSL

[VVAO12] Mario Vázquez-Villavicencio, Andrea Aburto, and Emilio Orgaz. The first steps of the Li-B-H cluster formation. *International Journal of Quantum Chemistry*, 112(5):1507–1513, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varadwaj:2015:FTH

[VVJ15] Arpita Varadwaj, Pradeep R. Varadwaj, and Bih-Yaw Jin. Fluorines in tetrafluoromethane as halogen bond donors: Revisiting address the nature of the fluorine's σ_{hole}. *International Journal of Quantum Chemistry*, 115(7):453–470, April 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Veis:2016:QCB

[VVN+16] Libor Veis, Jakub Višňák, Hiroaki Nishizawa, Hiromi Nakai, and Jiří Pittner. Quantum chemistry beyond Born–Oppenheimer approximation on a quantum computer: a simulated phase estimation study. *International Journal of Quantum Chemistry*, 116(18):1328–1336, September 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Valle:2018:SRS

[VVS+18] Raffaele Guido Della Valle, Elisabetta Venuti, Tommaso Salzillo, Aldo Brillante, Matteo Masino, and Alberto Girlando. Simulated Raman spectra of four tetraphenylbutadiene polymorphs. *International Journal of Quantum Chemistry*, 118(5), March 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

VicozodaSilva:2010:CCC

[VVVB10] João Viçozo da Silva, Jr., Luciano N. Vidal, Pedro A. M. Vazquez, and Roy E. Bruns. Coupled cluster and configuration interaction quantum calculations of infrared fundamental intensities. *International Journal of Quantum Chemistry*, 110(11):2029–2036, September 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Varadwaj:2018:HMD

[VVY18] Arpita Varadwaj, Pradeep R. Varadwaj, and Koichi Yamashita. Halogen in materials design: Fluoroammonium lead triiodide (FNH_3PbI_3) perovskite as a newly discovered dynamical bandgap semiconductor in 3D. *International Journal of Quantum Chemistry*, 118(15):e25621:1–e25621:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Vyboishchikov:2008:PAE

[Vyb08] Sergei F. Vyboishchikov. Partitioning of atomization energy. *International Journal of Quantum Chemistry*, 108(4): 708–718, ???? 2008. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wagner:2014:PQM

[Wag14] Lucas K. Wagner. Perspectives: Quantum Monte Carlo for Ab Initio calculations of energy-relevant materials. *International Journal of Quantum Chemistry*, 114(2):94–101, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:NMC

[Wan11] Y. J. Wang. Noncovalent modification of carbon nanotubes by conjugated polymer: a theoretical study. *International Journal of Quantum Chemistry*, 111(14):3897–3903, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:FPS

[Wan13] Shaoqing Wang. First-principles studies on the impact of proton disorder on physical properties of ice. *International Journal of Quantum Chemistry*, 113(5):661–666, March 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:CFR

[WB17] Xiaohong Wang and Joel M. Bowman. Calculating Feshbach resonances in HCO using an extension of Q_{im}-path theory. *International Journal of Quantum Chemistry*, 117 (2):139–145, January 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wei:2014:AWB

[WC14] Gao-Feng Wei and Wen-Li Chen. Arbitrary l-wave bound states of the Schrödinger equation for the hyperbolical molecular potential. *International Journal of Quantum Chemistry*, 114(23):1602–1606, December 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2012:ARH

[WCGD12] Zhizhong Wang, Yongjuan Chang, Xinxin Gong, and Liyi Dai. Active role of hydrogen bond and ambient water in Meyer–Schuster rearrangements in high-temperature water. *International Journal of Quantum Chemistry*, 112(3): 647–652, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:BES

[WCL+17] Guang-Zhao Wang, Hong Chen, Xu-Kai Luo, Hong-Kuan Yuan, and An-Long Kuang. Bandgap engineering of $SrTiO_3$ /$NaTaO_3$ heterojunction for visible light photocatalysis. *International Journal of Quantum Chemistry*, 117(20):??, October 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wolf:2014:RQM

[WCM14] Sarah Wolf, Emanuele Curotto, and Massimo Mella. Review: Quantum Monte Carlo methods for constrained systems. *International Journal of Quantum Chemistry*, 114 (10):611–625, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:ESS

[WCS+13] Cheng Wang, Wenwen Cui, Jingling Shao, Xiaolei Zhu, and Xiaohua Lu. Exploration on the structure, stability, and isomerization of planar C_nB_5 ($n = 1$–7) clusters. *International Journal of Quantum Chemistry*, 113(23):2514–2522, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2010:NMM

[WCY+10] Yin-Feng Wang, Wei Chen, Guang-Tao Yu, Zhi-Ru Li, and Chia-Chung Sun. Novel metal-[metal oxide]-nonmetal sandwich-like superalkali compounds $Li_3OMC_5H_5$ (M = Be, Mg, and Ca): How to increase the aromaticity of Li ring? *International Journal of Quantum Chemistry*, 110 (10):1953–1963, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:SCC

[WDJ+17] Jia Wang, Xing Dai, Wanrun Jiang, Tianrong Yu, and Zhigang Wang. The self-consistent charge density functional tight-binding theory study of carbon adatoms using tuned Hubbard U parameters. *International Journal of Quantum Chemistry*, 117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:NEI

[WDR+11] Zhi-Ping Wang, Phuong Mai Dinh, Paul Gerhard Reinhard, Eric Suraud, and Feng Shou Zhang. Nonadiabatic effects in the irradiation of ethylene. *International Journal of Quantum Chemistry*, 111(2):480–486, February 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2019:IDT

[WDS19] Lijuan Wang, Jianhong Dai, and Yan Song. The impact of diperfluorophenyl and thienyl substituents on the electronic structures and charge transport properties of the fused thiophene semiconductors. *International Journal of Quantum Chemistry*, 119(5):e25824:1–e25824:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Walewski:2014:QDB

[WDSL14] Łukasz Walewski, Przemysław Dopieralski, Oleg V. Shishkin, and Zdzisław Latajka. Quantum delocalization of benzene in the ring puckering coordinates. *International Journal of Quantum Chemistry*, 114(8):534–542, April 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:SPM

[WFS13] Jie-Min Wang, Heng-Qiang Feng, and Jin-Feng Sun. Spectroscopic parameter and molecular constant investigations for low-lying electronic states of P ion. *International Journal of Quantum Chemistry*, 113(7):902–907, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2018:CSI

[WG18] Chong Wang and Chen Guo. Computational study on the interaction of nucleobases with boron-rich boron nitride nanotubes. *International Journal of Quantum Chemistry*, 118(22):e25757:1–e25757:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2010:TIS

[WGLX10] Guixiang Wang, Xuedong Gong, Yan Liu, and Heming Xiao. A theoretical investigation on the structures, densities, detonation properties, and pyrolysis mechanism of the nitro derivatives of phenols. *International Journal of Quantum Chemistry*, 110(9):1691–1701, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wilson:2012:RMS

[WH12] S. Wilson and I. Hubač. On the representation matrices for the symmetric group adapted to electron-pair and electron-group wave functions using graphical methods of spin algebras. *International Journal of Quantum Chemistry*, 112 (18):3098–3109, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wulf:2018:TSH

[WH18] Toshiki Wulf and Thomas Heine. Toward separation of hydrogen isotopologues by exploiting zero-point energy difference at strongly attractive adsorption site models. *International Journal of Quantum Chemistry*, 118(9):e25545:1–e25545:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Watts:2014:TSC

[WHM14] Joshua Watts, Elizabeth Howell, and John K. Merle. Theoretical studies of complexes between Hg(II) ions and l-cysteinate amino acids. *International Journal of Quantum Chemistry*, 114(5):333–339, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:TSD

[WHS+13] Jinhu Wang, Qianqian Hou, Xiang Sheng, Jun Gao, Yongjun Liu, and Chengbu Liu. Theoretical study on the

deglycosylation mechanism of rice BGlu1 β-glucosidase. *International Journal of Quantum Chemistry*, 113(8):1071–1075, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2014:TSV

[WHY+14] Zerong Daniel Wang, Meagan Hysmith, Motoko Yoshida, Ben George, and Perla Cristina Quintana. Theoretical study of the vibrational frequencies of carbon disulfide. *International Journal of Quantum Chemistry*, 114(6):429–435, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Winkler:2010:LED

[Win10] Peter Winkler. Legendre expansion of the Debye interaction. *International Journal of Quantum Chemistry*, 110 (15):3129–3135, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Witwicki:2018:DFT

[Wit18] Maciej Witwicki. Density functional theory and ab initio studies on hyperfine coupling constants of phosphinyl radicals. *International Journal of Quantum Chemistry*, 118(23):e25779:1–e25779:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2011:TAH

[WJ11] Dongling Wu and Dianzeng Jia. Theoretical analysis on the hydrogen bonding and reactivity that associated with the proton transfer reaction of carboxylic acid dimers and their monosulfur derivatives. *International Journal of Quantum Chemistry*, 111(12):3017–3023, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wen:2010:GSE

[WJL+10] Jun-Qing Wen, Zhen-Yi Jiang, Jun-Qian Li, Li-Ke Cao, and San-Yan Chu. Geometrical structures, electronic states, and stability of Ni_n Al clusters. *International Journal of Quantum Chemistry*, 110(7):1368–1375, June 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:DFT

[WJL+11] Xiao-Qing Wang, Zhen-Yi Jiang, Jun-Qian Li, Qing-Li He, and San-Yan Chu. Density functional theory study of geometry and stability of small Zr_n ($n = 2--10$) clusters. *International Journal of Quantum Chemistry*, 111(1):182–190, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2015:CST

[WJY15] Cuihong Wang, Yue Jiang, and Guangwu Yang. Comprehensive study of threonine adsorption on carbon nanotube: a dispersion complemented density functional theory-based treatment. *International Journal of Quantum Chemistry*, 115(22):1606–1612, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Walter:2017:ATD

[WKE17] Christof Walter, Veronika Krämer, and Bernd Engels. On the applicability of time-dependent density functional theory (TDDFT) and semiempirical methods to the computation of excited-state potential energy surfaces of perylene-based dye-aggregates. *International Journal of Quantum Chemistry*, 117(6):??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wei:2017:PEE

[WLC+17] Yuan-Xin Wei, Hai-Bei Li, Jian-Bo Cheng, Wen-Zuo Li, and Qing-Zhong Li. Prominent enhancing effects of substituents on the strength of $\pi\cdots\sigma$-hole tetrel bond. *International Journal of Quantum Chemistry*, 117(23):??, December 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2010:QCS

[WLD+10] Sangwook Wu, Shubin Liu, Charles H. Davis, Darrel W. Stafford, and Lee G. Pedersen. Quantum chemical study of the mechanism of action of vitamin K carboxylase in solvent. *International Journal of Quantum Chemistry*, 110 (15):2744–2751, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:TSR

[WLG+11] Yong-Cheng Wang, Hui-Wen Liu, Zhi-Yuan Geng, Ling-Ling Lv, Yu-Bing Si, Qing-Yun Wang, Qiang Wang, and Dan-Dan Cui. Theoretical study of the reactions of lanthanide ions (Ce^+, Pr^+) with CO_2 in the gas phase. *International Journal of Quantum Chemistry*, 111(9):2021–2030, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2019:FPS

[WLH+19] Xiao Wang, Huazhong Liu, Marko Huttula, Youhua Luo, Meng Zhang, and Wei Cao. First-principles studies of lithium adsorption and diffusion on silicene with grain boundaries. *International Journal of Quantum Chemistry*, 119(13):e25913:1–e25913:??, July 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:TSI

[WLL11] Wenjun Wang, Wenjing Li, and Qingzhong Li. Theoretical study of the interaction between $LiNH_2$ and HMgH. *International Journal of Quantum Chemistry*, 111(3):675–681, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:ISR

[WLL+13] Jinghui Wang, Feng Li, Yan Li, Yinfeng Yang, Bin Wang, Shuwei Zhang, and Ling Yang. Insight into the structural requirements of benzimidazole derivatives as interleukin-2 inducible T-cell kinase inhibitors by computational explorations. *International Journal of Quantum Chemistry*, 113(21):2385–2396, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wen:2019:TPN

[WLL19] Mei Wen, Zhuo Zhe Li, and An Yong Li. Theoretical predictions of the nitrogen heterocyclic compounds with metal and noble gas (metal = Cu, Ag, Au). *International Journal of Quantum Chemistry*, 119(19):e25990:1–e25990:??, October 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wan:2019:UBI

[WLS+19] Di Wan, Huidong Li, Liming Shi, Xueke Wu, Qunchao Fan, Hao Feng, Robert Bruce King, and Henry F. Schaefer III. Unsaturation in binuclear iron carbonyl complexes of the split (3 + 2) five-electron donor hydrocarbon ligand bicyclo[3.2.1]octa-2,6-dien-4-yl: Role of agostic hydrogen atoms. *International Journal of Quantum Chemistry*, 119(22):e26010:1–e26010:??, November 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2014:ICK

[WLWL14] Shang-Ying Wu, Yun-Min Lee, Jong-Shinn Wu, and Ming-Chang Lin. Ab initio chemical kinetics for the unimolecular decomposition of Si_2H_5 radical and related reverse bimolecular reactions. *International Journal of Quantum Chemistry*, 114(4):278–288, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2012:DSM

[WLWT12] Jing-Mei Wang, Zhi-Minhg Li, Quan-Rui Wang, and Feng-Gang Tao. A DFT study on the mechanisms for the cycloaddition reactions between 1-Aza-2-azoniaallene cations and carbodiimides. *International Journal of Quantum Chemistry*, 112(3):809–822, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2012:ECS

[WLZ+12a] Jin-Yun Wang, Chen-Sheng Lin, Min-Yi Zhang, Guo-Liang Chai, and Wen-Dan Cheng. Effect of cage size on the third-order optical properties of endohedral metallofullerenes $Sc_3N@C_{2n}$ ($2n = 68, 70, 78$, and 80): a theoretical study. *International Journal of Quantum Chemistry*, 112(3):759–769, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2012:TSO

[WLZ+12b] Jin-Yun Wang, Chen-Sheng Lin, Min-Yi Zhang, Guo-Liang Chai, and Wen-Dan Cheng. Theoretical study on the one-, two-, and three-photon absorption properties of exohedral functionalized derivative of $Sc_3N@C_{80}$. *International Journal of Quantum Chemistry*, 112(4):1198–1208, February 5,

2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2018:PJT

[WLZ18] Ya Wang, Yang Liu, and Xiaonan Zheng. Pseudo Jahn–Teller origin tracking for symmetry breaking in halogenabenzene: How can a bird fly? *International Journal of Quantum Chemistry*, 118(19):e25704:1–e25704:??, October 05, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wende:2019:OVT

[WMK+19] Florian Wende, Martijn Marsman, Jeongnim Kim, Fedor Vasilev, Zhengji Zhao, and Thomas Steinke. OpenMP in VASP: Threading and SIMD. *International Journal of Quantum Chemistry*, 119(12):e25851:1–e25851:??, June 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2010:MRC

[WML10] Fen Wang, Qingxi Meng, and Ming Li. Mechanism of rhodium-catalyzed hydroacylation of propylene using formaldehyde: a computational study. *International Journal of Quantum Chemistry*, 110(4):850–859, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:MOI

[WML11] Jing-Bo Wang, Jian-Yi Ma, and Xiang-Yuan Li. Molecular orientations at interfaces by extended polarizable continuum model. *International Journal of Quantum Chemistry*, 111(10):2187–2195, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weymuth:2014:GDM

[WR14a] Thomas Weymuth and Markus Reiher. Gradient-driven molecule construction: an inverse approach applied to the design of small-molecule fixating catalysts. *International Journal of Quantum Chemistry*, 114(13):838–850, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weymuth:2014:RIQ

[WR14b] Thomas Weymuth and Markus Reiher. Review: Inverse quantum chemistry: Concepts and strategies for rational compound design. *International Journal of Quantum Chemistry*, 114(13):823–837, July 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Weymuth:2015:SDT

[WR15] Thomas Weymuth and Markus Reiher. Systematic dependence of transition-metal coordination energies on density-functional parametrizations. *International Journal of Quantum Chemistry*, 115(2):90–98, January 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2018:MSC

[WRW+18] Yueshen Wu, Benjamin Rudshteyn, Ingolf Warnke, Dequan Xiao, and Victor S. Batista. Mechanistic study of CO/ CO_2 conversion catalyzed by a biomimetic Ni(II)-iminothiolate complex. *International Journal of Quantum Chemistry*, 118(9):e25555:1–e25555:??, May 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:MET

[WSCL11] Y. Wang, S. L. Shang, L. Q. Chen, and Z. K. Liu. Magnetic excitation and thermodynamics of $BaFe_2$ As_2. *International Journal of Quantum Chemistry*, 111(14):3565–3570, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2011:TSS

[WSL+11] Julong Wu, Zhicheng Sun, Xiaojun Li, Bing Ma, Maosheng Tian, and Shirong Li. Theoretical study on the smallest endohedral metallofullerenes: TM@C_{20} (TM = Ce and Gd). *International Journal of Quantum Chemistry*, 111 (14):3786–3792, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2016:IEB

[WSML16] Weihua Wang, Zheng Sun, Lingpeng Meng, and Xiaoyan Li. Intriguing E$\cdots$E' bonding in $[Nap(EPh)(E'Ph)]^{\bullet+}$ (E, E' = O, S, Se, Te). *International Journal of Quantum*

Chemistry, 116(14):1090–1096, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Widom:2010:BBB

[WSV10] Allan Widom, Yogendra Srivastava, and Vincenzo Valenzi. The biophysical basis of Benveniste experiments: Entropy, structure, and information in water. *International Journal of Quantum Chemistry*, 110(1):252–256, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:TSS

[WTH+11] Jinhu Wang, Ke Tang, Qianqian Hou, Xueli Cheng, Yongjun Liu, and Chengbu Liu. Theoretical studies on the structural rearrangement of ligand binding pocket in human vitamin D receptor. *International Journal of Quantum Chemistry*, 111(14):3928–3937, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2019:DHM

[WTP+19] Jiajun Wang, Jing Teng, Lizhi Pu, Jing Huang, Ying Wang, and Qunxiang Li. Double-hole-mediated coupling of anionic dopants in perovskite $NaNbO_3$ for efficient solar water splitting. *International Journal of Quantum Chemistry*, 119(14):e25930:1–e25930:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2015:OFH

[WTW+15] Yanhua Wang, Jianying Tong, Weihong Wu, Zhijian Xu, and Yunxiang Lu. Organic fluorines as halogen bond donors: Theoretical study and crystallographic evidence. *International Journal of Quantum Chemistry*, 115(14):884–890, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wei:2011:DFT

[WTZ+11] Donghui Wei, Mingsheng Tang, Wenjing Zhang, Jing Zhao, Ling Sun, Chufeng Zhao, and Homgming Wang. A density functional theory study of the enantioselective reduction of prochiral ketones promoted by chiral spiroborate esters.

International Journal of Quantum Chemistry, 111(3):596–605, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2011:SPN

[Wu11] Junyong Wu. Structure, properties, and nature of the BrF-HX complexes: An Ab initio study. *International Journal of Quantum Chemistry*, 111(15):4247–4254, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:SAT

[WvRSW+11] Hong-Jian Wang, Paul v. R. Schleyer, Judy I. Wu, Yan Wang, and Hai-Jun Wang. A study of aromatic three membered rings. *International Journal of Quantum Chemistry*, 111(5):1031–1038, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:WCE

[WW11] Y. J. Wang and L. Y. Wang. Water chain encapsulated in carbon nanotube revealed by density functional theory. *International Journal of Quantum Chemistry*, 111(15):4465–4471, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2014:MDO

[WWB+14] Cheng-Long Wang, Jian Wang, Fu-Quan Bai, Jie Chen, and Hong-Xing Zhang. Molecular design of organic dyes with diketopyrrolopyrrole for dye-sensitized solar cell: a theoretical approach. *International Journal of Quantum Chemistry*, 114(9):560–567, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wallace:2017:CCC

[WWC17] Andrew J. Wallace, Bryce E. Williamson, and Deborah L. Crittenden. Coupled cluster calculations provide a one-to-one mapping between calculated and observed transition energies in the electronic absorption spectrum of zinc phthalocyanine. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2015:CBE

[WWD+15] Bo Wang, Li Wang, Xing Dai, Yang Gao, Wanrun Jiang, Jie Han, Zhigang Wang, and Rui-Qin Zhang. Correlation between electron delocalization and structural planarization in small water rings. *International Journal of Quantum Chemistry*, 115(13):817–819, July 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2018:HMC

[WWGW18] Hua Wu, Hui Wang, Zihan Guo, and Junqing Wen. Hydrogen migration in Coulomb explosion of cyclohexane to C_2 H_4^+ and C_4 H_8^+: Theoretical and experimental studies. *International Journal of Quantum Chemistry*, 118(22): e25764:1–e25764:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:DLD

[WWHZ13] Li Wang, Jinmiao Wen, Hongqing He, and Jinglai Zhang. A dual-level direct dynamics study on the hydrogen abstraction reaction of oxygen atom with methylhydrazine. *International Journal of Quantum Chemistry*, 113(21):2338–2344, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:LOE

[WWL+11] Yin-Feng Wang, Yi Wang, Zhi-Ru Li, Zhuo Li, Hong-Liang Xu, and Chia-Chung Sun. The lithium-orientation effect on the hyperpolarizability in the short zigzag-edged monolithiated aza-Möbius graphene ribbon $[2, 7]$ isomers. *International Journal of Quantum Chemistry*, 111(10):2406–2415, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:LFM

[WWL17] Yu Wang, Jian Wang, and Hans Lischka. Lagrange function method for energy optimization directly in the space of natural orbitals. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:RMH

[WWLZ17] Xiaoli Wang, Yongcheng Wang, Shuang Li, and Yuwei Zhang. Reaction mechanism of hydrogen cyanide catalyzed by gas-phase titanium. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:TSI

[WWQG17] Liang Wang, Xing Wang, Ping Qian, and Hong Guo. Theoretical study of interaction of heteroaromatic compounds with a cluster model of kaolinite tetrahedral surface. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wen:2011:QCS

[WWX+11] Zhengcheng Wen, Zhihua Wang, Jiangrong Xu, Junhu Zhou, and Kefa Cen. Quantum chemistry study on the mechanism of the reaction between ozone and 2,3,7,8-TCDD. *International Journal of Quantum Chemistry*, 111 (5):1081–1091, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:TIS

[WXB+11] Jian Wang, Bao-Hui Xia, Fu-Quan Bai, Lei Sun, and Hong-Xing Zhang. Theoretical investigation on the spectroscopic properties of cyclometallated iridium (III) complexes and the deprotonation influence on them in solution. *International Journal of Quantum Chemistry*, 111(15):4080–4090, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:CSM

[WXZ+11] Wenliang Wang, Jingfan Xin, Yue Zhang, Weina Wang, and Yanxia Lu. Computational study on the mechanism for the gas-phase reaction of dimethyl disulfide with OH. *International Journal of Quantum Chemistry*, 111(3):644–651, March 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2015:PPF

[WYM15] Xingyong Wang, Tianying Yan, and Jing Ma. Perspectives: Polarizable force fields based on physical models and quantum chemical calculations. *International Journal of Quantum Chemistry*, 115(9):545–549, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:QCS

[WYWL13] Chunling Wang, Xiaoke Yang, Endong Wang, and Baiqing Li. Quantum chemistry studies of adenosine 2503 methylation by S-adenosylmethionine-dependent enzymes. *International Journal of Quantum Chemistry*, 113(9):1409–1415, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2010:NAM

[WZ10a] Huiling Wang and Yusen Zhang. A new approach to molecular phylogeny of H5N1 avian influenza viruses in Asia. *International Journal of Quantum Chemistry*, 110(10):1964–1971, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2010:KIL

[WZ10b] Yan Wang and Wenwen Zhang. Kirchhoff index of linear pentagonal chains. *International Journal of Quantum Chemistry*, 110(9):1594–1604, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2012:ACH

[WZC+12] Huanwen Wu, Ning Zhang, Zhiji Cao, Hongming Wang, and Sanguo Hong. The adsorption of CO_2, H_2CO_3, HCO^{3-} and CO_3^{2-} on Cu_2O (111) surface: First-principles study. *International Journal of Quantum Chemistry*, 112(12):2532–2540, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:RCC

[WZHZ13] Li Wang, Jianxiang Zhao, Hongqing He, and Jinglai Zhang. Rate constants calculation of hydrogen abstraction reactions CH_3 CHBr + HBr and CH_3CBr_2 + HBr. *International Journal of Quantum Chemistry*, 113(7):997–1002,

April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2013:NTS

[WZM+13] Kun Wang, Jian-Guo Zhang, Tian-Tian Man, Man Wu, Shao-Wen Zhang, Tong-Lai Zhang, and Li Yang. Novel theoretical studies of the dehydrogenation of $LiBH_2NH_3$. *International Journal of Quantum Chemistry*, 113(9):1358–1364, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2017:HAB

[WZW17] Weizhou Wang, Yu Zhang, and Yi-Bo Wang. Highly accurate benchmark calculations of the interaction energies in the complexes $C_6H_6 \cdots C_6X_6$ (X = F, Cl, Br, and I). *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2011:ISC

[WZX11] Kedong Wang, Jicai Zhang, and Guoliang Xu. Ab initio studies of the conformers and conformational distribution of gas-phase N,N-dimethylaminopropanol. *International Journal of Quantum Chemistry*, 111(15):4296–4302, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wang:2015:QTP

[WZX+15a] Lifei Wang, Qin Zhang, Feng Xu, Xiao-Dong Cui, and Yujun Zheng. Quantum tunneling process for double well potential. *International Journal of Quantum Chemistry*, 115 (4):208–215, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wu:2015:RXF

[WZX15b] Jianming Wu, Yuwei Zhou, and Xin Xu. Reviews: The X1 family of methods that combines B3LYP with neural network corrections for an accurate yet efficient prediction of thermochemistry. *International Journal of Quantum Chemistry*, 115(16):1021–1031, August 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Wei:2010:TSM

[WZZL10] Xiaofeng Wei, Dongju Zhang, Changqiao Zhang, and Chengbu Liu. Theoretical study of the Michael addition of acetylacetone to methyl vinyl ketone catalyzed by the ionic liquid 1-butyl-3-methylimidazolium hydroxide. *International Journal of Quantum Chemistry*, 110(5):1056–1062, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2018:HRS

[XCD18] Jing Xu, Xiyue Cheng, and Shuiquan Deng. The high reactive site and the unusually short Sc — C bond of the scandium phosphinoalkylidene complex, an explanation from first-principles calculation. *International Journal of Quantum Chemistry*, 118(22):e25691:1–e25691:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2018:TBB

[XCL+18] Hui-Li Xu, Jian-Bo Cheng, Hai-Bei Li, Xin Yang, and Qing-Zhong Li. Tetrel bonds between $PhSiF_3$ /Ph$T H_3$ (T = Si, Ge, Sn) and H_3Z O (Z = N, P, A s) : a pentacoordinate silicon (I V) complex. *International Journal of Quantum Chemistry*, 118(17):e25660:1–e25660:??, September 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2015:TII

[XCY15] Chang Xu, Longjiu Cheng, and Jinlong Yang. Theoretical investigation on icosahedral $C_{60}(FeCp)_{12}$: a hybrid of C_{60} and ferrocene. *International Journal of Quantum Chemistry*, 115(22):1621–1628, November 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2010:PCP

[XDM+10] Sichuan Xu, Shengrong Deng, Liying Ma, Qiang Shi, Maofa Ge, and Xingkang Zhang. The proton-coupled proton transfer mechanism, H_2 O catalysis, and hydrogen tunneling effects in the reaction of $HNCH_2$ with HCOOH in the interstellar medium. *International Journal of Quantum Chemistry*, 110(14):2671–2682, November 15, 2010. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2019:TIS

[XF19] Zhen-Zhen Xu and Hong-Jun Fan. A theoretical investigation on the structures of $(NH_3)\cdot (H_2SO_4)\cdot (H_2O)_{0–14}$ clusters. *International Journal of Quantum Chemistry*, 119(7): e25850:1–e25850:??, April 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2014:QSM

[XFW+14] Wen Guo Xie, Dan Qing Fang, Wen Juan Wu, Rong Zhang, Guo Hua Zeng, Shao Jie Ma, Jing Heng Wu, and Yong Shen. 3D-QSAR studies and molecular design on a novel series of pyrimidine benzimidazoles as Lck inhibitors. *International Journal of Quantum Chemistry*, 114(9):598–609, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xing:2018:TSS

[XGH18a] Minmin Xing, Ling Guo, and Zijun Hao. Theoretical study of the single noble metal stabilized on metal oxide clusters catalyze the water-gas shift reaction. *International Journal of Quantum Chemistry*, 118(22):e25767:1–e25767:??, November 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2018:MOP

[XGH+18b] Jing Xu, Sheng Guo, Fei Hou, Jing Li, and Lianming Zhao. Methanol oxidation on the PtPd(111) alloy surface: a density functional theory study. *International Journal of Quantum Chemistry*, 118(3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiao-Hong:2010:NBO

[XHZXXZ10] Li Xiao-Hong, Tang Zheng-Xin, and Zhang Xian-Zhou. Natural bond orbital analysis of some S-nitrosothiols biological molecules. *International Journal of Quantum Chemistry*, 110(8):1565–1572, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2012:CIE

[XLGA12] Peng Xie, Kai Liu, Fenglong Gu, and Yuriko Aoki. Counter-ion effects of A- and B-type poly(dG)·Poly(dC) and poly(dA)·Poly(dT) DNA by elongation method. *International Journal of Quantum Chemistry*, 112(1):230–239, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2010:QCT

[XLLZ10] Wen-Wu Xu, Xin-Guo Liu, Shi-Xia Luan, and Qing-Gang Zhang. Quasi-classical trajectory study on He+H /D /T reactions. *International Journal of Quantum Chemistry*, 110(4):860–864, March 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xue:2019:ASP

[XLZ+19] Yunsheng Xue, Yunping Liu, Ling Zhang, Han Wang, Qingquan Luo, Ran Chen, Yin Liu, and Ya Li. Antioxidant and spectral properties of chalcones and analogous aurones: Theoretical insights. *International Journal of Quantum Chemistry*, 119(3):e25808:1–e25808:??, February 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2012:WOD

[XMZ+12] Qin Xie, Qiang-Qiang Meng, Gui-Lin Zhuang, Jian-Guo Wang, and Xiao-Nian Li. Water oxidation on N-doped TiO_2 nanotube arrays. *International Journal of Quantum Chemistry*, 112(13):2585–2590, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiao:2014:TKS

[XNL+14] Ruiyang Xiao, Matthew Noerpel, Hoi Ling Luk, Zongsu Wei, and Richard Spinney. Thermodynamic and kinetic study of ibuprofen with hydroxyl radical: a density functional theory approach. *International Journal of Quantum Chemistry*, 114(1):74–83, January 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xia:2018:QMS

[XS18] Xiuli Xia and Yuanzhi Shao. Quantum mechanical studies of full-shell noble metal nanoclusters in water. *Interna-*

tional Journal of Quantum Chemistry, 118(20):e25709:1–e25709:??, October 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2012:UHA

[XSLF12] Hujun Xie, Tingting Sun, Qunfang Lei, and Wenjun Fang. Understanding hydrogenation of the adenine-thymine base pairs and their anions: a density functional study. *International Journal of Quantum Chemistry*, 112(2):609–618, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xie:2013:CBB

[XTLA13] Peng Xie, Hiroyuki Teramae, Kai Liu, and Yuriko Aoki. Computational biochemistry and biophysics: Electronic states of mixed base pairs systems of DNA and the effect of base composition and sequences on the band structures using screw axis translational symmetry. *International Journal of Quantum Chemistry*, 113(4):489–496, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Lad14, XTLA14].

Xie:2014:LER

[XTLA14] Peng Xie, Hiroyuki Teramae, Kai Liu, and Yuriko Aoki. Letters to the editor: Reply to the comment of J. Ladik on "Electronic states of mixed base pairs systems of DNA and the effect of base composition and sequences on the band structures using screw axis translational symmetry". *International Journal of Quantum Chemistry*, 114(4):303, February 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [XTLA13, Lad14].

Xu:2016:QTP

[Xu16] Feng Xu. Quantum tunneling in a periodically driven double well system: Entangled trajectory molecular dynamics method. *International Journal of Quantum Chemistry*, 116(14):1057–1063, July 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2019:TTD

[Xu19] Feng Xu. Tunneling time in driven double-well system using entangled molecular dynamics method. *International Journal of Quantum Chemistry*, 119(16):e25854:1–

e25854:??, August 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2010:AIS

[XWC10] Shuhong Xu, Chunlei Wang, and Yiping Cui. Aromaticity of ionic structures: Investigation and application of NICS value and 4 n + 2 rule. *International Journal of Quantum Chemistry*, 110(6):1287–1294, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2011:BCM

[XWC11a] Shuhong Xu, Chunlei Wang, and Yiping Cui. Bonding characters of M-Cd_4Te_4 and M-Cd_3Te_3 (M = Cr, Cu, Ag, Al, Cd, and Zn) clusters. *International Journal of Quantum Chemistry*, 111(12):3167–3173, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2011:TSI

[XWC11b] Shuhong Xu, Chunlei Wang, and Yiping Cui. Theoretical study on influence of ligand and solvent to CdS clusters. *International Journal of Quantum Chemistry*, 111(1):156–164, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2011:CSE

[XWCY11] Hong-Liang Xu, Fang-Fang Wang, Wei Chen, and Guang-Tao Yu. The complexant shape effect on first (hyper)polarizability of alkalides Li^+ $(NH_2\ CH_3)_4$ M^- (M = Li, Na, and K). *International Journal of Quantum Chemistry*, 111(12):3174–3183, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2018:QBS

[XWP+18] Tianlv Xu, Lingling Wang, Yang Ping, Tanja van Mourik, Herbert Früchtl, Steven R. Kirk, and Samantha Jenkins. Quinone-based switches for candidate building blocks of molecular junctions with QTAIM and the stress tensor. *International Journal of Quantum Chemistry*, 118(16): e25676:1–e25676:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiaohong:2012:PSS

[XX12] Li Xiaohong and Zhang Xianzhou. PCM study of the solvent and substituent effects on bond dissociation energies of the O — NO bond — a DFT study. *International Journal of Quantum Chemistry*, 112(2):603–608, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2013:TAH

[XXbX+13] Jie Xu, Lin Xu, Ming biao Xu, Lin Zhao, Xiao ming Wu, Shou chen Wen, and Wei hong Liu. Theoretical analyses of the host–guest interaction within chlorine hydrate. *International Journal of Quantum Chemistry*, 113(19):2228–2233, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2016:QST

[XXJ+16] Yuning Xu, Tianlv Xu, Dong Jiajun, Steven R. Kirk, and Samantha Jenkins. A QTAIM and stress tensor perspective of large-amplitude motions of the tetrasulfur tetranitride S_4N_4 molecular graph. *International Journal of Quantum Chemistry*, 116(13):1025–1039, July 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xi:2018:LMB

[XYL+18] Cong Xi, Le Yang, Chang Liu, Peng You, Lanlan Li, and Peng Jin. Lanthanide metals in the boron cages: Computational prediction of M @B_n (M = Eu, Gd; n = 38, 40). *International Journal of Quantum Chemistry*, 118(13): e25576:1–e25576:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2011:DSN

[XZ11] Zhijuan Xu and Lixin Zhou. A DFT study of a novel oxime anticancer trans platinum complex: Monofunctional and bifunctional binding to purine bases. *International Journal of Quantum Chemistry*, 111(9):1907–1920, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2011:CST

[XZCH11] Cai-Xia Xu, Guo-Min Zuo, Zhen-Xing Cheng, and Juan Han. Computational study toward understanding the photodissociation mechanism of sarin. *International Journal of Quantum Chemistry*, 111(15):4410–4417, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2018:MPC

[XZG+18] Hao Xu, Yanyan Zhu, Peng Guo, Chunmei Liu, Jiankai Shan, and Mingsheng Tang. Mechanisms of phosphine-catalyzed [4 + 3] annulation of allenoates with C, N-cyclic azomethine imines: a DFT investigation. *International Journal of Quantum Chemistry*, 118(15):e25626:1–e25626:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2016:QTE

[XZJ+16] Feng Xu, Lei Zhang, Liyun Jiang, Lifu Bao, and Hao Meng. Quantum tunneling effect in entanglement dynamics. *International Journal of Quantum Chemistry*, 116(1):7–12, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xiong:2012:TII

[XZL+12] Yan Xiong, Shuting Zhang, Xuege Ling, Xu Zhang, and Jinyue Wang. Theoretical investigation on identical anionic halide-exchange SN_2 reaction processes on N-haloammonium cation NH_3X + (X = F, Cl, Br, and I). *International Journal of Quantum Chemistry*, 112(12):2475–2481, June 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2010:CIH

[XZYS10] Lin Xu, Jian-Wei Zou, Qing-Sen Yu, and Peng Sang. Computational insights into halogen bonding between P Cl contact and several electron donors. *International Journal of Quantum Chemistry*, 110(6):1245–1251, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Xu:2010:PHE

[XZZ+10] Yu Xu, Fengjuan Zhao, Yan Zhang, Yulong Gu, Tongxiang Liu, and Jian Cui. Potential high-energy pentazolides: $HB(N_5)_3M_{1\sim2}(N_5)_3BH$ (M = Be, Mg, Ca, Zn, and Cd). *International Journal of Quantum Chemistry*, 110(6):1235–1244, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoshii:2015:SNU

[YAF+15] Noriyuki Yoshii, Yoshimichi Andoh, Kazushi Fujimoto, Hidekazu Kojima, Atsushi Yamada, and Susumu Okazaki. Software news and updates: MODYLAS: a highly parallelized general-purpose molecular dynamics simulation program. *International Journal of Quantum Chemistry*, 115 (5):342–348, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yakushevich:2010:NDD

[Yak10] L. V. Yakushevich. Nonlinear dynamics of DNA: Velocity of the kinks activated in homogeneous polynucleotide chains. *International Journal of Quantum Chemistry*, 110(1):270–275, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yakushevich:2011:DSD

[Yak11] L. V. Yakushevich. DNA structure and dynamics: Potential of interactions between two complementary DNA bases. *International Journal of Quantum Chemistry*, 111 (11):2482–2489, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2010:VCA

[Yam10] Wataru Yamaguchi. δ and σ vs. π conflicting aromatic pentagonal ring of tungsten with a planar pentacoordinate carbon at the ring center. *International Journal of Quantum Chemistry*, 110(5):1086–1091, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2011:TPT

[Yam11] Yoichi Yamaguchi. Transport properties of two-dimensionally fused zinc porphyrins from linear-response approach. *International Journal of Quantum Chemistry*, 111(12):3230–

3238, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yurdakul:2011:QCS

[YB11] Şenay Yurdakul and Serdar Badoğlu. Quantum chemical studies on prototautomerism of 1H-imidazo[4,5-c]pyridine. *International Journal of Quantum Chemistry*, 111(12): 2944–2959, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2012:OPH

[YBMK12] Ge Yao, Mary T. Berry, P. Stanley May, and Dmitri S. Kilin. Optical properties of host material for phosphor computational modeling. *International Journal of Quantum Chemistry*, 112(24):3889–3895, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Bian:2018:NDR

[yBZfC18] Jiang yu Bian, Yang Zhang, and Ying fei Chang. The negative differential resistance mechanism of a molecular device based on double-cage fluorinated fullerene C_{20} F_{18} $(NH)_2$ C_{20} F_{18}: a theoretical study. *International Journal of Quantum Chemistry*, 118(18):e25630:1–e25630:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuan:2013:TPS

[YC13] Yuan Yuan and Longjiu Cheng. Theoretical prediction for the structures of gas phase lithium oxide clusters: $(Li_2O)_n$ ($n = 1$–8). *International Journal of Quantum Chemistry*, 113(9):1264–1271, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yakar:2011:CIV

[YÇÖ11] Yusuf Yakar, Bekir Çakir, and Ayhan Özmen. Computation of ionization and various excited state energies of helium and helium-like quantum dots. *International Journal of Quantum Chemistry*, 111(15):4139–4149, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2017:NSM

[YD17] Shuang Yu and Yi-Hong Ding. New structural motif of 18 valence electron molecules with a planar tetracoordinate heavier group 14 center: Unique stabilization effect of a π-type skeleton. *International Journal of Quantum Chemistry*, 117(22):??, November 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2013:ICN

[YDW13] Zejin Yang, Patrick Duffy, and Feng Wang. Inheritance and correlation of nucleic acid pyrimidine bases. *International Journal of Quantum Chemistry*, 113(20):2312–2318, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2016:COP

[YF16] Feng Yu and Ling-Xiao Fu. Comparison of one-parameter and linearly scaled one-parameter double-hybrid density functionals for noncovalent interactions. *International Journal of Quantum Chemistry*, 116(15):1166–1172, August 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2017:DPN

[YFY17] Feng Yu, Ling-Xiao Fu, and Yu Yang. DSD-PBEP86-NL and DOD-PBEP86-NL functionals for noncovalent interactions: Basis set effects and tentative applications to large noncovalent systems. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yin:2011:SDF

[YGL+11] Shuhui Yin, Mingxing Guo, Lei Li, Yinghui Zhang, and Xiangping Li. Stereo-dynamics of the F + HCl $\rightarrow$ HF + Cl reaction. *International Journal of Quantum Chemistry*, 111 (15):4400–4409, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2010:DBB

[YGLL10] Wen-Zhi Yao, Jin-Chang Guo, Hai-Gang Lu, and Si-Dian Li. $D_{\infty h}$ B_2 $(BS)_2^{-/2-}$ and T_d $B(BS)_4^-$: Boron sulfide clusters containing BB multiple bonds and B^- tetrahedral cen-

ters. *International Journal of Quantum Chemistry*, 110 (14):2689–2696, November 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2014:EQT

[YH14a] Ciann-Dong Yang and Shih-Ming Huang. Electronic quantum trajectories in a quantum dot. *International Journal of Quantum Chemistry*, 114(14):920–930, July 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

You:2014:RTC

[YH14b] Zhi-Qiang You and Chao-Ping Hsu. Reviews: Theory and calculation for the electronic coupling in excitation energy transfer. *International Journal of Quantum Chemistry*, 114 (2):102–115, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2013:EBG

[YHL+13] Xiaohui Yu, Tingjun Hou, Youyong Li, Xuhui Sun, and Shuit-Tong Lee. Effective band gap reduction of titanium oxide semiconductors by codoping from first-principles calculations. *International Journal of Quantum Chemistry*, 113(23):2546–2553, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2015:RTI

[YHLC15] Guangtao Yu, Xuri Huang, Shaochen Li, and Wei Chen. Reviews: Theoretical insights and design of intriguing nonlinear optical species involving the excess electron. *International Journal of Quantum Chemistry*, 115(11):671–679, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yousefpour:2013:MDS

[YINM13] Abbas Yousefpour, Sepideh Amjad Iranagh, Yousef Nademi, and Hamid Modarress. Molecular dynamics simulation of nonsteroidal antiinflammatory drugs, naproxen and relafen, in a lipid bilayer membrane. *International Journal of Quantum Chemistry*, 113(15):1919–1930, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2013:CBBb

[YIY+13] K. Yamaguchi, H. Isobe, S. Yamanaka, T. Saito, K. Kanda, M. Shoji, Y. Umena, K. Kawakami, J.-R. Shen, N. Kamiya, and M. Okumura. Computational biochemistry and biophysics: Full geometry optimizations of the mixed-valence $CaMn_4O_4X(H_2O)_4$ (X = OH or O) cluster in OEC of PS II: Degree of symmetry breaking of the labile Mn — X — Mn bond revealed by several hybrid DFT calculations. *International Journal of Quantum Chemistry*, 113(4):525–541, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yasrebi:2017:TIW

[YJ17] Sara Yasrebi and Zahra Jamshidi. Theoretical investigation of the weak interactions of rare gas atoms with silver clusters by resonance Raman spectroscopy modeling. *International Journal of Quantum Chemistry*, 117(15):??, August 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yaghobi:2011:NOP

[YK11] M. Yaghobi and A. Koohi. Nonlinear optical properties of the M @ C_{60} endohedrals (M = Cs, Li, and Na). *International Journal of Quantum Chemistry*, 111(1):148–155, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2013:CFM

[YK13] Yonggang Yang and Oliver Kühn. Concepts and fundamental methods in molecular simulations: Path integral approach to the calculation of reaction rates for a reaction coordinate coupled to a dual harmonic bath. *International Journal of Quantum Chemistry*, 113(3):306–315, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yanai:2015:RDM

[YKM+15] Takeshi Yanai, Yuki Kurashige, Wataru Mizukami, Jakub Chalupský, Tran Nguyen Lan, and Masaaki Saitow. Reviews: Density matrix renormalization group for ab initio calculations and associated dynamic correlation methods: a review of theory and applications. *International*

Journal of Quantum Chemistry, 115(5):283–299, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoshikawa:2013:FWF

[YKN13] Takeshi Yoshikawa, Masato Kobayashi, and Hiromi Nakai. Frontiers in wave function theory: Divide-and-conquer-based symmetry adapted cluster method: Synergistic effect of subsystem fragmentation and configuration selection. *International Journal of Quantum Chemistry*, 113 (3):218–223, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2010:HBR

[YL10] Yong Yang and Ying Liu. Hydrogen bond of radicals: Interaction of HNO with HCO, HNO, and HOO. *International Journal of Quantum Chemistry*, 110(6):1264–1272, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yue:2011:DFI

[YL11] Yun Yue and Xiao-Jun Li. Density functional investigations of endohedral metallofullerenes TM@C_{24} (TM = Mn, Fe, Co, Ni, Cu, and Zn). *International Journal of Quantum Chemistry*, 111(1):96–102, January 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuan:2017:GXP

[YLC17] Meiling Yuan, Wentao Li, and Maodu Chen. Global X^2 A' potential energy surface of Li_2H and quantum dynamics of H + Li_2 ($X^1\Sigma_g^+$) Li + LiH ($X^1\Sigma^+$) reaction. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2019:ABN

[YLH+19] Le Yang, Ying Li, Debo Hao, Lanlan Li, Huifen Peng, and Peng Jin. Aggregation behavior and non-covalent functionalization of borofullerenes B_{28}, B_{38}, and B_{40}: a density functional theory investigation. *International Journal of Quantum Chemistry*, 119(14):e25921:1–e25921:??, July 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yi:2013:EMC

[YLW+13] Pinggui Yi, Zhengjun Liu, Zhaoxu Wang, Xianyong Yu, Jiming Zhou, Bo Hou, and Qingzhong Li. Effect of metal cations [Li^+, Na^+, K^+, Be^{2+}, Mg^{2+}, and Ca^{2+}] on the structure of 2-(3′-hydroxy-2′-pyridyl)benzoxazole: a theoretical investigation. *International Journal of Quantum Chemistry*, 113(9):1316–1324, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2012:SPN

[YLWrL12] Hui Yang, Ying Li, Di Wu, and Zhi ru Li. Structural properties and nonlinear optical responses of superatom compounds BF_4-M (M = Li, FLi_2, OLi_3, NLi_4). *International Journal of Quantum Chemistry*, 112(3):770–778, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuan:2018:GPE

[YLYC18] Meiling Yuan, Wentao Li, Jiuchuang Yuan, and Maodu Chen. A global potential energy surface and time-dependent quantum wave packet calculation of Au + H_2 reaction. *International Journal of Quantum Chemistry*, 118 (3):??, February 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2017:HRM

[YLZ+17] Zi-Yi Yu, Han Lai, Wen-Juan Zhao, Rui Wu, Xue-Sen Liu, and Li-Hua Gan. A hidden rule in metal sulfide fullerenes: a case study of $Sc_2S@C_{88}$. *International Journal of Quantum Chemistry*, 117(19):??, October 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yadav:2012:QTS

[YM12] Amarjeet Yadav and P. C. Mishra. Quantum theoretical study of mechanism of the reaction between guanine radical cation and carbonate radical anion: Formation of 8-oxoguanine. *International Journal of Quantum Chemistry*, 112(8):2000–2008, April 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yadav:2013:RHP

[YM13] Amarjeet Yadav and P. C. Mishra. Reactivities of hydroxyl and perhydroxyl radicals toward cytosine and thymine: a comparative study. *International Journal of Quantum Chemistry*, 113(1):56–62, January 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yasuda:2014:ECT

[YM14] Koji Yasuda and Hironori Maruoka. Efficient calculation of two-electron integrals for high angular basis functions. *International Journal of Quantum Chemistry*, 114(9):543–552, May 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoneda:2013:CMN

[YMY+13] Kyohei Yoneda, Shu Minamide, Taishi Yamada, Soichi Ito, Takuya Minami, Ryohei Kishi, Yasuteru Shigeta, and Masayoshi Nakano. Computational meso- and nanoscience: Antidot effects on the open-shell characters and second hyperpolarizabilities of rectangular graphene nanoflakes. *International Journal of Quantum Chemistry*, 113(4):605–611, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yahia:2018:QCD

[YNLD18] Wassila Yahia, Abdelmalek Khorief Nacereddine, Messaoud Liacha, and Abdelhafid Djerourou. A quantum-chemical DFT study of the mechanism and regioselectivity of the 1,3-dipolar cycloaddition reaction of nitrile oxide with electron-rich ethylenes. *International Journal of Quantum Chemistry*, 118(11):e25540:1–e25540:??, June 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ohnishi:2015:SNU

[yOITn15] Yu ya Ohnishi, Kazuya Ishimura, and Seiichiro Ten-no. Software news and updates: Massively parallel MP2-F12 calculations on the K computer. *International Journal of Quantum Chemistry*, 115(5):333–341, March 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yahya:2015:PMI

[YOS15] W. A. Yahya, K. J. Oyewumi, and K. D. Sen. Position and momentum information-theoretic measures of the pseudo-harmonic potential. *International Journal of Quantum Chemistry*, 115(21):1543–1552, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoshizawa:2020:MDP

[Yos20] Terutaka Yoshizawa. A mathematical discussion of Pons Viver's implementation of Löwdin's spin projection operator. *International Journal of Quantum Chemistry*, 120 (12):e26215:1–e26215:??, June 15, 2020. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Pon19].

Yang:2014:VOR

[YPDW14] Zejin Yang, Wenning Pang, Patrick Duffy, and Feng Wang. Valence orbital response to methylation of uracil. *International Journal of Quantum Chemistry*, 114(5):314–320, March 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoosefian:2011:SES

[YRN+11] Mehdi Yoosefian, Heidar Raissi, Emad Saleh Nadim, Farzaneh Farzad, Mustapha Fazli, Elham Karimzade, and Alireza Nowroozi. Substituent effect on structure, electron density, and intramolecular hydrogen bonding in nitroso-oxime methane. *International Journal of Quantum Chemistry*, 111(14):3505–3516, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2013:RIF

[YS13] Ciann-Dong Yang and Kuan-Chang Su. Reconstructing interference fringes in slit experiments by complex quantum trajectories. *International Journal of Quantum Chemistry*, 113(9):1253–1263, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2018:CEP

[YS18] Yun-Fang Yang and Yuanbin She. Computational exploration of Pd-catalyzed C-H bond activation reactions. *International Journal of Quantum Chemistry*, 118(21):

e25723:1–e25723:??, November 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ysupova:2011:TTE

[YSA+11] A. A. Ysupova, A. G. Shamov, R. T. Ahmetova, V. A. Pervushin, and A. I. Hatsrinov. Titanium tetrachloride as electrophilic activator in the technology of inorganic polysulfides. *International Journal of Quantum Chemistry*, 111 (11):2575–2578, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yakubovich:2010:CCP

[YSG10] Alexander V. Yakubovich, Andrey V. Solov'yov, and Walter Greiner. Conformational changes in polypeptides and proteins. *International Journal of Quantum Chemistry*, 110 (1):257–269, January 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamanaka:2012:SRM

[YSK+12] S. Yamanaka, T. Saito, K. Kanda, H. Isobe, Y. Umena, K. Kawakami, J.-R. Shen, N. Kamiya, M. Okumura, H. Nakamura, and K. Yamaguchi. Structure and reactivity of the mixed-valence $CaMn_4\ O_5\ (H_2\ O)_4$ and $CaMn_4\ O_4\ (OH)(H_2\ O)_4$ clusters at oxygen evolution complex of photosystem II. Hybrid DFT (UB3LYP and UBHandHLYP) calculations. *International Journal of Quantum Chemistry*, 112(1):321–343, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yukcu:2012:CEM

[YŞÖ12] N. Yükçü, İ. Şenlik, and E. Öztekin. Calculation of electric multipole moment integrals with the different screening parameters via the Fourier transform method. *International Journal of Quantum Chemistry*, 112(2):414–425, January 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2010:TCB

[YSS+10] Kizashi Yamaguchi, Mitsuo Shoji, Toru Saito, Hiroshi Isobe, Satomichi Nishihara, Kenichi Koizumi, Satoru Yamada, Takashi Kawakami, Yasutaka Kitagawa, Shusuke Yamanaka, and Mitsutaka Okumura. Theory of chemical

bonds in metalloenzymes. XV. Local singlet and triplet diradical mechanisms for radical coupling reactions in the oxygen evolution complex. *International Journal of Quantum Chemistry*, 110(15):3101–3128, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2011:NGR

[YSW11] Jia-Feng Yu, Xiao Sun, and Ji-Hua Wang. A novel 2D graphical representation of protein sequence based on individual amino acid. *International Journal of Quantum Chemistry*, 111(12):2835–2843, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yoshikawa:2014:NRD

[YT14] Takehiro Yoshikawa and Toshiyuki Takayanagi. Nonadiabatic relaxation dynamics of water anion cluster and its isotope effects by ring-polymer molecular dynamics simulation. *International Journal of Quantum Chemistry*, 114 (10):636–641, May 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamabe:2019:ARI

[YTY19] Shinichi Yamabe, Noriko Tsuchida, and Shoko Yamazaki. The adenine ring influences the adenosine 5'-triphosphate hydrolysis. *International Journal of Quantum Chemistry*, 119(5):e25816:1–e25816:??, March 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2013:IIF

[Yu13] Feng Yu. Intermolecular interactions of formic acid with benzene: Energy decomposition analyses with ab initio MP2 and double-hybrid density functional computations. *International Journal of Quantum Chemistry*, 113(21): 2355–2360, November 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yurovsky:2013:SWY

[Yur13] Vladimir A. Yurovsky. On spin wavefunctions and Young orthogonal matrices. *International Journal of Quantum Chemistry*, 113(10):1436–1439, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See erratum [Yur15].

Yurovsky:2015:ESW

[Yur15] Vladimir A. Yurovsky. Erratum: On spin wavefunctions and Young orthogonal matrices. *International Journal of Quantum Chemistry*, 115(14):907, July 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic). See [Yur13].

Yang:2011:EQM

[YW11a] Ciann-Dong Yang and Hung-Jen Weng. Electronic quantum motions in hydrogen molecule ion. *International Journal of Quantum Chemistry*, 111(12):2980–2999, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2011:QBC

[YW11b] Ciann-Dong Yang and Hung-Jen Weng. Quantum bifurcation in a Coulombic-like potential. *International Journal of Quantum Chemistry*, 111(15):4330–4351, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2016:SQP

[YW16] Ciann-Dong Yang and Chia-Hung Wei. Synthesizing quantum probability by a single chaotic complex-valued trajectory. *International Journal of Quantum Chemistry*, 116(6): 428–437, March 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2012:BGDa

[YWH12a] Y. X. Yao, C. Z. Wang, and K. M. Ho. The benchmark of Gutzwiller density functional theory in hydrogen systems. *International Journal of Quantum Chemistry*, 112(1):240–246, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2012:BGDb

[YWH12b] Y. X. Yao, C. Z. Wang, and K. M. Ho. The benchmark of Gutzwiller density functional theory in hydrogen systems. *International Journal of Quantum Chemistry*, 112 (15):2766, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2012:SVF

[YWH+12c] Lei Yu, Yuhua Wang, Zhengguo Huang, Hongke Wang, and Yumei Dai. Structures, vibrational frequencies, topologies, and energies of hydrogen bonds in cysteine-formaldehyde complexes. *International Journal of Quantum Chemistry*, 112(5):1514–1525, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2011:NIP

[YWJ+11] Yinling Yang, Dongling Wu, Dianzeng Jia, Lang Liu, and Anjie Liu. New insight into the photochromic mechanism of 1,3-diphenyl-4-(4-fluoro)benzal-5-pyrazolone N (4)-phenyl semicarbazone. *International Journal of Quantum Chemistry*, 111(5):1048–1054, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ye:2018:CTD

[YWR+18] Chuanxiang Ye, Bin Wang, Can Ren, Teng Zhang, Yang Gao, Junmin Zhang, and Tingchao He. Chiral thiophene derivatives with optimal two-photon absorption in near-infrared window I and II. *International Journal of Quantum Chemistry*, 118(18):e25690:1–e25690:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2012:UCR

[YWY+12] Zhiwei Yang, Xiaomin Wu, Gang Yang, Yuangang Zu, and Lijun Zhou. Understanding the chiral recognitions between neuraminidases and inhibitors: Studies with DFT, docking, and MD methods. *International Journal of Quantum Chemistry*, 112(3):909–921, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2018:FPE

[YXM+18] Ping Yang, Tianlv Xu, Roya Momen, Alireza Azizi, Steven R. Kirk, and Samantha Jenkins. Fatigue and photochromism S_1 excited state reactivity of diarylethenes from QTAIM and the stress tensor. *International Journal of Quantum Chemistry*, 118(13):e25565:1–e25565:??, July 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamabe:2018:DSP

[YY18a] Shinichi Yamabe and Shoko Yamazaki. A DFT study of proton transfers for the reaction of phenol and hydroxyl radical leading to dihydroxybenzene and H_2O in the water cluster. *International Journal of Quantum Chemistry*, 118 (6), March 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamabe:2018:TRC

[YY18b] Shinichi Yamabe and Shoko Yamazaki. The tautomerization and ring closure in the Claisen rearrangement: a DFT study. *International Journal of Quantum Chemistry*, 118(18):e25677:1–e25677:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2012:SHM

[YYI+12] K. Yamaguchi, S. Yamanaka, H. Isobe, K. Tanaka, and N. Ueyama. Spin Hamiltonian models for artificial and native water splitting systems revealed by hybrid DFT calculations. Oxygen activation by high-valent Mn and Ru ions. *International Journal of Quantum Chemistry*, 112 (24):3849–3866, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamaguchi:2013:CBBa

[YYI+13] K. Yamaguchi, S. Yamanaka, H. Isobe, T. Saito, K. Kanda, Y. Umena, K. Kawakami, J.-R. Shen, N. Kamiya, M. Okumura, H. Nakamura, M. Shoji, and Y. Yoshioka. Computational biochemistry and biophysics: The nature of chemical bonds of the $CaMn_4O_5$ cluster in oxygen evolving complex of photosystem II: Jahn–Teller distortion and its suppression by Ca doping in cubane structures. *International Journal of Quantum Chemistry*, 113(4):453–473, February 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yamabe:2015:DSH

[YYS15] Shinichi Yamabe, Shoko Yamazaki, and Shigeyoshi Sakaki. A DFT study of hydride transfers to the carbonyl oxygen of DDQ. *International Journal of Quantum Chemistry*, 115(21):1533–1542, November 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yuan:2010:QCT

[YZ10] Ming-Hu Yuan and Guo-Jun Zhao. Quasi-classical trajectory stereodynamics study of the Li + HF($v = 0, j = 0$) $\rightarrow$ LiF + H reaction. *International Journal of Quantum Chemistry*, 110(10):1842–1847, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yin:2012:QMS

[YZ12] Hai-Feng Yin and Hong Zhang. Quantum mechanical study on plasmon resonances in small ring clusters. *International Journal of Quantum Chemistry*, 112(16):2816–2821, August 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yan:2013:RTE

[YZ13] Qi-Long Yan and Svatopluk Zeman. Reviews: Theoretical evaluation of sensitivity and thermal stability for high explosives based on quantum chemistry methods: a brief review. *International Journal of Quantum Chemistry*, 113 (8):1049–1061, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2010:TSE

[YZL+10] Bao-Zhu Yang, Xin Zhou, Tao Liu, Fu-Quan Bai, and Hong-Xing Zhang. Theoretical studies on the electronic structures and spectroscopic properties of a series of novel N C N-coordinating Pt(II) complexes. *International Journal of Quantum Chemistry*, 110(9):1605–1614, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2011:IDS

[YZL+11] Bao-Zhu Yang, Xin Zhou, Tao Liu, Fu-Quan Bai, and Hong-Xing Zhang. Ab initio and DFT study of the electronic structures and spectroscopic properties of pyrene ligands and their cyclometalated complexes. *International Journal of Quantum Chemistry*, 111(10):2258–2267, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2015:DTS

[YZW+15a] Xiao-Zhu Yang, Ting-Ting Zhang, Jia Wei, Jian-Feng Jia, and Hai-Shun Wu. DFT/TDDFT studies of the ancillary ligand effects on structures and photophysical properties of rhenium (I) tricarbonyl complexes with the imidazo[4,5-f]-1,10-phenanthroline ligand. *International Journal of Quantum Chemistry*, 115(20):1467–1474, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yao:2015:RBC

[YZW15b] Xiaojing Yao, Xiuyun Zhang, and Jinlan Wang. Reviews: The bonding characteristics and electronic and magnetic properties of organometallic sandwich clusters and nanowires. *International Journal of Quantum Chemistry*, 115(10):607–617, May 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2015:SZP

[YZZ15] Gang Yang, Chang Zhu, and Lijun Zhou. Stabilization of zwitterionic proline by DMSO. *International Journal of Quantum Chemistry*, 115(24):1746–1752, December 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yu:2016:DSL

[YZZ16] Xing Yu, Hongrui Zhu, and Yi Zeng. A DFT study of Lp $\cdots$ π/halogen bond competition in complexes of perhalogenated alkenes with oxygen/nitrogen containing simple molecules. *International Journal of Quantum Chemistry*, 116(16):1244–1253, August 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Yang:2015:TMB

[YZZH15] Zhao-Di Yang, Hui Zhang, Hong Zhao, and Baozhong Han. Trap mechanism based on frontier molecular orbitals of additives in polyethylene insulators: a theoretical study and molecular design strategy. *International Journal of Quantum Chemistry*, 115(20):1483–1489, October 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zborowski:2010:TSS

[ZAE10] Krzysztof K. Zborowski, Ibon Alkorta, and José Elguero. A theoretical study of the sulfenate–sulfoxide rearrangement. Effect of the hydrogen bond complexation. *International Journal of Quantum Chemistry*, 110(13):2391–2397, November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zagoulaev:2011:MNS

[Zag11] Serge N. Zagoulaev. Magnetic neutron scattering anti-Bragg solution. *International Journal of Quantum Chemistry*, 111(11):2579–2591, September 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2013:PNA

[Zak13] Maxim Zakharov. Performance of numerical atom-centered basis sets in the ground-state correlated calculations of non-covalent interactions: Water and methane dimer cases. *International Journal of Quantum Chemistry*, 113(15):1899–1918, August 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharov:2016:EEC

[Zak16] A. Yu. Zakharov. Exact equation for classical many-body systems: Passage from dynamics to equilibrium. *International Journal of Quantum Chemistry*, 116(3):247–251, February 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zoppi:2018:RCT

[ZB18] Laura Zoppi and Kim K. Baldridge. Reviews: From charge-transfer excitations to charge-transport phenomena in organic molecular crystals. *International Journal of Quantum Chemistry*, 118(1):??, January 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ziegler:2017:CSS

[ZBBB17] Eric W. Ziegler, James Clayton Baum, Alan B. Brown, and Gail S. Blaustein. A computational study of substituent effects on the stability and geometry of carbazole–pyridine complexes. *International Journal of Quantum Chemistry*,

117(4):??, February 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2019:DFT

[ZBG+19] Huimin Zhang, Huining Bai, Yuen Guo, Donghui Wei, Hui Chen, Yanyan Zhu, and Wenjing Zhang. A density functional theory study on mechanism and substituent effects of a base-free and catalyst-free synthesis of functionalized dihydrobenzoxazoles. *International Journal of Quantum Chemistry*, 119(6):e25836:1–e25836:??, March 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:RRP

[ZBK15] Yiteng Zhang, Gennady P. Berman, and Sabre Kais. Reviews: The radical pair mechanism and the avian chemical compass: Quantum coherence and entanglement. *International Journal of Quantum Chemistry*, 115(19):1327–1341, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2011:QMC

[ZCC11] Hong Zhang, Xin-Lu Cheng, and Simone Chiesa. Quantum Monte Carlo calculations of bond dissociation energies for some nitro and amino molecules. *International Journal of Quantum Chemistry*, 111(15):4452–4456, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhuo:2010:HLC

[ZCG10] Lin Zhuo, Feng Chen, and Bing Cong Gou. High-lying core-excited quartet states in Li-like N^{4+} and F^{6+} ions. *International Journal of Quantum Chemistry*, 110(5):1108–1116, April 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2016:DFC

[ZCG+16] Run-Ning Zhao, Rui Chen, Fan Gu, Yan-Hong Yuan, and Ju-Guang Han. A density functional computational investigation on electronic properties of the stable irregular boron fullerenes with 20–56 atoms. *International Journal of Quantum Chemistry*, 116(6):421–427, March 15, 2016. CO-

DEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:ERD

[ZCG+17] Yuan Zhang, En Cao, Shoubao Gao, Xin Huang, Qingtian Meng, and Yuzhi Song. Exploring the reaction dynamics of $O(^3P) + H2 + (X^2\Sigma_g^+)$ OH^+ $(X^3\Sigma^-) + H(^2S)$ reaction with time-dependent wave packet method. *International Journal of Quantum Chemistry*, 117(7):??, April 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Ziella:2011:SGE

[ZCP11] D. H. Ziella, M. C. Caputo, and P. F. Provasi. Study of geometries and electronic properties of $AgSi_n$ clusters using DFT/TB. *International Journal of Quantum Chemistry*, 111(7–8):1680–1693, June/July 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2018:SCF

[ZCTG18] Wen-Juan Zhao, Ai-Hua Cao, Jian-Lei Tian, and Li-Hua Gan. Structural connectivity and formation mechanism of monometallic cluster fullerenes $YCN@C_n$ (n = 68-84). *International Journal of Quantum Chemistry*, 118(16): e25647:1–e25647:??, August 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2016:COS

[ZCW16] Hu Zhou, Xianlang Chen, and Jianguo Wang. CO oxidation over supported Pt clusters at different CO coverage. *International Journal of Quantum Chemistry*, 116(12):939–944, June 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2016:DFT

[ZCX+16] Guohua Zhang, Yun Chen, Weiyu Xie, Fang Liu, and Chuntian Chen. Density functional theory study on the possibility of Si-, Ge-, and Sn-doped carbon nanotubes as efficient support materials for platinum. *International Journal of Quantum Chemistry*, 116(7):515–523, April 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:EEI

[ZCZ+12] Yuhua Zhang, Dezhan Chen, Honghong Zhang, Jianbiao Liu, Shizhen Mi, and Guiqiu Zhang. Effect of electrostatic interaction on the mechanism of dehalogenation catalyzed by haloalkane dehalogenase. *International Journal of Quantum Chemistry*, 112(3):889–899, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zamani:2013:GSS

[ZDF13] Mehdi Zamani, Hossein A. Dabbagh, and Hossein Farrokhpour. Gas storage of simple molecules in boron oxide nanocapsules. *International Journal of Quantum Chemistry*, 113(20):2319–2332, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zou:2011:DSA

[ZDZL11] Xiu-Juan Zou, Kai Ning Ding, Yong Fan Zhang, and Jun Qian Li. A DFT study of acetonitrile adsorption and decomposition on the TiO_2 (110) surface. *International Journal of Quantum Chemistry*, 111(5):915–922, April 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakrzewski:2010:IEP

[ZDZO10] Viatcheslav G. Zakrzewski, Olga Dolgounitcheva, Alexander V. Zakjevskii, and J. V. Ortiz. Ab initio electron propagator methods: Applications to nucleic acids fragments and metallophthalocyanines. *International Journal of Quantum Chemistry*, 110(15):2918–2930, December 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zaitsevskii:2018:PEE

[ZE18] Andréi Zaitsevskii and Ephraim Eliav. Padé extrapolated effective Hamiltonians in the Fock space relativistic coupled cluster method. *International Journal of Quantum Chemistry*, 118(23):e25772:1–e25772:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zenkov:2011:CTT

[Zen11] Andrei V. Zenkov. Charge-transfer transitions and optic spectra of chromites: a model computation. *International Journal of Quantum Chemistry*, 111(14):3864–3872, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:REB

[ZF15] Rui-Qin Zhang and Wen-Jie Fan. Reviews: Economical basis sets and their uses in ab initio calculations. *International Journal of Quantum Chemistry*, 115(9):570–577, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zou:2012:BPJ

[ZFC12] Wenli Zou, Michael Filatov, and Dieter Cremer. Bond pseudorotation, Jahn–Teller, and pseudo-Jahn–Teller effects in the cyclopentadienyl cation and its pentahalogeno derivatives. *International Journal of Quantum Chemistry*, 112(20):3277–3288, October 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:MMB

[ZFC+17] Zhihui Zhang, Xuejun Feng, Qun Chen, Mingyang He, Yaoming Xie, R. Bruce King, and Henry F. Schaefer III. Metal–metal bonding in biscycloheptatrienyl dimetal compounds of the second-row transition metals. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2011:TIW

[ZFS+11] Qiang Zhao, Dacheng Feng, Youmin Sun, Jingcheng Hao, and Zhengting Cai. Theoretical investigations on the weak nonbonded $CS\cdots CH_2$ interactions: Chalcogen-bonded complexes with singlet carbene as an electron donor. *International Journal of Quantum Chemistry*, 111 (14):3881–3887, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeng:2013:BCQ

[ZFW+13] G. H. Zeng, D. Q. Fang, W. J. Wu, R. Zhang, W. G. Xie, J. H. Wu, and Y. Shen. Binding conformations, QSAR, and molecular design of Alkene-3-quinolinecarbonitriles as Src inhibitors. *International Journal of Quantum Chemistry*, 113(10):1467–1478, May 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:QDR

[ZGSM15] Jing Zhang, Shoubao Gao, Yuzhi Song, and Qingtian Meng. The quantum dynamics of the reactions N + H_2 (HD, D_2) and their vibrational excitation effect. *International Journal of Quantum Chemistry*, 115(4):231–238, February 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:INE

[ZH12] Ai-Jie Zhang and Guo-Zhong He. The investigation of nonadiabatic effects for the N + ND $\rightarrow$ N_2 + D reaction. *International Journal of Quantum Chemistry*, 112 (15):2710–2714, August 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:SNU

[ZH15] Pei-Yu Zhang and Ke-Li Han. Software news & updates: GQSD: the program for the graphic processing units accelerated quantum scattering dynamics. *International Journal of Quantum Chemistry*, 115(11):738–743, June 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2010:TSE

[Zha10] Xiang Zhang. Theoretical study on electronic structure of (CNC)Fe_2N_2 and its N_2 elimination mechanism. *International Journal of Quantum Chemistry*, 110(10):1880–1889, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2014:TSR

[Zha14] Xiang Zhang. Theoretical study on S_H2 reaction of methyl radical with three-membered ring. *International Journal of Quantum Chemistry*, 114(23):1594–1601, December 5,

2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:ORR

[Zha15] Xiang Zhang. Origins of regioselectivity in radical arylation of aniline: a computational study. *International Journal of Quantum Chemistry*, 115(23):1658–1667, December 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:QIL

[Zha17] Yan Zhang. Quantitative investigation of local electric field through absorption spectrum in dye-sensitized solar cells: Atomistic simulations. *International Journal of Quantum Chemistry*, 117(18):??, September 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:AAW

[ZHF12] Min-Cang Zhang and Guo-Qing Huang-Fu. Analytical arbitrary ℓ-wave solutions of the Manning–Rosen potential in the tridiagonalization program. *International Journal of Quantum Chemistry*, 112(4):1036–1040, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2017:SIT

[ZHI17] Li Xia Zhao, Yuh Hijikata, and Stephan Irle. Structural influence of transition metal (Sc, Y, and Lu) atoms inside gold nanoparticles. *International Journal of Quantum Chemistry*, 117(12):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2019:CHH

[ZHL+19] Jingru Zhang, Qingze Hu, Qingzhong Li, Steve Scheiner, and Shufeng Liu. Comparison of σ-hole and π-hole tetrel bonds in complexes of borazine with TH_3F and F_2TO/H_2 TO (T = C, Si, Ge). *International Journal of Quantum Chemistry*, 119(11):e25910:1–e25910:??, June 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2018:WLE

[Zho18] Panwang Zhou. Why the lowest electronic excitations of rhodamines are overestimated by time-dependent density functional theory. *International Journal of Quantum Chemistry*, 118(23):e25780:1–e25780:??, December 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zuehlsdorff:2019:MAS

[ZI19] Tim J. Zuehlsdorff and Christine M. Isborn. Modeling absorption spectra of molecules in solution. *International Journal of Quantum Chemistry*, 119(1):e25719:1–e25719:??, January 5, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zilberg:2014:PCR

[Zil14] Shmuel Zilberg. Perspectives: Chemical reaction with two different elementary transition states. *International Journal of Quantum Chemistry*, 114(18):1162–1168, ???? 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2013:UOT

[ZJC+13] Wei-Wei Zhu, Lin Jin, Zhong-Hua Cui, Shao-Wen Zhang, and Yi-Hong Ding. Understanding the oxidation of the tricarbon radical C_3H: a reaction pathway survey. *International Journal of Quantum Chemistry*, 113(23):2506–2513, December 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zoboki:2013:CFM

[ZJS13] Tamás Zoboki, Péter Jeszenszki, and Péeter R. Surján. Concepts and fundamental methods in quantum chemistry: Composite particles in quantum chemistry: From two-electron bonds to cold atoms. *International Journal of Quantum Chemistry*, 113(3):185–189, February 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:CMW

[ZK12] Yuchi Zhang and Dmitri S. Kilin. Computational modeling of wet TiO_2 (001) anatase surfaces functionalized by

transition metal doping. *International Journal of Quantum Chemistry*, 112(24):3867–3873, December 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zakharieva:2011:UCM

[ZKKR11] Olga Zakharieva, Alena Kremleva, Sven Krüger, and Notker Rösch. Uranyl complexation by monodentate nitrogen donor ligands. A relativistic density functional study. *International Journal of Quantum Chemistry*, 111(9):2045–2053, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2017:TME

[ZKW17] Min Zheng, Jissy A. Kuriappan, and Mark P. Waller. Toward more efficient density-based adaptive QM/MM methods. *International Journal of Quantum Chemistry*, 117(6): ??, March 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:PPI

[ZKWZ17] Laibin Zhang, Xiangmu Kong, Mei Wang, and Mengmeng Zheng. Photophysical properties of the isomorphic emissive RNA nucleobase analogues and effect of water solution, ribose, and base pairing: a theoretical study. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2010:MGP

[ZL10] Xiao-Xia Zhao and Feng-Ling Liu. Mechanism for the gas-phase hydrogen fluoride-mediated decomposition of peroxyacetyl nitrate (PAN) studied by DFT method. *International Journal of Quantum Chemistry*, 110(6):1214–1223, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2012:TIS

[ZL12] Guozheng Zhao and Ming Lu. Theoretical investigation on the structures, densities, and detonation properties of polynitrotetraazaoctahydroanthracenes. *International Journal of Quantum Chemistry*, 112(16):2794–2800, Au-

gust 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:HEC

[ZLE17] Pan-Pan Zhang, Zeng-Zhao Li, and Alexander Eisfeld. Hierarchy of equations to calculate the linear spectra of molecular aggregates: Time-dependent and frequency domain formulation. *International Journal of Quantum Chemistry*, 117(14):??, July 18, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2011:ASS

[ZLJ11] Lie-Hui Zhang, Xiao-Ping Li, and Chun-Sheng Jia. Approximate solutions of the Schrödinger equation with the generalized Morse potential model including the centrifugal term. *International Journal of Quantum Chemistry*, 111 (9):1870–1878, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2010:TSI

[ZLLS10] Min Zhang, Yan Li, Ze-Sheng Li, and Jia-Zhong Sun. Theoretical study on the influence of ancillary ligand on the spectroscopic properties and electronic structures of phosphorescent Pt(II) complexes. *International Journal of Quantum Chemistry*, 110(6):1142–1151, May 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeng:2015:PPG

[ZLR15] Tao Zeng, Hui Li, and Pierre-Nicholas Roy. Perspectives: Potential generation and path-integral Monte Carlo in study of microscopic superfluidity. *International Journal of Quantum Chemistry*, 115(9):535–540, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2018:IDE

[ZLS+18] Fengying Zhang, Qi Luo, Xiufang Song, Xinyu Song, and Yuxiang Bu. Intriguing diaza effects on magnetic coupling characteristics in diaza-benzo[k]tetraphene-bridged nitroxide diradicals. *International Journal of Quantum Chemistry*, 118(18):e25693:1–e25693:??, Septem-

ber 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2016:CAL

[ZLWL16] Dawei Zhang, Haisheng Li, Huixian Wang, and Liben Li. Counter anion in Li^+-encapsulated C_{60} can further enhance the rate of Diels–Alder reaction: a DFT study. *International Journal of Quantum Chemistry*, 116(24):1846–1850, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2013:PST

[ZLWY13] Wenhua Zhang, Zhenyu Li, Bing Wang, and Jinlong Yang. Perspectives: Scanning tunneling microscopy and density functional theory combined studies of rutile TiO_2 (1 1 0) surface chemistry: Watch surface processes at the atomic scale. *International Journal of Quantum Chemistry*, 113 (2):89–95, January 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2016:CAR

[ZLWZ16] Chengxi Zhao, Yunxiang Lu, Guimin Wang, and Weiliang Zhu. Cation–anion radical interactions between halopyridinium cations and metal dithiolene complexes $[M(C_2\ S_2)_2\ CN]^{-\bullet}$: a theoretical study of halogen bonds in conducting or magnetic molecular materials. *International Journal of Quantum Chemistry*, 116(24):1872–1881, December 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2014:CDS

[ZLY+14] Bo Zhu, Zhong Ling Lang, Li Kai Yan, Muhammad Ramzan Saeed Ashraf Janjua, and Zhong Min Su. A comparative DFT study on the mechanism of olefin epoxidation catalyzed by substituted binuclear peroxotungstates ($[SeO_4WO(O_2)_2MO(O_2)_2]^{n-}$ ($M = Ti^{IV}$, V^{V}, Ta^{V}, Mo^{VI}, W^{VI}, Tc^{VII}, and Re^{VII})). *International Journal of Quantum Chemistry*, 114(7):458–462, April 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2014:CSS

[ZLZ+14] Xueying Zhang, Xiaoyan Li, Yanli Zeng, Lingpeng Meng, and Shijun Zheng. A comparative study of some lithium

and hydrogen-bonded complexes: Ab initio and QTAIM studies. *International Journal of Quantum Chemistry*, 114 (6):400–408, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zierkiewicz:2017:NIB

[ZMB+17] Wiktor Zierkiewicz, Mariusz Michalczyk, Dariusz Bieńko, Danuta Michalska, and Thérèse Zeegers-Huyskens. Nature of the interaction between ammonia derivatives and carbon disulfide. A theoretical investigation. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2013:DFT

[ZMZ13] Li-Jiao Zhao, Xin-Yan Ma, and Ru-Gang Zhong. A density functional theory investigation on the formation mechanisms of DNA interstrand crosslinks induced by chloroethylnitrosoureas. *International Journal of Quantum Chemistry*, 113(9):1299–1306, May 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zerbetto:2016:TRM

[ZP16] Mirco Zerbetto and Antonino Polimeno. Tutorial review: Multiscale modeling for interpreting nuclear magnetic resonance relaxation in flexible molecules. *International Journal of Quantum Chemistry*, 116(22):1706–1722, November 15, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2012:TSR

[ZPB12] Hongmei Zhao, Lu Pan, and Wensheng Bian. A theoretical study on the reaction mechanisms of O(^{3} P)+1-butene. *International Journal of Quantum Chemistry*, 112(3):858–872, February 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zerbetto:2010:CON

[ZPM10] Mirco Zerbetto, Antonino Polimeno, and Eva Meirovitch. C^{++} OPPS, a new software for the interpretation of protein dynamics from nuclear magnetic resonance measurements. *International Journal of Quantum Chemistry*, 110(2):387–405, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2010:BPA

[ZPR10] C.-G. Zhang, G. Periyasamy, and F. Remacle. Bonding patterns of $[Ag_2\text{-alanine}]^{0,\pm}$ hybrid complexes and the implementation of molecular logic gates. *International Journal of Quantum Chemistry*, 110(12):2237–2246, October 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhu:2016:RMZ

[ZPW16] Bao-Lin Zhu, Xian-Yong Pang, and Gui-Chang Wang. Reaction mechanism and Z-selectivity for chelated Ru-catalyzed AROCM of endic anhydride and propene: A DFT study. *International Journal of Quantum Chemistry*, 116(1):35–41, January 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:RML

[ZPZ15] Ruiting Zhang, Zhijun Pan, and Wei Zhuang. Reviews: Modeling the low frequency vibrational spectroscopy of ionic solutions. *International Journal of Quantum Chemistry*, 115(9):564–569, May 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2010:NNI

[ZQCJ10] Yuexing Zhang, Dongdong Qi, Xue Cai, and Jianzhuang Jiang. Nature of the near-IR band in the electronic absorption spectra of neutral bis(tetrapyrrole) rare earth(III) complexes: Time-dependent density functional theory calculations. *International Journal of Quantum Chemistry*, 110(8):1559–1564, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2013:CSI

[ZQJW13] Ting-Ting Zhang, Xiao-Xia Qi, Jianfeng Jia, and Hai-Shun Wu. Computational studies on the injection, transport, absorption, and phosphoresce properties of a series of cationic iridium (III) complexes $[Ir(C\wedge N)_2\,(L)_2\,]^+$ ($C\wedge N$ = ppy, tpy, dfppy, bzq). *International Journal of Quantum Chemistry*, 113(7):1010–1017, April 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:TIT

[ZQW+17] Wei Zhang, Yan Qiao, Yang Wang, Mingsheng Tang, and Donghui Wei. Theoretical investigation toward organophosphine-catalyzed [3 + 3] annulation of Morita–Baylis–Hillman carbonates with azomethine imines: Mechanism, origin of stereoselectivity, and role of catalyst. *International Journal of Quantum Chemistry*, 117(11):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2017:IVS

[ZQXP17] Xiu-Jun Zheng, Ning Qu, Li-Chun Xuan, and Qing-Jiang Pan. Infrared vibrational spectra, electronic structures, and formation reactions of polypyrrolic mono — and bis-actinyl complexes: a relativistic DFT study. *International Journal of Quantum Chemistry*, 117(13):??, June 5, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2013:DYG

[ZR13] Laibin Zhang and Tingqi Ren. Distinguishing yy-G tautomers by their spectroscopic signatures: a theoretical investigation. *International Journal of Quantum Chemistry*, 113(8):1225–1233, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeroual:2019:MSM

[ZRGE+19] Abdellah Zeroual, Mar Ríos-Gutiérrez, Mohammed El Idrissi, Habib El Alaoui El Abdallaoui, and Luis R. Domingo. An MEDT study of the mechanism and selectivities of the [3 + 2] cycloaddition reaction of tomentosin with benzonitrile oxide. *International Journal of Quantum Chemistry*, 119(18):e25980:1–e25980:??, September 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zimmermann:2010:EEA

[ZRLV10] Tomáš Zimmermann, Julien Ruppen, Baiqing Li, and Jiří Vaníček. Efficient evaluation of the accuracy of molecular quantum dynamics on an approximate analytical or interpolated ab initio potential energy surface. *International Journal of Quantum Chemistry*, 110(13):2426–2435,

November 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2011:DFS

[ZRR+11] Shuang Zhao, Yunlai Ren, Yunli Ren, Jianji Wang, and Weiping Yin. Density functional study of Ag_n Pd and Ag_n PdH clusters. *International Journal of Quantum Chemistry*, 111(10):2428–2435, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2013:IIS

[ZRY+13] Laibin Zhang, Tingqi Ren, Xiuqin Yang, Liuzhu Zhou, and Xiaoming Li. Intermolecular interactions of a size-expanded guanine analogue with gold nanoclusters. *International Journal of Quantum Chemistry*, 113(19):2234–2242, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zadeh:2011:QTA

[ZS11] Farnaz Heidar Zadeh and Shant Shahbazian. The quantum theory of atoms in positronic molecules: The subsystem variational procedure. *International Journal of Quantum Chemistry*, 111(9):1999–2013, August 5, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhikol:2012:ESI

[ZS12] Oleg A. Zhikol and Oleg V. Shishkin. Estimating stacking interaction energy using atom in molecules properties: Homodimers of benzene and pyridine. *International Journal of Quantum Chemistry*, 112(18):3008–3017, September 15, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zarate:2011:DTS

[ZSAP11] Ximena Zarate, Eduardo Schott, and Ramiro Arratia-Pérez. A DFT/TDDFT study of porphyrazines and phthalocyanine oxo-titanium derivatives as potential dyes in solar cells. *International Journal of Quantum Chemistry*, 111(15):4186–4196, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zarate:2013:MST

[ZSASS13] Ximena Zarate, Eduardo Schott, Leonor Alvarado-Soto, and Todd C. Sutherland. A molecular study of tetrakis(*p*-methoxyphenyl)porphyrin and its Zn(II) complex as discotic liquid crystals. *International Journal of Quantum Chemistry*, 113(20):2287–2294, October 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2014:TID

[ZSHL14] Jing Zhang, Xiang Sheng, QianQian Hou, and Yongjun Liu. Theoretical investigation on the dissociation of (R)-benzoin catalyzed by benzaldehyde lyase. *International Journal of Quantum Chemistry*, 114(6):375–382, March 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2016:RMM

[ZSHL16] Junfeng Zhao, Xiaoli Sun, Xuri Huang, and Jilai Li. Reaction mechanisms of methanol oxidation by $Fe^{IV}O$ biomimetic complex. *International Journal of Quantum Chemistry*, 116(9):692–701, May 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2010:TSS

[ZSQ+10] Hai-Bo Zhao, Shi-Ling Sun, Yong-Qing Qiu, Chun-Guang Liu, and Zhong-Min Su. Theoretical study on second-order nonlinear optical properties of spin crossover Fe(III) phenolate-pyridyl Schiff base complexes. *International Journal of Quantum Chemistry*, 110(10):1863–1870, August 15, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2013:TSM

[ZSS+13] Jinfeng Zhao, Chuanzhi Sun, Nan Sun, Lin Meng, and Dezhan Chen. Theoretical study on the mechanism of the reaction for alkene hydroaminations catalyzed by chiral aldehyde. *International Journal of Quantum Chemistry*, 113(22):2457–2463, November 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zazza:2010:CHP

[ZST+10] Costantino Zazza, Nico Sanna, Simone Tatoli, Massimiliano Aschi, and Amedeo Palma. Compound I in horseradish peroxidase enzyme: Magnetic state assessment by quadratic configuration interaction calculations. *International Journal of Quantum Chemistry*, 110(2):352–357, February 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhekova:2014:PRM

[ZSZ14] Hristina R. Zhekova, Michael Seth, and Tom Ziegler. A perspective on the relative merits of time-dependent and time-independent density functional theory in studies of the electron spectra due to transition metal complexes. An illustration through applications to copper tetrachloride and plastocyanin. *International Journal of Quantum Chemistry*, 114(15):1019–1029, August 5, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zaitsevskii:2013:ICG

[ZT13] Andréi Zaitsevskii and Anatoly V. Titov. Interaction of copernicium with gold: Assessment of applicability of simple density functional theories. *International Journal of Quantum Chemistry*, 113(13):1772–1774, July 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zheng:2011:TSM

[ZTC11] Jun-Hua Zheng, Hong-Wei Tan, and Guang-Ju Chen. Theoretical study on the mechanism of the DNA repair protein Fpg. *International Journal of Quantum Chemistry*, 111 (10):2454–2463, August 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2015:MCC

[ZW15] Li-Juan Zhao and Dong-Lai Wang. Monometallic cyanide cluster fullerene YCN@C_{78}: a theoretical prediction. *International Journal of Quantum Chemistry*, 115(12):779–784, June 15, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zicovich-Wilson:2012:BWT

[ZWE12] Claudio M. Zicovich-Wilson and Alessandro Erba. Beyond Wigner's theorems: the role of symmetry equivalences in quantum systems. *International Journal of Quantum Chemistry*, 112(21):3543–3551, November 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2018:NGP

[ZWL18] Yong Zhang, Jiemin Wang, and Wentao Li. New global potential energy surface of the MgH_2 system and dynamics studies of the reaction H + MgH $\rightarrow$ Mg + H_2. *International Journal of Quantum Chemistry*, 118(18):e25687:1–e25687:??, September 15, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:FPS

[ZWLC12] M.-Y. Zhang, J.-Y. Wang, C.-S. Lin, and W.-D. Cheng. First-principles simulations of two photon absorption spectra of dynamic structural chromophores in green fluorescent protein. *International Journal of Quantum Chemistry*, 112 (13):2607–2614, July 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2016:SNU

[ZWSF16] Jing Zhang, Andrew L. Weisman, Patrick Saitta, and Richard A. Friesner. Software news & updates: Efficient simulation of large materials clusters using the Jaguar quantum chemistry program: Parallelization and wavefunction initialization. *International Journal of Quantum Chemistry*, 116(5):357–368, March 5, 2016. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2010:FDS

[ZWWY10] Laibin Zhang, Hongming Wang, Meishan Wang, and Chuanlu Yang. Functionalization of diamond (001)-2 $\times$ 1 surface by cycloaddition of 1,3-cyclohexadiene: a theoretical study. *International Journal of Quantum Chemistry*, 110(9):1748–1755, August 5, 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2019:CDC

[ZWZK19] Laibin Zhang, Mei Wang, Mengmeng Zheng, and Xiangmu Kong. Computational design and characterization of new thieno-expanded tricyclic purine analogs. *International Journal of Quantum Chemistry*, 119(8):e25870:1–e25870:??, April 15, 2019. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:TCB

[ZX12] X.-G. Zhang and T. Xiang. Tunable Coulomb blockade and giant Coulomb blockade magnetoresistance in a double quantum dot system. *International Journal of Quantum Chemistry*, 112(1):28–32, January 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2013:LHR

[ZXY13] Dong-Xia Zhao, Zhen-Zhen Xu, and Zhong-Zhi Yang. Local HSAB rationalization of Diels–Alder reactions by means of ab initio and ABEEM $\sigma\pi$ methods: Stereoselectivity and reaction rate. *International Journal of Quantum Chemistry*, 113(8):1116–1127, April 15, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2013:PRP

[ZY13] Hong Zhang and Haifeng Yin. Plasmon resonances and plasmon-induced charge transport in linear atomic chains. *International Journal of Quantum Chemistry*, 113(19): 2200–2205, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2013:CIG

[ZYL+13] Run-Ning Zhao, Yanhong Yuan, Fuyi Liu, Ju-Guang Han, and LiuSi Sheng. A computational investigation on the geometries, stabilities, antioxidant activity, and the substituent effects of the L-ascorbic acid and their derivatives. *International Journal of Quantum Chemistry*, 113 (19):2220–2227, October 5, 2013. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhuo:2014:SMM

[ZYL+14] Hongying Zhuo, Hong Yu, Qingzhong Li, Wenzuo Li, and Jianbo Cheng. Some measures for mediating the strengths

of halogen bonds with the B–B bond in diborane(4) as an unconventional halogen acceptor. *International Journal of Quantum Chemistry*, 114(2):128–137, January 15, 2014. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2017:TPS

[ZYSW17] Xiang-Biao Zhang, Bin-Bin Yu, Sheng-Meng Si, and Song Wang. Theoretical prediction on the synthesis of 2,3-dihydropyridines through Co(III)-catalysed reaction of unsaturated oximes with alkenes. *International Journal of Quantum Chemistry*, 117(8):??, April 15, 2017. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2011:TST

[ZYZ+11] Gui-Ling Zhang, Hong-Liang Yuan, Hui Zhang, Yan Shang, and Miao Sun. Theoretical studies on the transport property of oligosilane with *p–n* junction. *International Journal of Quantum Chemistry*, 111(15):4214–4223, December 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhai:2015:DES

[ZZ15] Liangjun Zhai and Yujun Zheng. Dynamical entanglement of stretching–stretching and stretching–bending vibrations in SO_2. *International Journal of Quantum Chemistry*, 115 (19):1405–1411, October 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhou:2018:ADE

[ZZ18] Panwang Zhou and Li Zhao. Accurate description of excited state intramolecular proton transfer that involves zwitterionic state using optimally tuned range-separated time-dependent density functional theory. *International Journal of Quantum Chemistry*, 118(15): e25618:1–e25618:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2012:BDE

[ZZC12] Jun Zhao, Hui Zeng, and Xinlu Cheng. Bond dissociation energies for removal of the hydroxyl group in some alcohols from quantum chemical calculations. *International Journal of Quantum Chemistry*, 112(3):665–671, February 5,

2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2015:CIH

[ZZC15] Honghong Zhang, Xue Zhao, and Dezhan Chen. A computational investigation of the hydrogenation of imines catalyzed by rhodium thiolate complexes. *International Journal of Quantum Chemistry*, 115(1):1–5, January 5, 2015. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zeng:2011:IAS

[ZZL+11] Yanli Zeng, Xueying Zhang, Xiaoyan Li, Shijun Zheng, and Lingpeng Meng. Ab initio and AIM studies on typical π-type and pseudo-π-type halogen bonds: Comparison with hydrogen bonds. *International Journal of Quantum Chemistry*, 111(14):3725–3740, November 15, 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2012:TIE

[ZZR+12] Zi-Long Zhang, Lu-Yi Zou, Ai-Min Ren, Chun-Gang Min, Ying Sun, and Ying-Fang Liu. Theoretical investigations on electronic structures and photophysical properties of novel bridged triphenylamine derivatives. *International Journal of Quantum Chemistry*, 112(5):1473–1490, March 5, 2012. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2011:DDS

[ZZW11] Yue Zhang, Tianlei Zhang, and Wenliang Wang. Direct dynamics study on mechanism and kinetics of the biradical self-reaction of HOO. *International Journal of Quantum Chemistry*, 111(12):3029–3039, October 2011. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhang:2010:TSH

[ZZX10] Xiaowen Zhang, Weihua Zhu, and Heming Xiao. Theoretical studies on heats of formation, detonation properties, and bond dissociation energies of monofurazan derivatives. *International Journal of Quantum Chemistry*, 110(8):1549–1558, July 2010. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).

Zhao:2018:MAM

[ZZZ+18] Dong-Xia Zhao, Jian Zhao, Zun-Wei Zhu, Chao Zhang, and Zhong-Zhi Yang. A model of atoms in molecules based on potential acting on one electron in a molecule: I. Partition and atomic charges obtained from ab initio calculations. *International Journal of Quantum Chemistry*, 118(15):e25610:1–e25610:??, August 5, 2018. CODEN IJQCB2. ISSN 0020-7608 (print), 1097-461X (electronic).