A Complete Bibliography of Publications in *Advances in Quantum Chemistry*

Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: `beebe@math.utah.edu`, `beebe@acm.org`, `beebe@computer.org` (Internet)
WWW URL: `https://www.math.utah.edu/~beebe/`

24 January 2024
Version 2.36

Title word cross-reference

$+$ [BRW08, GAI08, TBM01]. $1.9\AA$ [YKS+12]. 10 [AGO07]. $1s$ [LPC24, PTC+13, PTBH13, UYT97, VT24]. 2 [DAB+23, SRZE04]. 20 [AGO07]. 217 [Gos02a]. $21^{\rm st}$ [KvH99]. $2 \leq Z \leq 10$ [OE17]. 2×2 [KC19]. 3 [KMR01, SRZE04]. $3+1^1$ [SBK15]. $3d$ [MTA00, TSON00]. 5 [HBGvM19]. $5d$ [SED+98]. $5f^2$ [MCC03]. 9 [JGCRC16]. $=$ [HOI+08, KIT+08]. $^+$ [ARS99, BB14, KM98, SJO05, SM23, TM13]. $^-$ [CCM05, JMWG19, SEL01, TM13]. ^{1} [BRW08, VT24]. ^{13} [CPBS05]. $^1\Sigma_g^+$ [Kom05]. ^{2} [SP99]. $^{2+}$ [CLK15, Mam19, SCTH+07]. $^{2-}$ [CSZ99]. ^{2h} [DE05]. ^{3} [Bel19]. $^{3+}$ [ADA03, JSG+14, JS21]. $^{4+}$ [IOA03, TBM01]. ^{8} [RF13]. ^{9} [RF13]. $\bullet$ [PEMC23]. ^{n} [CPBS05]. $^{n+}$ [LM03]. $^{n\pm}$ [NM03]. $_0$ [MFMCN01]. $_1$ [SP99]. $_{1-x}$ [NIO03]. $_{1.75}$ [NM00]. $_{1/8}$ [GWM+03]. $_{10}$ [LC03]. $_{12}$ [HOI+08]. $_2$ [APNM03, BRW08, CSZ99, DLMS03, GP14, Hog18e, Hog21, Jan97, Lyo08, Mar08b, MCC03, Miy03, MKK+00, Mur03, NM00, OTA97, Sak03a, SP99, Sau05b, SH19, SCE19, SS04, SEL01, TMM03, YKS+12, YIYM03, ŻM23]. $_{2,3}$

[OTA97]. $_{20}$ [PM16]. $^{+}_{2}$ [BMR+24, CLK15]. $^{-}_{2}$ [Miy03]. $_{3}$ [CY00, CSZ99, DLMS03, GWM+03, HSS+04, IKN+08, JMWG19, KIT+08, MVL01, NeMM03, NIO03, NP03, OTA97, Sau05b, SSS05, YTC+05]. $_{33}$ [SMAS08]. $^{-}_{3}$ [MGAUP23]. $_{4}$ [CL00, CSZ99, DA14, DLMS03, Jan97, OM03, RZTSW23, Sau05b, SIY+19, YKS+12]. $_{5}$ [SIY+19, YKS+12]. $_{5 \leq n \leq 8}$ [RK04]. $_{6}$ [APNM03, ADA03, CSZ99, HOI+08, KDG97, MKK+01]. $_{60}$ [LM03, NM03, PEMC23, SCN03]. $_{67}$ [SMAS08]. $_{7}$ [CL00]. $_{7/8}$ [GWM+03]. $_{c}$ [DB01]. $_{n}$ [CMVPFC16, UMD08]. $_{x}$ [NIO03]. $_{X}$ — $_{Y}$ [DE05]. α [Ada97b, Ada00, CL00, FSB+97, Fuk03, GG20, Gut97, IFAY08, Kaw97, KNM+08, LSZ+00, MYW00, MW08, MKK+00, MTA00, Mur08, Nak00, NHYU03, OTA97, Ros97, SBA+03, SBK+08, SNMI00, SYIY03, Tan00, UMD08, YFK+97]. B [ZBM98, Wen21]. β [CCT02, DNM+14, KS88, MTA00, RMN+14, dLHD10]. β^{-} [RF13]. : [ADA03]. D [Apo01, BG23, DB01, CCA13]. d^5 [DST+03]. $e^{\pm}$ [HHU+21, WHB+24]. E_i [HHU+21]. f [BKC68]. g [MWL+05, SJO05, Sau05b]. $G \otimes (g \oplus h)$ [LPDB03]. $H \otimes 2h$ [LC03]. I [ZBM98]. $J > 0$ [ACDV01]. K [GVFR98]. L [HMH+18]. $\leq$ [HHU+21]. $\leq E_i \leq$ [WHB+24]. M [HMH+18]. $\mu - S_2$ [CSZ99]. N [LK90, CMVPFC16, Gal73, GSTvE98, RRMAF08, VT24]. ns [VT24]. p [BK70, CCCC15]. π [FH65, Fow03, Ohn67]. $\psi^{(\alpha *)}$ [AFE13]. q [KMR01]. R_3 [MKB04]. s [GW01]. s^2 [AR03]. Σ^{+} [SZP21]. T [AHPD+03]. T_3 [MKB04]. $T \otimes (e \oplus t_2)$ [LPDB03]. Y [BMC97]. Z [SGK+08, DTC04].

-2-azabuten-4-yl [NeMM03]. **-Al** [OTA97]. **-Bromopropane** [RRMAF08]. **-Bromouracil** [HBGvM19]. **-Carboxylic** [JGCRC16]. **-carotene** [CCT02]. **-Cyclodextrin** [DNM+14, RMN+14, dLHD10]. **-Decay** [RF13]. **-Decay-Induced** [KS88]. **-Deformed** [KMR01]. **-Dimensional** [CCA13, KMR01]. **-doped** [IOA03]. **-Edge** [OTA97]. **-Electron** [FH65, Gal73]. **-ETOs** [AFE13]. **-Family** [DLMS03]. **-helices** [GG20]. **-K** [KC19]. **-lone** [AR03]. **-Method** [FSB+97]. **-Nitroaniline** [CCCC15]. **-Parameter** [Apo01]. **-Particle** [GSTvE98]. **-Phenyloxirane** [JJD05]. **-Representability** [LK90]. **-Schrödinger** [BG23]. **-site** [DAB+23]. **-States** [BK70]. **-Subshells** [HMH+18]. **-Tartaric** [HSR98]. **-Type** [GW01]. **-Values** [BKC68]. **-Wave** [DB01].

/Ã [SP99]. **/alumina** [Hog23c]. **/K** [MTA00].

0.1-2 [Sim07].

1 [BG23, HHU+21]. **1-** [NeMM03]. **11-tetraazacyclotetradecane** [MYW00]. **1s** [HPB17].

2-azolyl [NeMM03]. **2-bis** [YKY+00]. **2-Cyclohexenone** [GBHM14]. **2-Hydroxy-acetamide** [SDGW98]. **2012** [Hog13g, Hog14].

3-Dipolar [RGA99]. **3P** [RT18].

4-Center [AA18]. **4-dioctyloxyphenyl** [YKY+00]. **40** [Miy03].

= [BMC97, BJMB14, CMVPFC16].

A1N [SYIY03]. **Ab-Initio** [DO09]. **Absolute** [MYM08]. **absorbed** [LYM03]. **Absorbing** [RDNFH98]. **Absorption** [CCCC15, CLÅ05, JGCRC16, Jos08, KsKsN08, KNM+08, MYW00, MW08, Mur08, Tak19, YFK+97, IOA03, Mur03, SP99, YNNU03]. **Abstract** [KS97b]. **academic** [SBK+08]. **Accelerating** [ST07, BG23]. **Accounting** [DKV+19]. **Accumulative** [BR65]. **Accuracy** [BR65, Hal64, KE98, Koł70, Pau13, Ros97]. **Accurate** [BC80, CS77, SZP21, ŚBG14, Bis19, EÜSB21, KHPP23, LH20, VT24]. **Accurately** [Hog18e]. **ACES** [PM16]. **acetamide** [SDGW98]. **Acetic** [PWZ+08]. **achiral** [QSW20]. **Acid** [BWH08, HSR98, JGCRC16, KLG+08, KV08, PWZ+08, Tur07]. **Acid-Water-Ammonia** [KV08]. **Acidities** [Sey12]. **Acids** [PP68]. **Acknowledgement** [Ano04a]. **Across** [DE05]. **Acrylonitrile** [RGA99]. **Actinyl** [HTS+00]. **Activation** [Bro98a, Bro98b, OM03, RZTSW23]. **Active** [Bro98a, Bro98b, YMI+21]. **Activity** [Jan97, ST17]. **Adaptation** [KCM70]. **Adapted** [KMJ97, CAG+21, KHPP23]. **ADC** [Hät05]. **Adding** [Sim05]. **addition** [KBH23, PEMC23]. **Adiabatic** [AdMB99, BVHK03, DST+03, JSG+14, Koł70, ML18, Nag01, NFW+98, SJO05, Sim99, BMR+24, JS21]. **Adjoint** [Löw96b]. **Adjustment** [LJK+08]. **adsorbed** [Hog21, HDFT24, KBH23]. **Adsorption** [GBHM14, SN08]. **Adv** [Miy03]. **Advanced** [BKB+19, MK23, YKC+08, SBA+03]. **Advances** [ABC+98, Ano13a, Ano13b, Ano19a, BSB13, Brä21a, BB22b, BB24a, Cam12, CS04, HPL98, Hog13a, Hog13b, Hog18b, Hog23a, JKMB19a, Löw64a, Löw65a, Löw67a, Löw68a, Löw70a, Löw72a, Löw73a, Löw74a, Löw75a, Löw77a, Löw78a, Löw80a, Löw81a, Löw81b, Löw82a, Löw82b, Löw85a, Löw86a, LSZ88, LSZ89, LSZT90, LSZ91, LSZ92a, LSZ92b, LSZ94, LSZ95, LSZ96, LSZ+97b, LSZ+97a, LSZ+98b, LSZ+98c, LSZ+98a, LSZB99, LSZ+99b, LSZ+99a, LSZ+00, LSZB00, MPU19, NBS10, SBM+01a, SBM+01b, SB02, SBA+03, SB03, SBC+03, SBCT04a, SBCT04b, SBK04, SO05b, SB05, SBLJ05, SB06, SB07, SBSL08, SBK+08, SBGJ08, SBC09b, SB09a, SBC09a, SBC10, Sab11, SB11, SB12a, SB13a, Sab15, SB17a, SB17b, SB18a, SS99, AP03, SSK03]. **Advancing** [LÖS02]. **Advantages** [HB14]. **Adventurer** [OS05, SO05b]. **Advisory** [Ano94a, Ano98a]. **Aerosol** [KSG08]. **Affect** [Tak19]. **Affinity** [KDG97, Bel19, GPEB21]. **after** [MBAPS19]. **Ag** [ARS17, SHBC19, WHB+24]. **Aging** [Löw65c]. **Aharonov** [Sjö04]. **Al** [KBH23, KKA97, MGAUP23, OTA97, WHB+24]. **alcohol** [GC01]. **Algebra** [LMSP01, Löw92a, Pal04]. **Algebraic** [AČP88, FMA08, QGW01, WN05, Yas17, Yas23]. **Algorithm**

[ACDV01, Kou15]. **Alkali** [Jan65, ML18, SCN03, Tak19, SJAB+22, STO+00]. **Alkali-Metal-Doped** [SCN03]. **Alkaline** [KRL01, STO+00]. **Alkaline-Earth** [KRL01]. **Alkyl** [PL98]. **All-Electron** [MSM17]. **all-metal** [MGAUP23]. **all-particle** [SA23b]. **Alleged** [Sjö04]. **Allosteric** [ST17]. **alloyed** [TMM03]. **Alloys** [KKA97, MLR+98, YM00]. **Almost** [LGJP99]. **Almost-Linear** [LGJP99]. **Along** [BŚG17, Nag01]. **Alpha** [BRL13]. **Alphas** [Sab97]. **Alternative** [Ave98]. **alumina** [Hog23c]. **Aluminate** [MW08]. **aluminium** [PGV97]. **aluminum** [CCL03, Hog21, MST+03]. **Ambient** [ASGG08]. **amine** [NeMM03]. **Ammonia** [KV08]. **among** [IFAY08]. **Amorphous** [Mur08, SMAS08]. **analogy** [YMI+21]. **Analysis** [Ada00, Bel11, BE04, BRL13, Fuk08a, HSR98, KÖO23, Kle77, Len68, Löw92a, Mur08, Nal00, Nic10, OTA97, SJO05, STO+00, Shi12, Sid18, SYIY03, TP03, Uda00, UMD08, WmG18, YKC+08, Bis19, CCM+19, IOA03, MST+03, Sak03a]. **Analytic** [BGW73, BG73, Gre73, OE17, ZP17]. **Analytical** [Brä12, Cam12, CH03, GC10, GC92, HPU+17, HJ88, Lin17b, Rui23, WN05, BB21]. **Analyzing** [Köv08]. **Angles** [CLK15]. **Angular** [Har05, MFLK15, WP06]. **Anharmonic** [EÜSB21]. **Anion** [Lin05, Bel19, MGAUP23]. **Anionic** [RK04, JMWG19]. **Anions** [Fuk15, Sim99]. **Anisidine** [DNM+14]. **anisotropy** [ZLL+20]. **annihilating** [AP03]. **Annihilation** [FJS+04, SSK03]. **Anniversary** [Ano03a, Ano19b]. **Announcement** [Ano88a, Ano89a, Löw88a]. **ANO** [AT91]. **Anomalies** [GMP98]. **Anomalous** [HBKS03]. **Ansatz** [TA04]. **Answer** [Miy03, SEL01]. **Anthracene** [JGCRC16]. **Anthracene-** [JGCRC16]. **Anthropogenic** [AVB08]. **Antibinding** [FRM70]. **Antiferromagnetic** [Fuk08a]. **Antiferromagnetism** [Fuk15]. **Antihydrogen** [FJS+04]. **Antilinear** [SS03]. **Antimatter** [Gre08, Fro02]. **Antimatter-The** [Gre08]. **Antiproton** [PBK04]. **Antisymmetric** [Sal74]. **Antisymmetrized** [Wei04]. **AO** [CB92]. **Aperiodic** [Löw65c]. **Apology** [The96]. **Appendix** [Gos02a]. **Applicability** [DSW04, SIY+19]. **Application** [ASGG08, AGL05, AR03, CH03, Dru78, GC92, GW17, HPB17, KE97, Lin17c, Öhr17, PM16, PL98, RPSB00, Ray95, Rei73, Tan00, WD70, YMI+21, YTC+05, MKK+01]. **Applications** [AČP88, ABB90, CCSZ01, EG99, HM21, JG08, LB92, MNR+98, OE17, PSAP10, SBGJ08, SSV98, SGM+13, Sva98, ZLC+10, BPK23, Hog14, NBS12, PBOL02, Ros97, LFM89]. **Applied** [Byl98, Cru09c, OO05]. **Applying** [SSCL97]. **Approach** [ADRAB16, AL04, BKB+19, Chi03, CH03, CHSC03, CC97, DGKCT15, DR90, FMA08, GMLSC+10, GC10, Glu19, GCAGM17, HPRR10, HL90, IM80, KMHL13, Kob68, KD11, Ler85, LHL18, Löw85c, MH98, McW98, MKN10, MM99, NAY+08, NFW+98, Oli12, PČ75, PTC+13, Pul77, SG80, TA04, Tap09, dLHD10, vL03, EW03, MU03, SA23b, SKS+19, Zap01]. **Approached** [vS07]. **Approaches** [BBB10, KB86, LvWH+01, MC10, PGP17, STZY18, SS99, CTC22, JS21, Ort22, WLM23]. **Approaching** [CCC17]. **Approximate** [KB98, LGJP99, Lin02, MKB04, Nes67, PJH05, RAR15, MPU19, QSW20].

Approximating [HPB17]. **Approximation** [BG73, CHR13, Hur73, Koł70, Lyk64, NA04, Pol03, QGW01, SED+98, Sid18, BG23, GWW19, Köv03]. **Approximations** [BB99b, LV90]. **Aqueous** [BWH08, CCM05, MYW00, MW08, PWZ+08, dLHD10, MST+03]. **Arbitrary** [LR72]. **Architecture** [PWZ+08]. **Architectures** [Oli12]. **Aromatic** [AVB08, DSW04, FLV99]. **Aromaticity** [Ran18, MGAUP23]. **aromatics** [RZTSW23]. **Arsenide** [KSY08]. **Art** [AdMB99, AH19b]. **Artificial** [Duc97, MP22, SSCL97, YMI+21]. **Aspects** [ACDK72, Bis94, Coh04, Dau70, DDPC95, Fow03, GEO91, KK85, Löw65c, Löw85c, Löw98, PP68]. **Assessment** [BB99b]. **Assignment** [CÅ01, NM00]. **Assisted** [ALND10, DBC+99, PLA01, Dra20, MS03]. **Associated** [Löw88b, LFM89, OTA03]. **Asymmetric** [MFLK11, ORL23]. **Asymptotes** [HM21]. **Asymptotic** [BE04, JSF08, KKGG98, LRCR98, SPH14, Sid18, BKL21]. **ATiO** [KIT+08]. **Atmosphere** [ASGG08]. **Atmospheres** [JGNJ08]. **Atmospheric** [BRW08, GAI08, JG08, KSG08, KLG+08, KV08, MCG+08, Mar08b, NAY+08, ZZ08, SBGJ08]. **Atmospherically** [ILS08]. **Atom** [Bel09, BMM13, CTO18, Cru09c, FVB99, FAS+98, GV09, GW18, HG17, Jan65, KO18, Kle77, KMJ97, Lau09, LK09, MFLK11, Mic15, Mic17, RT18, RAR+08, STZY18, Bar23, Bel22, JS21, Mic02, Mic22, MBAPS19, NA19]. **Atom-by-Atom** [FVB99]. **Atomic** [AFE13, AJ04, AT91, ADRAB16, AAAC04, BS98, BKC68, Bli65, CCA13, DKMP98, DY08, Dru78, DKV+19, Eks98, GP91, Glu19, GM91, Hal64, HPU+17, HMH+18, Har18, HOI+08, HM21, Hyl64, KS77, Kob68, KGI+19, LK13, Lin17c, LA12, MG22, Nor98, OPPZ06, Ono00, PR98, RLF17, San98, SOS15, SBF+08, SCM09, Ste73, TSON00, TAM04, WMM+98, Bun23, CTC22, CAP19, HPL98, LSZ+00, NBA20, RSP21, SBSL08, SKK23, SA23b]. **Atomic-Beam** [Eks98]. **Atomic-Number** [Ono00]. **atomicity** [BFHS23]. **Atomization** [PEZB98, SYM+08]. **Atoms** [AAE+01, AAM04, Ano08h, Aqu09, ACDK72, AA05, BND81, Bad09, BGW73, BG73, Byl98, Dol09, DGKCT15, ERC88, FSB+97, FMA08, Glu19, GSTvE98, Gre73, GVFG09, HUS+11, IS01, JSF08, Jan65, Jør74, KRL01, KMJ97, LASV18, ML18, Mat96, MKN10, Nes75, Nic10, OE17, PV09, PJH05, Phi98, RR05, RP18, RRMAF08, RF13, Saa01, YTF78, BH24, CM24, FCAG19, FTG22, GW23, HHU+21, MKK+01, SJAB+22, Tők19, WHB+24]. **Attachment** [JA07, SSS05]. **Attempt** [FHHE82, Zap01]. **attochemistry** [SBH+20]. **attosecond** [WLM23]. **Auger** [ÅCL92, Köv03, Köv08, MM96]. **Augmented** [SED+98, Sla64]. **Author** [Ano64a, Ano65a, Ano67a, Ano68a, Ano70a, Ano72a, Ano73a]. **Autoionizing** [AA05]. **Automated** [WN05]. **automatic** [Bun23]. **Auxiliary** [Per98a]. **Average** [GMLSC+10]. **Averaged** [ILS08]. **axons** [JJ20]. **azabuten** [NeMM03]. **Azide** [PL98]. **Azido** [IFAY08]. **Azido-Bridged** [IFAY08]. **azolyl** [NeMM03].

B [HOI+08, Miy03, SP99, Mam19, SCT16]. **Ba** [KIT+08, GVFG09]. **Back** [Lin17b]. **bacteriophytochromes** [Dur20]. **Bad** [QSG98]. **BAg** [BU97]. **Balance** [PM14, Vis05]. **Band** [Cse97, KSY08, Kri03, PGN04, SS90, Sla64, SSV98]. **Band-Structure** [PGN04]. **Bands** [BWK97]. **Barkas** [Por04]. **Barkas-Effect** [Por04]. **Barnett** [SPH14]. **Barrier** [Hog18e, PEZB98, PLA01]. **Base** [JA07, KN01]. **Based** [ATL+18, AR03, BB13, GEO91, HZ89, KS97b, LFM89, OTA97, OYI+00, WmG18, BSL+19, SRZE04, YNNU03, ŻMM23]. **Bases** [CL07, MFLK15, PP68]. **Basic** [AYÖ17]. **Basicities** [Sey12]. **Basis** [AT91, AH19b, BL18, CTSOS99, Dau64, Gil94, GW01, IM80, MW98, Mon05, OOSS17, PTC+13, Pul77, QGW01, SPAS05, SW98, SDGW98, VWP+98, WM97, CCM+19, CAG+21, CAP19, GW23, RA19, SKGŚ23, Wen21]. **BaTiO** [CY00, IKN+08]. **Batteries** [YKC+08]. **BAu** [BU97]. **BC** [ACDV01, Mur03]. **BCu** [BU97]. **Be** [RLF17]. **Be-Like** [RLF17]. **Beam** [Eks98]. **Beginnings** [HKS90]. **Behavior** [ARS17, JSF08, KG12, Lev14]. **Behaviour** [LRCR98]. **Benchmark** [MWL+05]. **Benford** [MG22]. **Benzene** [JH99, KBS03, LGK+99, RAR+08]. **Bersuker** [Ano03a]. **Bessel** [HPB17]. **Bethe** [CTSOS99, ORL23, Por04]. **Between** [FLV99, GV09, KMJ97, OBHM17, Suc98, AR03, BVHK03, LR72, Nal06, PMK23, RR05, Ste73, VG22, YMI+21]. **Beyond** [GS04b, Lin98, HO16]. **Bi** [LFM89, KNI+08]. **Bi-Variational** [LFM89]. **Bimolecular** [Sko12]. **Binary** [MKK+00, MYM08, LCC22, TSTH03]. **Binding** [FRM70, KRL01, PEMC23, Ort22, PGV97]. **Biogenic** [ZZ08]. **Biographic** [Ano99a]. **Biological** [AGMdV+13, BGG+07, Bic13, Löw65c, MBO+07]. **Biology** [FHHE82, Rei73, SL20]. **Biomolecules** [HS19, JJD05, Sab07, SOS11, Bel21, SB07]. **Biophysics** [Jeh65]. **biosynthesis** [Hes22]. **Biphospholylidene** [PM16]. **Bipolar** [Sil14]. **Bipolaronic** [DB01]. **Birefringences** [RC05]. **Bis** [YKY+00]. **bisphenol** [BTB+20]. **Bivariate** [Lev14]. **Black** [Mur08]. **Bloch** [Löw98, Por04]. **Blocks** [Brä04]. **Board** [Ano88d, Ano89d, Ano90c, Ano91c, Ano92e, Ano92f, Ano95c, Ano96d, Ano97f, Ano97g, Ano98m, Ano98n, Ano98o, Ano99i, Ano99j, Ano01i, Ano03g, Ano08g, Ano09g, Ano09h, Ano10e, Ano10f, Ano11e, Ano12e, Ano19i, Hog13e, Ano99k, Ano13e]. **Body** [AAE+01, AA01, BMM13, BŚG14, DDPC95, FP06, GAM+13, Har04, Har05, HA13, Har17, HW01, HMW01, Khe19, KT98, KB86, KO19, MC10, Mat78, MK18, SW98, Shi12, WDD16, vL03, BKL21]. **Bohm** [Sjö04]. **Bohmian** [GMB04]. **Bond** [Apo01, CCSZ01, CS04, DE05, GVCN82, Joh73, Krs16, Nak00, NSM11, San92, SH95, SKT+08, SYM+08, SSS05, TLOK97, YM97, BLC23, OTA03, STO+00]. **Bonded** [FCC04, GAI08]. **Bonding** [Bra67, HTS+00, KTMA08, LK14, Lin05, MC10, Ono00, Ort99, PWZ+08, SH95, SIY+15, SMAS08, TSON00, WD70, BFHS23, LYM03, NHM03, ŻMM23]. **Bonds** [DE05, Nal09, She15]. **Boranes** [BMC97]. **Born** [TA04, BG73, CHR13, NBA20, SZP21, SA23b, Tap01]. **Boron**

[BU97, HOI+08, Oli12, Bel19]. **Boron-Coinage** [BU97]. **Both** [RC05, CTO22]. **Bottom** [Oli12]. **Bottom-Top** [Oli12]. **Bound** [AAE+01, CTSSO19, KO19, RLF17, Shi12, CBSM20, JMWG19, RA19]. **Boundaries** [Cru09c, LK09, PB20c, OTA03]. **boundary** [Bel22, Sak03b]. **Bounds** [GP91, Wei72]. **Boxes** [Aqu09]. **Br** [FPL97, HOI+08]. **brain** [NTT20, PB20a]. **Breaking** [Apo01, She15]. **Breakings** [Ber03]. **Breaks** [Sim07]. **Breit** [LT98]. **Bridged** [IFAY08]. **Brillouin** [HW01, HMW01, MH98]. **Bromine** [FPL97]. **Bromopropane** [RRMAF08]. **Bromouracil** [HBGvM19]. **BSSE** [VWP+98]. **Built** [RP72]. **bulk** [SKK23].

C [CPBS05, CSZ99, BMC97, CTSSO19, JMWG19, LM03, NM03, PM16, PEMC23, SCN03]. **Ca** [CY00, GVFG09]. **Ca-Doped** [CY00]. **Cage** [Kat03]. **Cages** [CKC09]. **Calculate** [GM05]. **Calculated** [AA05, Hal64, PJH05, VWP+98, NHYU03]. **Calculating** [Dau64, SA23b]. **Calculation** [Ada97a, Ada97b, CTSOS99, CTSDÖ04b, CL00, DKMP98, FCH15, Gal73, GDL98, GSTvE98, HJ88, IOI+00, IFAY08, Kaw97, Khe19, KNI+08, KSY08, McG04, MKK+00, OE17, PR05, PBK04, SPAS05, SP99, SSO19, TMN10, YKC+08, YTC+05, IOA03, KTA03, MAS03, SH19]. **Calculations** [ÅVM96, AFE13, AT91, ABGM03, ASGG08, AAG03, AAAC04, BGW73, LJK+08, BC80, Bis94, BR65, BŚG14, CMFA99, Chr72, DRV82, DDPC95, DA14, EEL96, EM17, Fuk00, Fuk15, GVCN82, HSS+04, HBT+00, Hog18e, IKN+08, IS01, JMWG19, KE98, KNM+08, LF09, Löw80b, LÅJM95, MYW00, MWL+05, MK18, MCM14, MSM17, Nes67, Odd78, OTA97, OYI+00, Ohn67, ÖB81, PS05a, PTC+13, PB75, PL98, PWZ+08, QGW01, San92, SJO05, SED+98, SNMI00, SIY+15, Sla64, ŚBG14, Tan00, Uda00, UMD08, VI01, YFK+97, ZDZO11, vS07, AP03, Bun23, Fuk03, GW23, MOB+03, NBA20, PS21, PMK23, RA19, Ros97, SM23, SSK03, Yam03, YNNU03]. **calculus** [Ber02, VT24]. **CaMn** [SIY+19, YKS+12]. **Can** [MRS+99]. **Cancer** [BB11]. **Canonical** [CDK15, LB92, MDÖ05]. **CaO** [TP03]. **Capacity** [MYM08]. **caps** [LC03]. **Capture** [LK13, MA04, MTA00, Bel21, MG22]. **Car** [PWZ+08]. **carbide** [RZTSW23]. **Carbides** [SNM+97]. **Carbon** [BRL13, Mur08, RT18, LYM03, MOB+03]. **carbonitriles** [JMWG19]. **Carboxylic** [JGCRC16]. **Career** [Nor98]. **Carlo** [AGL05, CCT02, CCM05, CC97, HB14, Hog18e, Hog21, Hog23c, HDFT24, KBH23, MCA+18, NFW+98, RMMP17, RP18, SH19, TAU17, vS07]. **Carlo/Quantum** [CCM05, CCT02]. **carotene** [CCT02]. **Cartesian** [CB92]. **Cascade** [HS19]. **Case** [GVFR98, HOI+08]. **Cases** [CHSC03]. **CASSCF** [CTG98]. **CASVB** [CTG98]. **Catalysis** [Bro98a, Bro98b, Hog23c, KBH23]. **catalyst** [Hog21]. **Catalysts** [HB14, Hog18e, LDP+04]. **Cation** [KBS03, LGK+99, OTA97, LMK19, TMK21]. **Cationic** [DNM+14, RK04]. **Cations** [ARS99, CL07, KTMA08, CTSSO19, FB20]. **Cauchy** [PJH05]. **Cause** [Sim07]. **Cavity** [CTO18, Lau09]. **CC2** [Hät05]. **CC3** [PJH05]. **CCSD** [BB99b]. **Cd** [HHU+21]. **CdI** [BKC68]. **Ce** [NM00]. **Cell** [BB13].

Cells [KD11, GTB23]. **Cellular** [BB15]. **Center** [AA18, Bis67, CB92, ZP17, Rui23]. **Century** [BB99a, KvH99]. **CeO** [NM00]. **Ceramic** [Fuk00]. **Ceramics** [CY00, Tan00, Sak03b]. **CETO'S** [CB92]. **CF** [UMD08]. **CH** [MVL01, RZTSW23, Sau05b]. **Challenge** [RC05]. **Challenges** [DC99]. **Change** [FU00, Löw88b, LFM89]. **Changes** [YKY+00]. **Changing** [HB14, LA12]. **Channel** [Les75]. **Channeled** [GP04]. **Channels** [Sch94, SIY+15]. **Chaotic** [IBB+19]. **Chapter** [BMR+24, BH24, CM24, HDFT24, Kar24, LPC24, VT24, WHB+24]. **Character** [NeMM03]. **Characteristics** [SKT+08, YM00, SSK03]. **Characterization** [DDPC95, MM96]. **Charge** [BLKS78, CHR13, CCSZ01, CS77, FLV99, HPRR10, Jeh65, JS21, KKA97, LA12, MF04, OYI+00, SCTH+07, Bel22, GJP23, TBM01]. **Charge-Changing** [LA12]. **Charge-Transfer** [FLV99]. **Charged** [Ano08h, Ano08j, AK12, CHR13, KH03, LT98, PGN04, Sig05, TTLB04, AGS+19, BKL21, Tők19]. **Charged-Particle** [Sig05]. **Charges** [NA04, OPPZ06, SKK23, WD22]. **Charles** [Sab00]. **Chem** [Miy03]. **Chemical** [AT91, ACC99, BS04, BR20, Cal13, CT82, Dau67, DW98, FF72, GDL98, Gut06, HTS+00, Joh73, Jør74, JGNJ08, Kar97, KTMA08, Kuk14, Ler85, MÅ01, MM99, Nal03, NSM11, NHM03, Ono00, Ort99, PSAP10, RNL14, SJO05, Sey12, SH95, She15, SKT+08, SYM+08, SW81, Sko12, Sla81, SGM+13, TMN10, TSON00, Tap01, Tap09, WD70, YM97, BPK23, Brä03, BFHS23, LYM03, PBOL02, STO+00, ŻMM23]. **Chemical-QSPR** [Sey12]. **Chemisorption** [SG80]. **Chemistry** [AVB08, Ano04l, Ano13a, Ano13b, Ano19a, Bel11, BSB13, BR20, Brä21a, BB22b, BB24a, CCC17, CS77, CB18, Cra99, DKV+19, Duc97, EBR92, FHHZ88, HPL98, Hog13a, Hog13b, Hog18b, Hog23a, Jan65, JKMB19a, KS97b, Kla81, KV08, LBH+17, Lar17, LDP+04, Löw64a, Löw65a, Löw67a, Löw68a, Löw70a, Löw72a, Löw73a, Löw74a, Löw75a, Löw77a, Löw78a, Löw80a, Löw81a, Löw81b, Löw82a, Löw82b, Löw85a, Löw86a, LSZ88, LSZ89, LSZT90, LSZ91, LSZ92a, LSZ92b, Löw92a, LSZ94, LSZ95, LSZ96, LSZ+97b, LSZ+97a, LSZ+98b, LSZ+98c, LSZ+98a, LSZB99, LSZ+99b, LSZ+99a, LSZ+00, LSZB00, MCG+08, MRS+99, Mat64, Mez96, MP97, MG23a, NAY+08, NBS10, Nic11, OS05, Oli12, Oni12, Oni15, OO82, Pyy78, QSG98, Ryc98, SBM+01a, SBM+01b, SB02, SBA+03, SB03, SBC+03, SBCT04a, SBCT04b, SBK04, SO05b]. **Chemistry** [SB05, SBLJ05, SB06, SB07, SBSL08, SBK+08, SBGJ08, SBC09b, SB09a, SBC09a, SBC10, Sab11, SB11, SB12a, SB13a, Sab15, SB17a, SB18a, SSCL97, SBK15, Sut98, Tap17, VWOS89, BB21, Dra20, Fro02, Hog14, HO16, LÖS02, NBA20, SCT15, SCT16, SB17b]. **Chiral** [LDP+04, QSW20]. **Chirality** [CL05]. **Chirped** [CM24, MCP12, ML18]. **chromium** [CCL03]. **Chromophore** [BHM17]. **CI** [Ave98, BE01, Har18, PB75, RSP21, Rui23, TR98]. **Circular** [CE72, PR05]. **Circulenes** [SKT+03]. **Cl** [RAR+08, CTSSO19, RRMAF08]. **Cl-Atom** [RAR+08]. **Classical** [AdMB99, GMB04, HM19, MT04, Per20, PS05b, PSAP10, Sig05, Sim99, WDD16, BPK23, EW03]. **Classical-quantum**

[Per20]. **Classification** [FHHE82]. **clean** [SH19]. **close** [JS21]. **close-coupling** [JS21]. **Closed** [Bra77, Cru09c, JSF08, KRL01]. **Closed-** [Bra77]. **Closed-Shell** [JSF08]. **Closed-Subshell** [KRL01]. **Cluster** [Ada97a, Bra77, Cam12, CL00, FP06, GEO91, HJ99, HS86, KE97, KE00, KB86, KMR01, LEK01, LGJP99, MDBM98, MH98, MP89, MMSK16, MSM17, OTA97, OYI^{+}00, PJH05, PM16, PB99, RR05, ST17, SB99, SIY^{+}19, SG80, WN05, YKS^{+}12, BPK23, CCM^{+}19, EÜSB21, Fuk03, GWW19, GPEB21, Köv03, LMK19, MKB04, MK23, TMK21, TM21]. **Clusters** [BHV^{+}00, Bor03, CMVPFC16, EGCL91, HL97, HOI^{+}08, ILS08, Kap98, KRL01, KIHA97, LJ17, MLR^{+}98, RK04, RMMP17, Saa01, Tak19, EOH03, Fuk03, LSZ^{+}97a, STO^{+}00]. **CO** [HB14, Hog21, HDFT24, KBH23, SNMI00, CMVPFC16, FU00, NHYU03, Yam03]. **Co-** [NHYU03]. **Coalescence** [KNN17]. **Code** [SGM^{+}13]. **Codes** [Pau13]. **Coefficient** [MYM08]. **Coefficients** [ASGG08, HJ99]. **Cognition** [SS17]. **Cognitive** [Sri01]. **Coherence** [TS10, CM24]. **Coherent** [GP04, Ram98, RAR15, Wei04, WMM^{+}98]. **Coinage** [BU97]. **cold** [ŻM23]. **Collective** [BS72, SCE19, JJ20]. **Colliding** [Saa01]. **Collinear** [Per98b]. **Collision** [Les75, MMM19, Tők19]. **Collisional** [BKB^{+}19, MHWvdA97]. **Collisions** [AGMdV^{+}13, Bel09, BMM13, BR17, BB14, CHR13, CCSZ01, DGKCT15, FAS^{+}98, FJS^{+}04, KMHL13, Kle77, LK13, Mic74, MF04, MM13, RGFC13, SCTH^{+}07, Bel21, Bel22, JS21, TBM01, ŻM23]. **Colour** [VTM98]. **Combinations** [LDNP99]. **Combined** [KBS03, LGJP99, TMN10, TL10, MKK^{+}01]. **Combining** [MP97, SBC10]. **Combs** [MCP12, ML18]. **Comment** [Miy03]. **Communication** [Nal09, NSM11]. **communications** [Nal23]. **Compact** [HS05, VT24]. **Companions** [Cra99]. **Comparative** [BRL13, GV09, JJD05, KIT^{+}08]. **Comparison** [BKC68, LvWH^{+}01, Löw98, PS05a, QGW01, RR05, Sau05b]. **Competing** [Dur20]. **Competition** [PMK23]. **competitive** [SCJ^{+}23]. **Complete** [CCA13]. **Complex** [Byl98, DST^{+}03, LBH^{+}17, Löw88b, LFM89, NeMM03, Nes75, STZY18, SIY^{+}15, SIY^{+}19, Ste73, YAJHR03, YTF78, ALA21, ALA23]. **Complexation** [ARS99]. **Complexes** [DB68, JA07, Mam19, MYW00, MHWvdA97, YFK^{+}97]. **Component** [SW98, YZDM01, Bar23]. **Components** [AGO07, QSG98, BB22a]. **Composed** [PTC^{+}13]. **Composition** [MKK^{+}00]. **Compounds** [AVB08, Ber74, GAI08, HSR98, IFAY08, LvWH^{+}01, MYM08, Sey12, YM97, dLHD10, KOT^{+}00, TMM03]. **Compton** [KS77, OE17, ÖEO23, VG22]. **Computation** [BR65, CTS04, Nic10, RGFC13, EÜSB21]. **Computational** [BBB10, Duc97, LDP^{+}04, Mar08b, NAY^{+}08, OO05, RRMAF08, ST17, San98, SBK15, Tur07, LSZ^{+}97b]. **computationally** [Wen21]. **Computations** [AH19b, Ano04l, Har18, LBV01, MRS^{+}99]. **Computer** [FMA08, GBPSR10, MFMCN01]. **Computer-Algebraic** [FMA08]. **Computing** [Bis19, BPK23]. **Concentrated** [FIK^{+}03]. **concept** [JJ20]. **Concepts** [GDL98, SCT15, SCT16, vL03]. **Conceptual** [Kar08]. **concerted**

[Hes22]. **Concluding** [Uda97]. **Condensate** [DB01]. **Condensed** [Ber03, Kar97, TMN10]. **Condition** [CCC17]. **Conditions** [KNN17, Bel22]. **Condon** [AHPD$^+$03, AHPD$^+$03, Pal04, SP99]. **conduction** [JJ20]. **Conductive** [TY85]. **Conductors** [KTMA08, Oni15]. **Conference** [Ano97a]. **Configuration** [ATL$^+$18, AA03, Bel19, Bun18, EEL96, EM17, GC92, LHL18, RMMP17, RP18, RT18, SS99, CAG$^+$21, SKS$^+$19, WLM23]. **Configurations** [MFLK11, WD70]. **Confined** [Aqu09, Bad09, BC09, CTO18, CKC09, CLK15, DO09, GV09, GVFG09, Lau09, LK09, MFLK11, PV09, SPM09, SCM09, SBC09b, SBC09a, WD22]. **Confinement** [Cru09c, LKD05, BLC23, MBAPS19]. **Confirming** [Fuk15]. **Conformation** [HZ89]. **Conformational** [HSR98, Pul77]. **conformations** [GC01]. **Conformers** [SDGW98]. **Conical** [Pet98]. **Conical-Intersection** [Pet98]. **Conjugate** [Gos02b]. **Conjugated** [Nal09, RPSB00, SD04, TY85]. **Conjugation** [SS03]. **Conjunction** [Ano08h, ILS08]. **connected** [TM21]. **Connection** [AdMB99, BVHK03, Gut06, MC10, NFW$^+$98]. **Conoidal** [LK09]. **conscious** [Per20]. **Consequences** [Coo18]. **Considerations** [Mar08a, MG20]. **Consistency** [DDPC95, Per90]. **Consistent** [DKMP98, GDL14, Sla72, VWP$^+$98, WD70, LJKH13, LSC19, Ort22]. **Constant** [Nal00, SS22]. **Constants** [DE05, Gon98, Kar08, LvWH$^+$01, Moh98, RM04, SPAS05]. **Constrained** [GM17, Lev90, DAB$^+$23, Zap01]. **Constrained-Search** [Lev90]. **Constructed** [SW98]. **Construction** [KS97b, SO19c]. **Contact** [MFCT15]. **contacts** [MOB$^+$03]. **Contemporary** [Sla81]. **Contents** [Ano67b, Ano68b, Ano70b, Ano72b, Ano73b, Ano74a, Ano75a, Ano77a, Ano78a, Ano80a, Ano81a, Ano81b, Ano82a, Ano82b, Ano85a, Ano98b, Ano98c, Ano01a, Ano01b, Ano01c, Ano03b, Ano03c, Ano04b, Ano04c, Ano04d, Ano05a, Ano05b, Ano05c, Ano06a, Ano07a, Ano08a]. **continuous** [NBS10, NBS12]. **Continuum** [ABC$^+$98, BRL13, Cam12, JGCRC16, Jør74, KGW98, LJKH13, MFA21, Nic17, OOSS17, TS10, CTSSO19]. **Contracted** [VTPR97, VdLCPT98]. **Contribution** [MYM08, ST07, JMWG19]. **Contributions** [FAS$^+$98, OOSS17, Ram08, CTSSO19]. **Contributors** [Ano64b, Ano64d, Ano65b, Ano65d, Ano67c, Ano67e, Ano68c, Ano68e, Ano70c, Ano70e, Ano72c, Ano72e, Ano73c, Ano73e, Ano74c, Ano75c, Ano77b, Ano77d, Ano78c, Ano80b, Ano80e, Ano81c, Ano81d, Ano81i, Ano81j, Ano82e, Ano82c, Ano82d, Ano85b, Ano85c, Ano88b, Ano89b, Ano90a, Ano91a, Ano92a, Ano92b, Ano94b, Ano95a, Ano96a, Ano97b, Ano97c, Ano98g, Ano98h, Ano98i, Ano98f, Ano98d, Ano98e, Ano99b, Ano99c, Ano99d, Ano99e, Ano00a, Ano00b, Ano01d, Ano01e, Ano01g, Ano01f, Ano01h, Ano02, Ano03d, Ano03e, Ano03f, Ano04e, Ano04f, Ano04g, Ano05d, Ano05e, Ano05f, Ano06b, Ano07b, Ano08b, Ano08c, Ano08d, Ano09a, Ano09b, Ano09c, Ano10a, Ano10b, Ano11a, Ano11b, Ano12a, Ano12b, Ano13c, Ano14a, Ano15a, Ano15b, Ano16a, Ano17a, Ano17b, Ano17c, Ano18a]. **Contributors** [Ano19c, Ano19d, Ano19e, Ano20a, Ano20b, Ano21a, Ano21b, Ano22a, Ano22b, Ano23a, Ano23b, Ano24a, Hog13c, Hog18c, SB13b]. **Control**

[Kra99, ML18, MM99, CM24]. **Controlled** [ALND10, ST17]. **Conundrums** [Cal13]. **convection** [Nal23]. **Convergence** [Bas78, CÅ01, DDPC95, KMJ97, OB23, SW98, Sil14, VWP^{+}98, BG23]. **convergent** [SÁ23a]. **Cooling** [Phi98]. **cooperation** [SBK^{+}08]. **Cooperative** [Chi03, GWM^{+}03, NP03]. **Coordinate** [Lev90, TAM04, DAB^{+}23]. **Coordinates** [ACC99, Byl98, Har05, KO18, MFA21]. **Coordination** [Ber74]. **Copper** [HB14, MYW00, TP03, YFK^{+}97]. **Copyright** [Ano64c, Ano65c, Ano67d, Ano68d, Ano70d, Ano72d, Ano73d, Ano74b, Ano75b, Ano77c, Ano78b, Ano80c, Ano81e, Ano81f, Ano82f, Ano82g, Ano85d, Ano86a, Ano88c, Ano89c, Ano90b, Ano91b, Ano92c, Ano92d, Ano94c, Ano95b, Ano96b, Ano97d, Ano97e, Ano98j, Ano98k, Ano98l, Ano99f, Ano99g, Ano99h, Ano08e, Ano08f, Ano09d, Ano09e, Ano09f, Ano10c, Ano10d, Ano11c, Ano11d, Ano12d, Ano12c, Ano13d, Ano14b, Ano15c, Ano15d, Ano16b, Ano17d, Ano17e, Ano17f, Ano18b, Ano19f, Ano19g, Ano19h, Ano20c, Ano20d, Ano21c, Ano21d, Ano22c, Ano22d, Ano23c, Ano23d, Ano24b, Hog13d, Hog18d, SB13c]. **Core** [CS04, FVB99, OTA97, PGV97, CCM^{+}19, FB20, MKK^{+}01]. **Core-and-Bond** [CS04]. **Core-electron** [PGV97]. **Core-Hole** [OTA97]. **Correct** [LRCR98, Bel22]. **Corrected** [JGCRC16, LBV01, LRCR98]. **Correction** [AHPD^{+}03, Per90, Por04, LSC19, YNNU03]. **Corrections** [DKMP98, EM17, LT98, PEZB98, PSS98, SJO05, YZDM01, VG22]. **Correlated** [DBC17, HA13, Har17, Hät05, MS03, MS65, NA19, Ryc98, SBH^{+}20, Sau05b, SS99, SM23, SA23b, SCJ^{+}23, Tew21]. **Correlation** [AH19b, BŚG17, HS86, HB14, HM21, IL98, JSF08, Kap98, KB98, KD11, KvH99, LBV01, MW98, MP89, Nes98, She15, Sla72, ŚBG14, SCN03, SDGW98, UK05, VWP^{+}98, HO16, ORL23, SO19c, VdLCPT98]. **Correlations** [DB01, DB13, Gre98, OYI^{+}00, BFHS23, WD22]. **corresponding** [LPC24]. **Cosine** [AFE13]. **Cost** [GDL98]. **Cost-Effective** [GDL98]. **Coulomb** [Ave13, AA18, BH24, CCA13, DGA18, GAM^{+}13, GW23, Har04, KO18, LT98, LPC24, LJ17, Rui23, Sil14, SSS05]. **Coulomb-Breit** [LT98]. **Coulombic** [KNN17]. **Coulson** [SPH14]. **Coupled** [BPK23, Cam12, CCSZ01, FP06, GEO91, HJ99, HS86, KB86, LEK01, Les75, LGJP99, MDBM98, MH98, MFCT15, MKB04, MMSK16, MSM17, PM16, PB99, RR05, RMMP17, SB99, WN05, BB21, CCM^{+}19, EÜSB21, GPEB21, LMK19, MK23, TMK21, TM21, PJH05]. **Coupled-Channel** [Les75]. **Coupled-Cluster** [Cam12, FP06, HJ99, HS86, KB86, LEK01, MH98, PB99, SB99, WN05, BPK23, MKB04, EÜSB21, MK23, TMK21, TM21]. **Coupled-Cluster-Theory** [PM16]. **Coupling** [ÅVM96, BVHK03, Chi03, DE05, ERC88, Kry03, MRS^{+}99, Nal00, PB05, RM04, SPAS05, BMR^{+}24, JS21, SBC^{+}03]. **Couplings** [CPBS05, Lon99, SPAS05, SKS^{+}19]. **Cousins** [RK04]. **Covalency** [BFHS23, OYI^{+}00]. **Covalent** [She15]. **CPMD** [PWZ^{+}08]. **CPU** [LH20]. **Cr** [ADA03, IOA03]. **CrF** [MKK^{+}01]. **Criterion** [Per17]. **Critical** [BB99b, CCC17, HK03, IKN^{+}08, ZZ08]. **Cross**

[CTSDÖ04b, CTSDÖ04a, HMH^{+}18, Jos08, LC03, PBK04, RGFC13, MG22]. **Cross-caps** [LC03]. **Cross-Sections** [PBK04]. **Crossing** [SH95]. **Crossover** [LPDB03, NeMM03]. **Crystal** [ADA03, Jan65, MYW00, KC19]. **Crystalline** [HOI^{+}08]. **Crystals** [AAM04, ABGM03, BJV86, Chi03, GWM^{+}03, Jan65, KSY08, YKY^{+}00, IOA03]. **Cs** [BJMB14, BMPV99, APNM03, SSS05]. **CSCH** [SSS05]. **CSDA** [AGO07]. **CSDA-Ranges** [AGO07]. **Cu** [SMAS08, ARS99, FU00, Fuk03, KC19, Mam19, NHYU03, SHBC19, UJYU03, WHB^{+}24, YNNU03]. **Cu-** [NHYU03]. **Cubic** [APNM03, AHPD^{+}03, ABGM03, HJ99]. **Cuprate** [DB01]. **Cuprates** [Fuk15, Kri03]. **Current** [Del74, Har04, Kho04, OW08, SBSL08]. **Currents** [CPBS05, FTG22]. **Curve** [SH95]. **Curves** [HBT^{+}00, MCM14, MMSK16, MSM17, LMK19, SM23, TMK21]. **cusp** [LSC19]. **Cyanide** [ARS99]. **Cycloadditions** [RGA99]. **cyclobutanone** [MFMCN01]. **Cyclodextrin** [DNM^{+}14, RMN^{+}14, dLHD10]. **Cyclohexenone** [GBHM14]. **Cylindrical** [LKD05]. **Cytosine** [MBM99].

D [BRW08, SRZE04]. **D'Alembert** [Per17]. **Dalton** [BND81]. **Damage** [BB13, BB15, CL07, Tur07, vS07, SS22]. **Damages** [ST07]. **Darwinian** [BP20]. **Darwinism** [Brä22]. **Data** [KS97b, OO05]. **Dawn** [KvH99]. **DC** [KGI^{+}19, SD04, dLHD10]. **deactivation** [Dur20]. **Decades** [GMP98, KKK^{+}97, Nor98]. **Decay** [AK12, Gre08, KS88, MTA00, RF13, TMMS10, UYT97]. **Decoherence** [MCP12]. **decomposing** [Hog23c]. **Decomposition** [MC10, PL98]. **Decoupling** [NSM11]. **Dedication** [Ano96c]. **Defects** [Kuk14, MAS03]. **Definition** [Yas23]. **Deformations** [Kuk14, SIY^{+}19]. **Deformed** [KMR01]. **Degenerate** [SBDD03, AR03]. **Degrees** [Nal06]. **Degrees-of-Freedom** [Nal06]. **Del** [LSZ^{+}99a]. **Delocalization** [MFCT15]. **Delocalizations** [LR72]. **Delocalized** [Nal09]. **Delocalized/Conjugated** [Nal09]. **Dense** [DTC04, SPAS05]. **Densities** [AAAC04, BLKS78, TM13]. **Density** [AdMB99, ARS17, BR05, BK70, Bro98a, Bro98b, BŚG17, CDBG00, CD05, Cio90, CS77, Cru09c, Dah01, DR90, EG99, EEL96, Fuk15, GW17, GDL98, GBHM14, Gon98, GL90, GK90, Har90, HBT^{+}00, HL90, JGCRC16, Kho04, KMHL13, KS90, KB98, Kry81, LBV01, Lev90, LS03, LDNP99, Lon99, LSZT90, LSZ^{+}98a, LK90, LLBK^{+}98, MRS^{+}99, MTS04, McW98, Mic99, MT04, MNR^{+}98, Min22, MYM08, MOB^{+}03, Nag97, Nal00, Nal03, Nes03, Noo09, Öhr02, Oli90, PKYM01, Per98a, Per90, PEZB98, PGP17, PL98, RPSB00, RTV05, RP72, SRZE04, SS90, ŚBG14, UJYU03, VKI97, VRG90, WT99, WmG18, Yan90, YZDM01, vL03, BSL^{+}19, GTB23, VdLCPT98, Zap01]. **Density-Based** [WmG18, BSL^{+}19]. **Density-Dependent** [ŚBG14]. **Density-Functional** [EG99, Lev90, LS03, SS90, Min22]. **Density-Gradient** [KS90, PEZB98]. **Density-Matrix** [PKYM01]. **Dependence** [CDK15, FPL97, GP14, HK03, HBKS03, Ono00, ZLL^{+}20]. **Dependent** [ARS17, BBB10, GK90, HG17, JGCRC16, KMHL13, LHL18, Lin17c, Löw67c, MKN10, MCA^{+}18, Öhr15, Öhr17, ŚBG14, VTM98, WT99, LSZ^{+}99a, LSZB00, NA19, PS21, WLM23]. **Deposition** [CTS04, CTSDÖ05, CTCS05, CMJR+04, MBO+07, Sab97, Mic22]. **Deprotonations** [LDP+04]. **Depurated** [MMM18]. **Derivation** [FMA08, LK90, WN05]. **Derivative** [BB21, BB22a, IL98, Per90]. **Derivatives** [Cam12, HJ88, LDB95, WN05]. **Derived** [AAAC04, ŚBG14]. **Described** [Cam12, YTC+05]. **describing** [Hog23c]. **Description** [ABC+98, HL97, HS86, Sla81, Sut01, WD70, Nal23]. **Descriptions** [FVB99]. **descriptors** [BSL+19]. **Design** [Oli12, Oni15]. **Detachment** [ZDZO11]. **Determinant** [ATL+18, CAG+21]. **Determination** [ASGG08, SOS13, SSV98, SKS+19]. **Determine** [Fuk00]. **Determined** [Eks98, SBF+08]. **Determining** [BWK97, KS88, LASV18, Sme99]. **Detonation** [PM14]. **Deuteration** [LGK+99]. **Deuterium** [LJK+08]. **Development** [BMPV99, LDP+04, Nik70, OW08, OO05, TMN10, LH20]. **Developments** [Ber74, EEL96, HBE64, I'H64, LLBK+98, Pet98, SS98, San98, Sid18, SGM+13, TAM04, CCT02]. **DFT** [ABGM03, AR03, CKC09, KT15, LS07, Mam19, PS21, SKGŚ23]. **DFTB** [dLHD10]. **DFTB/UFF** [dLHD10]. **DH** [BMR+24]. **Diabatic** [TA04, Tap09]. **Diagnosis** [BSL+19]. **Diagnostics** [BB11, BB21]. **Diagonal** [DB13]. **Diagrammatic** [PČ75]. **Diagrams** [Sal74, SH95, WP06]. **Diamagnetic** [CE72, CPBS05, Vis05]. **Diamide** [HSR98]. **Diamond** [MTS04]. **Diaqua** [MYW00]. **Diastereoselectivity** [RGA99]. **Diatomic** [BC80, IS01, KGW98, Kob97, KK85, MK18, OO05]. **Dibromo** [MYW00]. **dications** [SM22]. **Dichroism** [CE72, PR05]. **Dielectric** [HL90, MTS04, MM13, AA19, VG22]. **Difference** [IS01, QGW01]. **Different** [LvWH+01, PS05a, CCT02, WLM23]. **Differentiability** [LS03]. **Differential** [FH65, SGB16, Ber02]. **Differentiation** [NSM11]. **Diffraction** [CS77]. **Diffusion** [FIK+03, TAU17]. **Difluoride** [MYW00]. **Dihedral** [CLK15]. **Dihydrates** [HTS+00]. **Dilated** [MM96]. **Dimensional** [CCA13, KMR01, RA19, SPD09]. **Dimensionally** [FCH15]. **Dimensions** [Ros98]. **Dimer** [BHM17, MCG+08, ORL23, SCJ+23]. **Dimers** [BU97]. **Dimethyl** [Fuk08b]. **Dimethylamine** [SSV98]. **dioctyloxyphenyl** [YKY+00]. **Dioxide** [PM16]. **Dioximato** [YKY+00]. **Dipolar** [RGA99, SJO05]. **Dipole** [AB73, BO86, CTO18, CCM05, JMWG19, OOSS17, PS05a, RM04, CTSSO19, PS21]. **Dipole-bound** [JMWG19]. **Dirac** [BH24, Cru09c, Lin02, Öhr16, QGW01]. **Dirac-Weizsäcker** [Cru09c]. **Direct** [DDPC95, GDL14]. **Directly** [Sal74]. **Discontinuity** [CTO18, Per90]. **Discotic** [YKY+00]. **Discoveries** [Wyb97]. **Discrete** [EG99, OW08, SGB16, SYIY03]. **Discussion** [KT15]. **disorder** [OTA03]. **Disordered** [Kar97]. **Dispersion** [HJ99, VG22]. **Dissimilarity** [SNM+97]. **Dissipative** [Brä02, Mic22]. **Dissociating** [Sut01]. **Dissociation** [BWH08, BŚG17, Hog18e, BLC23]. **Dissociative** [SSS05]. **Distances** [TTLB04]. **Distorted** [Bel22, BRL13, LK13, RGFC13]. **Distortion** [ITI+00, Kat03]. **Distortions** [LM03]. **Distortivity** [Fow03]. **Distributed** [GW01, MW98, QGW01, WM97]. **Distribution** [BWK97, CTSO04, OE17].

Distributions [CS77, KS77, AP03]. **Disulfide** [PM16]. **divalent** [FB20]. **DNA** [AGO07, CL07, Coo18, FB20, JA07, Krs16, KN01, Lad73, LS07, Löw65c, SOS11, Sim07, vS07]. **Do** [SS17]. **Does** [Tak19]. **domains** [Tew21]. **Doped** [CY00, HDB03, SCN03, TP03, Hog21, IOA03, Ito03]. **Dosimetry** [PGJ07]. **Dots** [SPD09]. **Double** [MCM14, PLA01, Bel22, SM22]. **Double-Barrier** [PLA01]. **Doubles** [HS86, LGJP99]. **Doublets** [DeB09]. **downfolding** [BPK23]. **Driven** [BGG+07, SBH+20, WLM23]. **Droplets** [GNM08]. **Due** [FU00]. **Dunham** [OO05]. **During** [UYT97, MU03]. **DV** [Ada97b, Ada00, CL00, FSB+97, Fuk03, Fuk15, Gut97, IFAY08, Kaw97, KNM+08, LSZ+00, MYW00, MW08, MKK+00, Mur08, Nak00, NHYU03, OTA97, Ros97, SBA+03, SBK+08, SNMI00, Tan00, UMD08, YFK+97]. **DV-X** [Ada00, CL00, LSZ+00, MYW00, MKK+00, Nak00, SBK+08, SNMI00, Tan00]. **dye** [GTB23]. **dye-sensitized** [GTB23]. **Dyes** [BMPV99]. **Dynamic** [FAS+98, NeMM03]. **Dynamical** [AAM04, Brä04, CTSDÖ04a, NP03]. **Dynamically** [ILS08]. **Dynamics** [ACC99, BR82, BHV+00, BJV86, CTSDÖ04b, CMJR+04, DW98, För94, GMB04, HHK+98, HS19, HG17, HPRR10, HBGvM19, IBB+19, ILS08, JGNJ08, KD11, MCG+08, Mat96, Mic17, PWZ+08, RFG+98, Saa01, Sab97, SGM+13, TA04, dLHD10, GTB23, Mic02, Mic22, MFMCN01, NTT20, SBH+20, WLM23].

E-Hy-CI [RSP21]. **E-learning** [MP22]. **Early** [BB11]. **Earth** [KRL01, STO+00]. **Easy** [Col68]. **Eckart** [YTC+05]. **Economical** [BR65]. **Edaravone** [RMN+14]. **Edge** [KsKsN08, MYW00, OTA97, YFK+97, CCM+19, NHYU03]. **Edited** [Ano90c]. **Editorial** [Ano88d, Ano89d, Ano91c, Ano92e, Ano92f, Ano95c, Ano96d, Ano97f, Ano97g, Ano98m, Ano98n, Ano98o, Ano99i, Ano99j, Ano99k, Ano01i, Ano03g, Ano08g, Ano09g, Ano09h, Ano10e, Ano10f, Ano11e, Ano12e, Ano19i, Hog13e, Ano13e]. **Editors** [Ano82h, Ano94a, Ano98a, Ano08l, Ano08n, Ano09i, Ano09j, Ano10g, Ano10h, Ano11f, Ano11g, Ano12i]. **educated** [SÁ23a]. **educational** [Kar02]. **Effect** [ADA03, BP82, BO86, Chi03, FE97, GWM+03, GBPSR10, HBKS03, ITI+00, KT98, MCC03, NM00, NP03, OTA97, Por04, SKT+03, SCM09, Sjö04, SCN03, VWP+98, NA19, WHB+24]. **Effective** [CHSC03, GW18, GDL98, KKGG98, MMM18, Mic74, Nag01, MMM19, SKGŚ23]. **Effectiveness** [AFE13]. **Effects** [AB73, ABC+98, BMPV99, Bas64, BS04, Bic13, BB14, BŚG17, CTSDÖ05, CTO18, CHSC03, CC97, DKV+19, ERC88, Fuk00, GMLSC+10, GM17, GC01, GVFG09, IKN+08, Jør74, JGNJ08, KH03, KD11, KBS03, Laz04, LGK+99, OYI+00, Ono00, Pet98, PSAP10, PGN04, RM04, SIY+19, SDGW98, TS10, UK05, WDD16, AA19, Kar24, SS22, VdLCPT98]. **Effects-Selected** [CHSC03]. **Efficient** [PTBH13, BG23, KBH23]. **Eigenfunctions** [Sal74]. **Eigenstates** [RP72]. **Eigenvalue** [YTF78, Gos02b]. **Eight** [LPC24]. **Einstein** [McW99]. **Ejection** [Sim99]. **Eka** [LvWH+01].

Eka-Lead [LvWH$^+$01]. **Elastic** [HHU$^+$21, SJAB$^+$22]. **Electric** [FPL97, IS01, KGI$^+$19, LDB95, Laz04, LHL18, SJO05, UK05, YÖ13]. **electrical** [BLC23]. **electrode** [KTA03, SYIY03]. **Electrodes** [OBHM17, KTA03]. **electrodynamic** [PMK23]. **Electrodynamics** [MDÖ05, Moh98, Sal11, Sau05a, SBG$^+$98, SAL10, SGK$^+$08]. **Electromagnetic** [BGG$^+$07, IBB$^+$19]. **Electron** [Ada00, AGO07, AYÖ17, Ave98, Ave13, BGG$^+$07, BL18, BS72, BC80, CTSDÖ04b, CO17, DBC$^+$99, DSR81, FH65, FJS$^+$04, Gal73, HHK$^+$98, HUS$^+$11, HPU$^+$17, HMH$^+$18, HS05, HSS$^+$04, HS86, HB14, HO16, HM21, Hyl64, JA07, KS88, Kap98, Kle77, KDG97, KD11, KvH99, LT98, LJ17, LK13, LR72, Lon99, Lyk64, MLPD$^+$98, MM96, MA04, MTA00, MSM17, NA04, Nes75, Nic17, NM03, OYI$^+$00, OM03, Ohn67, ÖB81, Ort99, PKYM01, RP72, RLF17, Sab97, Sal74, STZY18, SPM09, Sim99, Sim05, SHBC19, SSS05, SGK$^+$08, SS04, SGM$^+$13, SCN03, SDGW98, TM13, UK05, Yea05, ZDZO11, ZP17, AO03, AP03, Bel19, Bel21, Cru09c, FCAG19, GTB23, GPEB21, IOA03, Lar02, LSC19, MOB$^+$03, MU03, Ort22, PGV97, Rou20, SBH$^+$20, SPD09, WLM23]. **Electron-** [NM03]. **Electron-Capture** [MTA00, Bel21]. **Electron-Driven** [BGG$^+$07]. **Electron-Impact** [HMH$^+$18]. **Electron-Ion** [LJ17]. **Electron-Nuclear** [CTSDÖ04b]. **electron-nucleus** [LSC19]. **Electron-Pair** [TM13]. **Electron-phonon** [SHBC19]. **electron-positron** [AP03]. **electron-propagator** [Ort22]. **Electronegativity** [OPPZ06]. **Electronic** [Ada97a, ADRAB16, AB73, AH19b, AR03, AK12, BVHK03, Bas64, Bas78, BS04, BJMB14, BWK97, Bra67, CTO22, CD05, CMDN89, CCCC15, CY00, CL00, CCL03, CSZ99, Dau64, DO09, DA14, DB01, DB13, DBC17, EGCL91, EOH03, FP06, FCH15, FE97, Fuk00, Fuk15, GTB23, GSTvE98, GM91, GVFG09, Har18, HJ88, HOI$^+$08, HTS$^+$00, Hog13g, Hog14, Ito03, Jan97, KM98, KIT$^+$08, Ker82, KIHA97, KNI$^+$08, KC19, Kot68, Köv08, KE97, KE00, KTA03, Kuk14, LM97, Lin17a, LSZ$^+$97a, MC10, MTS04, Mic99, MKH$^+$97, MYM08, MMSK16, NIO03, Nal03, Nal06, Nal23, OTA03, PR05, PB75, PB99, PP68, RPSB00, SS98, Sal74, ST78, SNM$^+$97, Shi12, SNIM08, SMAS08, TY85, Tap01, TA04, Tap09, YKS$^+$12, YM00, AO03, BSL$^+$19, KOT$^+$00, LSZ$^+$99a, LSZB00, MMM22]. **electronic** [SCE19, SKS$^+$19, YIYM03]. **Electronically** [MT04]. **Electrons** [ACDK72, BG73, FVB99, She15, Sim07, Suc98, ST07, AA19, NBA20, SJAB$^+$22, SM23]. **Electronuclear** [TA04]. **Electrostatic** [Jør74, PTBH13, ST78, FSP23, ŻMM23]. **Element** [AAE$^+$01, BS05a, Fuk15, SGB16]. **Elemental** [ASGG08]. **Elementary** [CDP82, Gre08, MCG$^+$08]. **Elements** [CD05, KE98, KRL01, MTA00, RP72, Bar23, TMM03]. **Elliptic** [PS05b]. **Elpasolites** [APNM03]. **Elucidation** [Oni15, SIY$^+$19]. **Embedded** [KE97, KE00]. **Embedding** [LC03, LJKH13, OK11, MG21]. **Emerald** [IOI$^+$00, ITI$^+$00]. **Emission** [JGCRC16, Kaw97, MKK$^+$00, MTA97, SS04, Uda00, UMD08, Mur03]. **Emitted** [AVB08]. **Emitters** [BWVD$^+$13]. **Empirical** [BRL13, HSS$^+$04].

Employing [FP06, Kou15]. **Encaged** [Dol09]. **encoded** [BB22a]. **Endo** [RGA99]. **Endo/Exo** [RGA99]. **Endohedral** [CTO18]. **Energetic** [AGMdV+13, Ber14, CHR13, Kuk14, MF14, PGJ07, Sab14a, TR14]. **Energetics** [LYM03, PL98]. **Energies** [AGO07, Gal73, HMH+18, HL90, JSF08, LM03, PEZB98, PGP17, RR05, SOS11, SYM+08, VI01, ZDZO11, Bel22, CTSSO19, CTO22, CTC22, MKK+01, Ort22, PEMC23, SSO19, TBM01]. **Energy** [AJ04, Apo01, AL04, BB99b, Ber14, Bic13, LJK+08, Bun18, CTS04, CTSDÖ05, CTCS05, CMDN89, CMJR+04, CMVPFC16, DKMP98, DDPC95, GP91, GC92, Glu19, GS04b, HBT+00, HL90, IL98, Kho04, KSY08, KB98, Köv08, LBH+17, LJ17, Les75, LDNP99, LASV18, Mic22, MW98, MF04, MM13, MBO+07, MCM14, MMSK16, MSM17, Nak00, Nes75, Oli12, Per98a, PB14, PLA01, RGFC13, Sab97, SOS13, SPD09, SJO05, SOS15, SW98, Sim07, Sla64, SSS05, TMN10, Tők19, WN05, YZDM01, Bun23, GG20, Kar24, Lar02, LMK19, NA19, PGV97, SH19, SM23, TMK21, ŻM23]. **Engels** [Miy03]. **Engineering** [DO09]. **Enhance** [PB14]. **Enhancement** [LASV18]. **Enlarge** [MRS+99]. **Ensemble** [PGP17]. **Ensembles** [CDK15]. **Entanglement** [KO19]. **Entropy** [Kou15, Brä22]. **envelopes** [BB22a]. **Environment** [GBPSR10]. **EOMXCC** [PB99]. **EPR** [Coo18, TP03]. **equal** [NBA20]. **Equalization** [OPPZ06]. **Equation** [Löw85c, Löw98, MFCT15, MKN10, MKB04, Öhr16, QGW01, VTPR97, WN05, Yas17, BG23, BH24, ORL23, Yas23]. **Equation-of-Motion** [WN05, MKB04]. **Equations** [BE01, BS05a, Cal85, Kob97, LK90, Per17, SGB16, SKGŚ23, VdLCPT98]. **Equilibria** [KZR86]. **Equilibrium** [Spe78]. **Equivalence** [EBR92]. **Error** [Bun18, VWP+98]. **Errors** [KB98, Bun23]. **Estimating** [Apo01]. **Estimation** [Sey12, SIY+19]. **Ethanedione** [YKY+00]. **Ether** [Fuk08b]. **ethylene** [RZTSW23]. **ETOs** [AFE13]. **ETS** [ŻMM23]. **ETS-NOCV** [ŻMM23]. **Euristic** [ST78]. **eV** [AGO07, HHU+21, Sim07, WHB+24]. **Evaluating** [Hog18e]. **Evaluation** [AYÖ17, CB92, KS77, KNM+08, ÖÖ13, SB99, ALA23, BSL+19, MKK+01, Rui23]. **Even** [KGW98]. **Even-Tempered** [KGW98]. **Evolution** [Brä19, Löw67c, Tos08]. **Evolving** [SIY+15, SIY+19]. **Exact** [Bel06, BC09, DeB09, GC10, KB98, Kob97, KNN17, MRHdCK15, Ort99, SPM09, vL03]. **examined** [MG22]. **Examining** [Brä12]. **Example** [Lyo08, MCM14]. **Exchange** [Jan65, KB98, LRCR98, LDNP99, MRHdCK15, MF04, Sla72, ŚBG14, SCTH+07, Bel22, JS21, ORL23, SO19c]. **Exchange-Correlation** [Sla72, ŚBG14, ORL23, SO19c]. **Exchange-Energy** [LDNP99]. **Exchanges** [PLA01]. **Excitation** [ATL+18, Bel09, BLKS78, GP04, LM03, PGP17, RR05, SOS13, SOS11, SOS15, Tak19, AGS+19, CTSSO19, CTO22, CTC22, FCAG19, GJP23, Lar02, MKK+01, SSO19]. **Excitations** [FLV99, Kuk14, CCM+19, SCE19]. **Excited** [AB73, Hät05, HBKS03, KM98, LKD05, MT04, Nag97, Nag01, Oli90, PB99, RM04, Sme99, WN05, Dur20, MK23, Nag03, OB23, PS21, SZP21]. **Excited-State** [AB73, WN05, Dur20]. **exciton** [GJP23]. **existing** [BPK23].

Exo [RGA99]. **Exotic** [Ano08h]. **Expansion** [BR65, MKN10, MP89, Sil14, CAP19]. **Expansions** [AA01, FP06, FMA08, KS90, SPH14, Sid18, SCJ$^+$23]. **Experiment** [RC05, VWOS89, PMK23]. **Experimental** [ASGG08, BKC68, BLKS78, LGK$^+$99, Miy03, RAR$^+$08, ZBM98, Hog14]. **Experimentalist** [vS07]. **Experimentation** [LDP$^+$04]. **Experiments** [Ano08h]. **Explicit** [Vis05, SS22]. **Explicitly** [Ryc98, SA23b, SCJ$^+$23, Tew21, TM21]. **Exploding** [LJ17]. **exploration** [PB20a]. **Explored** [ABGM03]. **Exploring** [ORL23, WLM23]. **Exponential** [AA15, CB92, FP06, Hog13g, HM21, Nik70, ZP17]. **Exponential-Type** [AA15]. **Exponentially** [Har17]. **Expression** [PTBH13, SYM$^+$08, Yas17]. **Expressions** [Vis05, TM21]. **Extended** [BC00, Cal85, CDBG00, DB01, FP06, LK90, May80, Mon05, Uda00, Min22, Ort22]. **extended-Koopmans-theorem** [Ort22]. **Extending** [BBB10]. **Extension** [GVFR98, Lev14, RP18]. **Extensive** [LJK$^+$08]. **Extensivity** [EM17, SB99]. **External** [SD04, TA04, NA19]. **extremely** [MG21].

F [Kom05, CTSSO19, CCM05, UYT97]. **F12** [Tew21]. **Facility** [Ano08j]. **Factor** [LASV18]. **Factors** [AHPD$^+$03, SJO05]. **failure** [Sak03b]. **Family** [DLMS03, VT24]. **Far** [Eks98]. **Fast** [Ave13, Bel06, Bel09, BMM13, DeB09, LK13, SS04, Bel21]. **Faults** [FU00, UJYU03]. **Favorite** [FCC04]. **Fe** [CSZ99, ARS99, YNNU03]. **Fears** [Sut98]. **Features** [Kry03, Lin17a]. **Fermi** [Cru09c, CTC22, MYM08, SO19c]. **Fermion** [Per98a, LSZT90, PČ75]. **Ferroelectricity** [IKN$^+$08]. **Feshbach** [SW81]. **Few** [Har04, KO19, LT98, Mic17, Shi12, Mic02]. **Few-Atom** [Mic17, Mic02]. **Few-Body** [Har04, KO19, Shi12]. **Few-Electron** [LT98]. **Feynman** [FMA08, GM91]. **Field** [BVHK03, FPL97, FSB$^+$97, Glu19, GDL14, HG17, HPRR10, IBB$^+$19, JH99, Kob68, KGI$^+$19, Laz04, LJKH13, Nic10, Nic17, Per98a, PLA01, Sla72, WD70, EÜSB21, NA19, Ort22]. **Field-Assisted** [PLA01]. **Field-Free** [Nic10]. **Field-Induced** [Nic10, Nic17]. **Fields** [AAM04, DSW04, Gre08, IS01, SBG$^+$98, SD04, TA04, VRG90, BB22a]. **Fifth** [KB86]. **Fifth-Order** [KB86]. **Fifty** [Cra99]. **film** [KBH23]. **Films** [KsKsN08]. **Finite** [AAE$^+$01, BS05a, DR90, Fuk15, IS01, KCM70, OOSS17, QGW01, SGB16, WDD16, SKGŚ23]. **Finite-Difference** [IS01]. **Finite-Element** [AAE$^+$01, BS05a, SGB16]. **First** [Ada97b, CHR13, DA14, Fuk08a, Fuk08b, HPRR10, HBGvM19, IOI$^+$00, KIT$^+$08, KSY08, KG12, MTS04, MCC03, OYI$^+$00, PM16, Sak03a, WN05, Yam03, YKC$^+$08, KTA03, VdLCPT98]. **First-order** [MCC03]. **First-Principle** [HPRR10]. **First-Principles** [Ada97b, DA14, Fuk08a, Fuk08b, HBGvM19, IOI$^+$00, KIT$^+$08, KSY08, MTS04, OYI$^+$00, YKC$^+$08, Sak03a]. **Fischer** [CL05]. **Fission** [BHM17, SKS$^+$19]. **Fitted** [MRHdCK15]. **Five** [VT24]. **Floquet** [LMSP01, Pal04]. **Fluctuation** [Jeh65]. **Fluids** [CCCC15]. **Fluorescence**

[HBE+98]. **Fluoride** [UMD08]. **Fluorides** [TSON00]. **Fluorine** [SPAS05]. **Fluorine-Fluorine** [SPAS05]. **Fock** [BB99b, DKMP98, OE17, ÖEO23, BGW73, CBSM20, DAB+23, FCH15, GV09, GW23, Hur73, HMC73, LBV01, LEK01, LMK19, LFM89, LM92, May80, MMM18, MK18, MMSK16, Nes67, Sme99, TMK21]. **Fock-Space** [LEK01]. **folding** [LL20]. **Following** [AGS+19]. **footing** [NBA20]. **Force** [DSW04, Gon98, Krs16, PTLGOM12, Suc98, TTLB04, EÜSB21]. **Forces** [Kap98, LR72, MS67, Sal11, ST78]. **Forcing** [KSG08]. **Foreword** [Ano08i, Köv97]. **Formal** [Noo09]. **Formalism** [BMP03, CS04, Cru09c, GM91, Löw85c, MM13, OO05]. **Format** [Ano88a, Ano89a, Löw88a]. **Formation** [KV08, MCG+08, BMR+24, JMWG19]. **Forming** [ST17]. **Formulae** [SIY+19, Wyb97]. **Formulas** [ZP17]. **Formulation** [Lev90, MDÖ05, Yan90]. **Formulations** [MDBM98]. **formyl** [HDFT24]. **Foundation** [Brä19]. **Foundations** [CO17, Hal91, LK90, MG21]. **Four** [BMR+24, BL18, BMM13, GMP98, Har05, HA13, Har17, MYW00, Nor98, QSG98, RLF17, BMC97]. **Four-Body** [BMM13, Har05, HA13, Har17]. **Four-Electron** [BL18, RLF17]. **four-membered** [BMC97]. **Fourier** [AYÖ17, FCH15, Mon05, ÖÖ13]. **Fr** [BJMB14]. **Fractionation** [Lyo08, Mar08a]. **Fragmentation** [SCTH+07, ST07]. **Fragments** [GVFR98, ZDZO11]. **Frame** [YTC+05]. **Framework** [ATL+18, CCVB94, Gut97, LJKH13, Tap17, LT21, SKGŚ23]. **Franck** [AHPD+03, Pal04, SP99]. **Frank** [KT15, Ano03h, Kai15, SCT15, SCT16]. **Free** [KT15, Mat64, MFLK11, Nic10, TMN10, VKI97, vS07, GG20]. **Free-Energy** [TMN10]. **Free-Radical-Induced** [vS07]. **Freedom** [Nal06]. **Freeon** [Mat96]. **Frequencies** [BLKS78]. **Frequency** [MCP12, ML18]. **Friction** [TTLB04, BMR+24]. **Friend** [Lin99, OB22a, Öhr05]. **Froissart** [DeB09]. **Front** [Ano19j]. **frontier** [PEMC23]. **frustrated** [SPG+22]. **Full** [BE01, HS86, SED+98]. **Fullerene** [CKC09, KOT+00]. **Fullerene-like** [CKC09]. **Fullerenes** [CPBS05, Dol09, HDB03, Kat03, ZDZO11]. **Fully** [Bun23, CTG98, HA13]. **Function** [BMP03, DDPC95, FP06, KD11, MTS04, EW03]. **Functional** [ARS17, Bro98a, Bro98b, BŚG17, Cio90, Cru09c, DR90, EG99, EEL96, Fuk15, GW17, GDL98, GBHM14, Gon98, GL90, GK90, Har90, HBT+00, HL90, IL98, JGCRC16, KMHL13, KB98, LBV01, LRCR98, Len68, Lev90, LS03, LK90, LLBK+98, MRS+99, Mez96, MNR+98, Nag97, Nal03, Nes03, Noo09, Oli90, Oni12, Per98a, Per90, PGP17, PL98, RTV05, Rou20, SRZE04, SS90, VKI97, VRG90, WT99, Yan90, YZDM01, vL03, GTB23, LSZT90, LSZ+98a, MGAUP23, Min22, MPU19, MOB+03, Zap01]. **Functionals** [AdMB99, GP91, KB98, LDNP99, Löw96b, MRHdCK15, Nal00, vL03]. **Functioning** [KN01]. **Functions** [AFE13, BL18, BS05a, Bis67, BR65, BC00, BC09, CDBG00, CD05, CTG98, Dah01, Dau64, DGA18, FU00, GAM+13, GM17, Gil94, Har17, Har18, HPB17, KO18, Kla81, KNN17, LV90, Lev14, McG04, MS65, MFA21, Nes03, PS05a, PS05b, RMMP17, Ryc98, SJO05, SW98, SPH14, SNIM08, ZP17, ALA21, ALA23, LPC24, Per20, SA23b, TM21, VT24, VG22, Wen21]. **Fundamental** [DE05, GM05, Moh98, QSW20, SBF^{+}08]. **Fundamentals** [GM17, MNR^{+}98, Spe78]. **Further** [AFE13, TAM04, MG21]. **Future** [HKS90, OW08].

GaAs [Ito03]. **Gallium** [KSY08]. **Gap** [Cal85, IFAY08, SS90]. **Gaps** [Kri03]. **Gas** [BG73, HSR98, Jan65, MRS^{+}99, NA04, RAR^{+}08, HM19]. **Gas-Phase** [HSR98, MRS^{+}99, RAR^{+}08]. **Gaseous** [ASGG08]. **Gauge** [Woo98]. **Gaussian** [ALA21, BL18, DR90, Gil94, GW01, HO16, HPB17, KGW98, MW98, PTC^{+}13, QGW01, SW98, SA23b, WM97]. **Gaussian-Type** [DR90, SW98, ALA21]. **Geminal** [Wei04]. **Genealogical** [Sal74]. **General** [Brä08, CMDN89, Kry03, KNN17, LM92, LH20, Löw88b]. **Generalizations** [OPPZ06]. **Generalized** [AAG03, AAAC04, AA05, BLKS78, CTSOS99, FP06, GAM^{+}13, GJP23, HW01, I'H64, Mic15, MFA21, SED^{+}98, TA04, Tap09, Gos02b]. **Generated** [PTBH13, Sal74]. **Generation** [AAM04]. **Generator** [TAM04, DAB^{+}23]. **Genetics** [Löw65c]. **Gentleman** [SO19b]. **GeO** [GP14]. **Geometric** [Nal06, PB14]. **Geometrical** [HJ88, LDB95, SIY^{+}19]. **Geometry** [BHM17]. **GeV** [HHU^{+}21]. **Giuseppe** [LSZ^{+}99a]. **Giving** [PTBH13]. **Glance** [KG12]. **Glasses** [KE97, KE00]. **Glassy** [MKK^{+}00]. **Glycine** [SOS11]. **Gold** [BHV^{+}00, RK04, MOB^{+}03]. **Goldstone** [FMA08]. **Good** [Cra99, QSG98]. **Goscinski** [Ano04i, SBK04]. **Got** [SS17]. **GPCR** [ST17]. **Gradient** [FPL97, KS90, Laz04, LRCR98, PEZB98, SED^{+}98, YZDM01]. **Gradient-Corrected** [LRCR98]. **Gradients** [GC92, WN05]. **Grain** [Sak03b, OTA03]. **Grand** [CDK15]. **Graph** [Gut06, JH99, LC03, Yan81]. **Graphical** [LHL18]. **Graphite** [UMD08, KOT^{+}00]. **graphitic** [Mur03]. **graphitic-structured** [Mur03]. **Green** [BMP03, BC00, KD11, McG04]. **Green's** [DDPC95]. **Green's-Function** [DDPC95]. **Ground** [CMVPFC16, KM98, KT15, LPDB03, MS03, MW98, RM04, RT18, Bel19, Hog21, MK23]. **Ground-State** [KT15, Hog21]. **Group** [Col68, DSR81, LHL18, LB92, Mat78, RPSB00, Sme92]. **Groups** [DSW04, Gal73, KCM70, Mez96, Ray95, Ser74]. **GSI** [Ano08j]. **GTOs** [ALA23]. **Guesses** [Wyb97]. **Guide** [Öhr16, ZLC^{+}10]. **GW** [Mon05].

H [AGS^{+}19, BRW08, CSZ99, DLMS03, HOI^{+}08, Miy03, NeMM03, YKS^{+}12, CLK15, Hog18e, Hog21, LK14, MBAPS19, Sau05b, SH19, SSS05, SS04, SEL01, TM13, YIYM03]. **H-Bonding** [LK14]. **Hadron** [Pau13]. **Hadrontherapy** [Fra13]. **Hafnium** [KsKsN08]. **Haldane** [IFAY08]. **Half** [BB99a, Sme99]. **Halide** [Tak19]. **Halides** [Jan65, LF09]. **Halo** [DY08]. **halogen** [GC01]. **Halogens** [ASGG08]. **Ham** [Ano03h]. **Hamiltonian** [CHSC03, FTG22, LEK01, Löw85c, Löw88b, LFM89, Mic74, Öhr16, YZDM01]. **Harmonic** [AAM04, KMR01, LKD05, VTM98]. **harmonically** [WD22]. **Harmonics** [AYÖ17, AA01, AA15, CCA13, MFLK15, SR73]. **Harris**

[Kai15, SCT15, SCT16]. **Hartree** [BGW73, CBSM20, DAB+23, DKMP98, FCH15, GV09, GW23, Hur73, HMC73, LBV01, LFM89, LM92, May80, MMM18, MK18, Nes67, OE17, ÖEO23, Sme99]. **HBXYBH** [BMC97]. **He-like** [BH24, VT24]. **Heat** [MYM08]. **Heavy** [Ano08h, Bic13, KE98, NA04, RGFC13, Bar23, MKK+01, MMM22]. **HeH** [CLK15, SJO05]. **Heights** [PEZB98]. **helical** [Min22]. **helices** [GG20]. **Helium** [Aqu09, GV09, GW18, Kob68, KMJ97, PV09, SCJ+23, VT24]. **Helmholtz** [BS05a]. **Heme** [Kot68]. **Heredity** [Löw65c]. **Heterostructures** [Kra99]. **HF** [Kob97, MCM14, PS05a, Sau05b]. **Hg** [HHU+21]. **HgI** [BKC68]. **Hierarchical** [SPG+22]. **High** [AAM04, BB11, BB17, BS05a, LJK+08, Bor03, DTC04, DB01, DB13, DBC17, Hug98, KE98, Köv08, MF14, MM13, RGFC13, RSP21, San98, SPH14, SGK+08, Sva98, VTM98, Bel22, BB22a, Sak03b]. **High-** [SGK+08]. **High-Accuracy** [KE98]. **High-Energy** [Köv08, MM13, RGFC13]. **High-Order** [AAM04, BS05a, VTM98]. **High-Power** [Sva98]. **High-Precision** [LJK+08, RSP21, San98]. **High-Resolution** [BB11, BB17]. **High-T** [DB01]. **High-Temperature** [DB13, DBC17]. **Higher** [BB14, KNN17]. **Higher-Order** [KNN17]. **Highly** [Ano08h, Ano08j, HS05, LT98, Ram98, SS99, ŚBG14]. **HITRAP** [Ano08j]. **Hole** [NM03, OTA97, SS03, GJP23]. **Homogeneous** [LDNP99]. **homotopy** [JJ20]. **honor** [LSZ+99a]. **Honour** [SBK04]. **Hopes** [Sut98]. **Hot** [DTC04]. **Hubbard** [DAB+23, DB01, ORL23]. **Hückel** [BE04, I'H64]. **Hunches** [Wyb97]. **Hund** [KP77]. **Hy** [RSP21, RSP21]. **Hy-CI** [RSP21]. **Hybrid** [ATL+18, GMB04, MRHdCK15, EW03, Rui23]. **Hybridization** [BB99a]. **Hydrate** [HBT+00, MYW00, PWZ+08]. **Hydrates** [KKK+97, PWZ+08]. **Hydrazine** [RNL14]. **hydride** [CBSM20, YIYM03]. **Hydrides** [SKT+08, SYM+08]. **Hydrocarbon** [Bro98a, Bro98b, LF09]. **Hydrocarbons** [KH03, ZZ08]. **Hydrogen** [Aqu09, LJK+08, Bra67, CTO18, CLK15, DE05, EGCL91, FRM70, FCC04, FJS+04, GAI08, KO18, Kom05, KMJ97, Krs16, Lau09, LK09, LKD05, MC10, MFLK11, MW98, OOSS17, PV09, PWZ+08, SIY+15, YM97, YM00, Fuk03, Hog23c, HDFT24, JS21, KBH23, PMK23, SZP21, WLM23, YIYM03]. **Hydrogen-Antihydrogen** [FJS+04]. **Hydrogen-Atom** [KO18]. **Hydrogen-Bonded** [FCC04, GAI08]. **Hydrogen-Bonding** [MC10, PWZ+08]. **Hydrogen-like** [Lau09]. **Hydroxy** [SDGW98]. **Hylleraas** [Har05, Har18, Rui23]. **Hylleraas-CI** [Har18, Rui23]. **Hyperbolic** [AFE13, MFCT15]. **Hyperfine** [Bli65, EEL96, GMP98, Lon99]. **Hypergeometric** [CAP19]. **Hypergolic** [RNL14]. **Hyperguinones** [Mam19]. **Hypermatter** [Gre08]. **Hyperpolarizabilities** [HJ99, LÅJM95]. **Hyperquantization** [ACDV01]. **Hypershieldings** [LDB95]. **Hyperspherical** [ACC99, ACDV01, AA01, AA15, CCA13]. **hyperthermal** [HM19].

Icosahedral [JL03, LC03, SBDD03]. **Ignition** [RNL14]. **II**

[YKY$^+$00, BGW73, LFM89, LSZ$^+$98c, MYW00, NBS12, SIY$^+$15, SIY$^+$19, TP03, YFK$^+$97]. **III** [BG73, NeMM03, PM16]. **Illustrations** [JH99]. **Imaging** [BWVD$^+$13]. **Impact** [ARS17, HUS$^+$11, HPU$^+$17, HMH$^+$18, Heh18, KSG08, LJ17, SS04, ST07, MG22]. **Impenetrable** [Lau09]. **Implementation** [CTCS05, PM16, SGM$^+$13, LH20]. **Implementing** [TL10]. **Implications** [Brä12, JGNJ08]. **Implicit** [SS22]. **Importance** [LK90, AO03]. **Important** [BRW08]. **Improve** [PEZB98]. **Improvements** [AFE13]. **Impurities** [FE97, Fuk00]. **Impurity** [KNI$^+$08, MFCT15]. **Including** [KT98, CTO22, WHB$^+$24]. **Inclusion** [MKB04, dLHD10]. **Incorporating** [MKK$^+$00]. **Independence** [Kla81]. **Independent** [BBB10, BGW73, BG73, Gre73, Lyo08, Mar08a, PČ75]. **Index** [Ano64a, Ano64e, Ano65a, Ano65e, Ano67a, Ano67f, Ano68a, Ano68f, Ano70a, Ano70f, Ano72a, Ano72f, Ano73a, Ano73f, Ano74d, Ano75d, Ano77e, Ano78d, Ano80d, Ano81g, Ano81h, Ano82i, Ano82j, Ano85e, Ano86b, Ano88e, Ano89e, Ano90d, Ano91d, Ano92g, Ano92h, Ano94d, Ano95d, Ano96e, Ano97h, Ano97i, Ano98p, Ano98q, Ano98r, Ano98s, Ano99l, Ano99m, Ano99n, Ano00c, Ano00d, Ano01j, Ano01k, Ano04h, Ano08m, Ano12f, Ano12j, Ano13f, Ano13g, Ano13h, Ano14c, Ano14d, Ano15e, Ano15f, Ano16c, Ano17g, Ano17h, Ano17i, Ano18c, Ano19k, Ano19l, Ano19m, Ano20e, Ano20f, Ano21e, Ano21f, Ano22e, Ano22f, Ano23e, Ano23f, Ano24c, Apo01, Nak00, San92]. **Indices** [MNR$^+$98]. **Indirect** [SPAS05]. **INDO** [BMPV99]. **Induced** [BGG$^+$07, BWVD$^+$13, BR17, KS88, Kho04, Nic10, Nic17, Sal11, Sim99, SS04, TS10, Uda00, vS07, HDB03, Yam03]. **Industrial** [Hog18e, SBK$^+$08]. **Inelastic** [AGMdV$^+$13, BR17, FCAG19, MM13, RGFC13, AMAA22]. **Inference** [Kou15]. **Infinite** [Kla81, Bar23, LK09]. **infinite-order** [Bar23]. **Influence** [PGJ07, FB20, Kar02]. **Influenced** [SSS05]. **Influences** [Jør74]. **Information** [Nal03, Shi12, Nal23]. **Information-Theoretic** [Nal03, Nal23]. **Informed** [TR14]. **infrared** [EÜSB21]. **Ingvar** [Nor98]. **Initial** [Gre73]. **Initiated** [RAR$^+$08]. **Initio** [BŚG14, CL07, CH03, DRV82, DO09, DSW04, HPRR10, ILS08, Jan97, JcH18, KNI$^+$08, KTC01, LBH$^+$17, MBM99, PR05, PWZ$^+$08, QSG98, RNL14, RFG$^+$98, Sau05b, HO16, IKN$^+$08, SM23, ŚBG14, ZDZO11, CG80, Chr72, MWL$^+$05, San92, BMC97, Kap98, SSV98]. **Inlet** [SIY$^+$15]. **Inner** [HUS$^+$11, HMH$^+$18, HL97, MU03]. **Inner-Shell** [HUS$^+$11, HL97, MU03]. **Inorganic** [CH03, DB68, Oni12, SSK03, YMI$^+$21]. **input** [Hog21]. **Insertion** [HSS$^+$04, KTA03]. **Insight** [GTB23, LSZ$^+$99b]. **insights** [LCC22]. **Instabilities** [Cal85]. **Instability** [BE04]. **Integral** [CB92, GM91, Yan90]. **Integrals** [AYÖ17, Ave13, AA15, AA18, BL18, Gil94, HPB17, ÖÖ13, Ste73, Yas17, YÖ13, ZP17, ALA21, ALA23, KÖO23, Rui23]. **Integration** [Nal00]. **Intelligence** [Duc97, SSCL97, MP22]. **Intensities** [APNM03, BKC68, YTC$^+$05]. **Intensity** [BWK97, MTA00]. **Intensivity** [DDPC95]. **Interacting** [KT98, MHWvdA97]. **Interaction** [ATL$^+$18, AJ04, AA03, BMP03, Bun18, DKV$^+$19, EGCL91, EEL96, EM17, GC92, HK03, KMJ97, KK85, KN01, LHL18, MCC03, PKYM01, Per90, PGN04, RMN$^+$14, RFG$^+$98, RMMP17, RP18, RT18, SBCT04a, SBCT04b, Sab07, SS99, AA19, Bel19, CAG$^+$21, FB20, SB07, SHBC19, SKS$^+$19, WLM23]. **Interactions** [BP82, Bor03, CT82, DSW04, GP14, GM05, Jan65, Jeh65, KSG08, KH03, PP68, Rei73, Sau05a, FSP23]. **Interatomic** [Gon98]. **Interelectron** [AA18]. **Interest** [EBR92, MLR$^+$98]. **interesting** [SBA$^+$03]. **interface** [SYIY03]. **interfaces** [Per20]. **Interferences** [SS04]. **Intermediate** [LEK01, Bel22]. **Intermediates** [GAI08]. **Intermolecular** [MCG$^+$08, MS67, Sal11, ST78]. **International** [Moh08]. **internationalization** [Kar02]. **Interparticle** [BFHS23]. **Interpenetrating** [Sil14]. **Interplay** [LDP$^+$04, MCC03, Nal06, Sig05]. **Interpretation** [Brä04, Kar08, KP77, ST78, Ort22, NBS12]. **interpretations** [LT21]. **Interpreting** [Köv03]. **Intersection** [Pet98]. **Interstellar** [CG80]. **interstitial** [GWW19]. **Intra** [Chi03, PWZ$^+$08]. **Intra-Hydrate** [PWZ$^+$08]. **Intra-Site** [Chi03]. **Intramolecular** [LK14, MCG$^+$08]. **Intrinsic** [ITI$^+$00]. **Introduced** [KB98]. **Introducing** [Yas17]. **Introduction** [Ano19n, Ano19o, Ano19p, Sme92, TAU17, Tri90]. **Introductory** [Die97]. **Invariance** [Woo98]. **Invariances** [Kar08]. **Inversion** [GDL14, MMM18]. **investigate** [Hog21]. **Investigating** [KV08]. **Investigation** [Fuk08b, LK14, ST17, ZZ08, KÖO23]. **invoke** [Hes22]. **Involving** [Byl98, DSW04, HPB17, IL98, ALA21, ALA23, MKK$^+$01]. **Iodine** [Mar08b]. **Ion** [Bel09, BMM13, FRM70, FAS$^+$98, HBE$^+$98, JJ20, Jan65, KMHL13, LJ17, Mam19, MF04, MM13, Pau13, SS04, ST07, YKC$^+$08, Bel21, Bel22, CBSM20, MG22, SM23, VG22]. **Ion-Atom** [Bel09, BMM13, FAS$^+$98, Bel22]. **Ion-Matter** [MM13]. **Ion-Metal** [MF04]. **Ion-Solid** [FAS$^+$98]. **Ionic** [GL90, HPU$^+$17, MLR$^+$98, Sch94, FTG22]. **ionicity** [BFHS23]. **Ionization** [Bel09, BMM13, BRL13, CHR13, DC99, GS04b, GPEB21, HUS$^+$11, HPU$^+$17, HMH$^+$18, MCM14, UYT97, VTM98, MG22, MU03, SM22, BG73]. **ionizations** [CCM$^+$19]. **ionized** [MK23]. **Ionizing** [BGG$^+$07, Fra13]. **IONO** [Mar08b]. **Ions** [Ano08h, Ano08j, ABGM03, AL04, Bic13, BKB$^+$19, CHR13, CLK15, DGKCT15, DTC04, GP04, Khe19, LT98, MKH$^+$97, MA04, NM03, PGJ07, RGFC13, SBCT04a, SBCT04b, SOS15, SW98, SGK$^+$08, VI01, WMM$^+$98, CTC22]. **IR** [CÅ01, Jan97]. **Iron** [Kot68, MKH$^+$97]. **Irregular** [AYÖ17, SR73]. **Isaac** [Ano03a]. **ISM** [JMWG19]. **Isoelectronic** [Jør78, VI01, VT24]. **Isolobal** [YMI$^+$21]. **Isomer** [FCC04]. **Isomerism** [Sla81]. **Isomers** [PM16]. **isospin** [YMI$^+$21]. **Isotope** [DY08, JGNJ08, Lyo08, Mar08a]. **Isotopes** [Per98b]. **Isotopic** [BB14]. **Isovalent** [MVL01]. **Iterative** [BS05a, GDL14, SGB16]. **IV** [VT24].

J [BB21, CPBS05, DE05]. **J-coupled** [BB21]. **Jack** [OB22a]. **Jacobi** [CMDN89, CAP19]. **Jahn** [ABGM03, ADA03, BP82, BO86, Ber03, Chi03, CKRT03, DST$^+$03, FIK$^+$03, GWM$^+$03, HBKS03, KH03, KBS03, LPDB03, LC03, LM03, MS03, MCC03, NeMM03, OM03, Pol03, SKT$^+$03, SS03, SIY$^+$19, SCN03, YAJHR03]. **Jan** [Öhr05, SBLJ05]. **Jean** [Ano19b]. **Jens** [OS05, SO05b]. **Jones** [Hal91]. **Jordan** [Brä04]. **Jørgensen** [Odd05, SBLJ05]. **Journey** [CCC17, Cra99].

Junctions [BR05].

K-edge [CCM+19]. **Kelvin** [MYM08]. **Kepler** [CCA13]. **kernels** [ORL23]. **Ket** [IM80]. **Ket-Vectors** [IM80]. **keV** [TBM01]. **Key** [RNL14, vL03, RZTSW23]. **KH** [TMK21]. **Kind** [PS05b]. **Kinetic** [CTCS05, LASV18, NA04, Per98a, YZDM01]. **Kinetic-Energy** [YZDM01]. **Kinetics** [RNL14]. **KLi** [MMSK16]. **Knowledge** [KS97b, MRS+99]. **Knowledge-Based** [KS97b]. **Kohn** [GV09, KB98, LK90]. **Kołos** [MG23a, PMK23]. **Kondo** [FCAG19, FTG22]. **Koopmans** [Ort22]. **Kossel** [Jør78]. **Kr** [PJH05]. **Kramers** [AA03]. **KS** [SKGŚ23]. **KS-DFT** [SKGŚ23]. **Kummer** [BC09].

L [OTA97, YNNU03]. **Laboratory** [KNM+08, PEMC23]. **ladder** [CAP19]. **Laguerre** [DGA18, LPC24]. **Lamé** [MFLK15]. **LaMnO** [NP03]. **Lanczos** [SP99, SGB16]. **Landscapes** [Oli12]. **Large** [Chr72, EG99, SIY+15, TTLB04]. **Large-Scale** [SIY+15]. **Laser** [AAM04, ALND10, ADA03, BS98, DGKCT15, Glu19, ML18, PR98, Per98b, TS10, VTM98, IOA03, WLM23]. **laser-driven** [WLM23]. **Laser-Induced** [TS10]. **Laser-Modified** [DGKCT15]. **Lasers** [Sva98]. **Lattice** [DDPC95]. **Lattices** [Phi98]. **Laves** [TMM03]. **law** [MG22]. **layered** [KTA03]. **LCAO** [Del74, PTC+13]. **LDA** [ABB90]. **Lead** [LvWH+01]. **Leader** [Lin99]. **Learning** [Ber02, SS17, Dra20, MP22]. **Least** [LJK+08, Löw92a]. **Least-Squares** [LJK+08]. **Legacy** [Bun17]. **Length** [PR98]. **Lennard** [Hal91]. **Lennard-Jones** [Hal91]. **Level** [MYM08, MBO+07, SPD09, SGM+13]. **Levels** [ATL+18, LJK+08, Bun23]. **Li** [BB14, Khe19, KNI+08, KNM+08, RF13, TM13, YKC+08, ŻM23]. **Li-Ion** [YKC+08]. **Li-K** [KNM+08]. **Li-like** [Khe19]. **LiAlH** [DA14]. **LiCaAlF** [ADA03]. **Lie** [AČP88]. **Life** [PB20c, BP20, SB02]. **Lifetimes** [BS98, MAS03]. **Lifting** [FSP23]. **Ligand** [ARS17]. **Ligands** [YFK+97]. **Light** [DY08, Phi98, SBH+20]. **LiH** [PS05a]. **Like** [FPL97, RLF17, BH24, CKC09, Khe19, Lau09, VT24]. **Limit** [Bas78, Sau05a]. **Limited** [LK09]. **Limits** [Brä12, Ber02]. **Linderberg** [Öhr05, SBLJ05]. **Lindgren** [Löw98, Nor98]. **Line** [Eks98, HBKS03]. **Linear** [AL04, BR82, Bas78, BB13, Bis94, JJD05, Kla81, LGJP99, LPDB03, LDNP99, Löw92a, Löw96b, MCA+18, PS05a, PM16, Tap09, BLC23, PS05b]. **Linear-Response** [MCA+18, PM16]. **Linearized** [SED+98]. **Linearized-Augmented-Plane-Wave** [SED+98]. **Lines** [Glu19]. **Linked** [Bra77]. **Linked-Cluster** [Bra77]. **Liouvillian** [Löw85c]. **Liquid** [BRL13, Krs16, MLR+98, RFG+98, YKY+00]. **Liquids** [HPRR10]. **LiRb** [SM23]. **List** [Ano64d, Ano65d, Ano67e, Ano68e, Ano70e, Ano72e, Ano73e, Ano74c, Ano75c, Ano77d, Ano78c, Ano80e, Ano81i, Ano81j, Ano04i]. **Lithium** [YKC+08, KTA03, LYM03]. **Lived** [Lyo08, SM22]. **living** [Per20]. **LiX** [BJMB14]. **Local** [GL90, JcH18, Köv08, LLBK+98, MMM18, Nes03, PWZ+08, YIYM03].

Local-Scaling [LLBK+98]. **Localizability** [ACDK72]. **Localization** [GM17, PLA01]. **Localized** [CE78, KT98, KTC01, Nal09, MG21]. **Locally** [SPAS05]. **Loge** [ACDK72]. **Logical** [Brä12]. **lone** [AR03]. **Long** [DB13, JGCRC16, Lyo08, SM22, TMMS10]. **Long-Lived** [Lyo08, SM22]. **Long-Range** [DB13, JGCRC16]. **Loss** [AJ04, AL04, Bel09, Bic13, GS04b, Kho04, Tők19]. **Loss-Excitation** [Bel09]. **Loss-Ionization** [Bel09]. **Lost** [Heh18]. **Low** [DLMS03, DST+03, Jos08, KM98, LP97, LKD05, MF04, MMSK16, Nes75, RPSB00, SPD09, Sim07, SSS05, TM13, Bel19, Kar24]. **Low-dimensional** [SPD09]. **Low-Energy** [Sim07, SSS05]. **Low-Lying** [KM98, LKD05, MMSK16, TM13, RPSB00, Bel19]. **Low-Spin** [LP97]. **Low-Temperature** [DLMS03]. **Löwdin** [Bun17, Heh18, Kar02, LÖS02, LÖBS17, SB02, SB17a, SPH14]. **Löwdin's** [SS17]. **Lower** [BB14, Wei72]. **lowering** [TSTH03]. **Lowest** [GV09]. **Lunell** [Miy03]. **Lying** [KM98, LKD05, MMSK16, TM13, Bel19, RPSB00].

M&S [TR14]. **machine** [Dra20]. **Macrocyclic** [YFK+97, ZDZO11]. **Made** [Col68]. **Madelung** [KSY08]. **Magic** [KMR01]. **Magnesium** [MYM08]. **Magnesium-Zinc** [MYM08]. **Magnetic** [Bel06, BB11, CE72, DST+03, DeB09, GWM+03, IS01, JH99, JcH18, Laz04, Ram08, VRG90, Vis05, BB22a, TMM03]. **Main** [Dau64]. **make** [KHPP23]. **Making** [MKH+97]. **Maleonitrile** [RGA99]. **Manganese** [NeMM03]. **Manifestations** [SBC+03]. **Manipulation** [MCP12, WMM+98]. **Many** [AO03, AA01, Ave98, BŚG14, CB92, Cru09c, DDPC95, DSR81, HG17, HW01, HMW01, IOA03, Khe19, KT98, KB86, Löw88b, LFM89, MC10, Mat78, Mic15, Mic17, MK18, Nic17, NM03, PKYM01, RP72, Sal74, SW98, WDD16, vL03, LSZT90, Mic02, Mic22]. **Many-Atom** [HG17, Mic15, Mic17, Mic02, Mic22]. **Many-Body** [AA01, BŚG14, DDPC95, HW01, HMW01, Khe19, KT98, KB86, MC10, Mat78, MK18, SW98, WDD16, vL03]. **Many-Electron** [Ave98, DSR81, Nic17, PKYM01, RP72, Sal74, AO03, Cru09c, IOA03]. **many-fermion** [LSZT90]. **Many-Particle** [Löw88b, LFM89]. **Maruani** [Ano19b]. **Mass** [KS88, Lyo08, Mar08a, MRS+99]. **Mass-Independent** [Lyo08, Mar08a]. **Masses** [SBF+08]. **Master** [Kai15]. **match** [SÁ23a]. **Material** [FE97, GP14]. **materialism** [PB20a]. **Materials** [Ber14, DLMS03, Kuk14, MF14, Oni12, Oni15, SNIM08, TR14, AO03, LSZ+00, SBA+03, Sab14a]. **Mathematical** [CD05, EBR92, Gut06, Sut01, SCT15, SCT16]. **Matrices** [BMP03, BK70, Dah01, Har90, Kry81, RP72]. **Matrix** [LK90, McW98, Mic99, PKYM01, RPSB00, RP72, Öhr02]. **Matter** [Ano19j, Ber03, DTC04, Gre08, MM13, SBCT04a, SBCT04b, AA19]. **MCSTEP** [Yea05]. **Mean** [CTC22, HG17, SOS13, SOS11, SOS15, CTSSO19, CTO22, SSO19]. **Mean-Field** [HG17]. **meaningful** [SKGŚ23]. **Means** [ST78]. **Measured** [BS98, NHYU03]. **Measurements**

[BLKS78, KNM$^+$08, MRS$^+$99, MYW00, Tap11]. **Mechanical** [And80, AA01, Bel09, BB17, CC97, HPRR10, KZR86, Pul77, Wei72, vS07, BMR$^+$24, NBA20]. **Mechanics** [Brä08, CCM05, CL05, Deu99, MDÖ05, Öhr17, PD10, Sch94, Sig05, Spe78, TL10, CCT02, LT21, MG21, SBC10]. **mechanics/extremely** [MG21]. **Mechanism** [Ber03, Oni15, TBM01]. **Mechanisms** [ASGG08, FHHZ88, YAJHR03]. **Mechanistic** [BB13, BB15, Mar08a]. **Media** [AGMdV$^+$13, JJD05, Kar97]. **Mediated** [MBM99]. **medical** [BB21]. **membered** [BMC97]. **Memory** [SS17, JJ20, MG20]. **Mercury** [ASGG08]. **MEST** [Hog13g, Hog14]. **Metal** [Ada97a, ARS99, BU97, EGCL91, GP14, Kap98, KMR01, MF04, RR05, SS98, SNM$^+$97, SNIM08, SCN03, TLOK97, Tak19, TTLB04, FB20, FCAG19, FTG22, Hog23c, KBH23, MGAUP23, PBOL02, STO$^+$00, SYIY03]. **Metal-Cluster** [KMR01]. **metal-film** [KBH23]. **Metallic** [Bro98a, Bro98b, Saa01, AMAA22]. **Metalloporphyrins** [DRV82]. **Metals** [Ber74, FHHE82, MA04, SED$^+$98, STO$^+$00]. **Metastability** [PB14]. **Metastable** [CKRT03]. **Methane** [RZTSW23, Hog23c, HDFT24]. **Methanol** [FCC04]. **Method** [Ada97b, Ada00, Ave98, CTCS05, CL00, CB18, DKMP98, EG99, FSB$^+$97, FCH15, Fuk15, GW17, GEO91, GVFR98, Glu19, GDL14, I'H64, IFAY08, KE97, LEK01, Löw88b, LFM89, Löw92a, LM92, MW08, May80, MMM18, MM96, Mon05, MKK$^+$00, Mur08, MKB04, MMSK16, Nak00, NFW$^+$98, OW08, OE17, PB99, RPSB00, RP18, SGB16, SS99, SNMI00, Sla64, SGM$^+$13, TMN10, TAM04, WD70, WmG18, Yea05, BH24, DAB$^+$23, GPEB21, Hog23c, HDFT24, KBH23, LMK19, MKK$^+$01, ÖEO23, TMK21]. **Methodologies** [BRL13]. **Methodology** [GDL98, ZLC$^+$10, CCT02]. **Methods** [AdMB99, AČP88, AH19b, And80, ACDK72, Bel09, Byl98, Dau64, FP06, GC92, HPU$^+$17, Har04, Hät05, HZ89, HG17, HM21, HMW01, JG08, LGJP99, LJKH13, LB92, Löw85c, ML18, Mic74, Mic17, MP89, Nic10, ÖÖ13, PS05a, RR05, STZY18, San98, Sau05b, SBK15, TAU17, TL10, WN05, WDD16, Bar23, CCM$^+$19, EÜSB21, Hog14, JMWG19, LH20, Min22, SBGJ08, SBC10]. **Methylamine** [SSV98]. **Metrology** [PR98]. **MeV** [AGO07, WHB$^+$24]. **Mg** [FU00, NHYU03]. **Mg-** [NHYU03]. **MgB** [SCE19]. **mGluR5** [ST17]. **MgO** [OTA97]. **MI** [GVFR98]. **Michael** [Sab00]. **Microscopic** [Chi03, MTS04, Brä02]. **Minimum** [Kou15]. **Mixed** [MLR$^+$98, Mon05, PSAP10, SIY$^+$19]. **Mixed-Quantum** [PSAP10]. **Mixed-Quantum/Classical** [PSAP10]. **Mixed-Valence** [SIY$^+$19]. **Mixing** [AR03, SH95]. **mixture** [LCC22]. **MM** [BBB10, MC10, SBC10, SIY$^+$15, TL10, ZLC$^+$10]. **Mn** [NeMM03, YNNU03]. **MnO** [GWM$^+$03]. **MO** [Yas17, CDP82, Del74, YNNU03, RZTSW23]. **Mo-** [RZTSW23]. **Mobile** [KTMA08]. **mobility** [ZLL$^+$20]. **Model** [ABC$^+$98, BMPV99, BGW73, BB13, BE04, BG73, BWH08, BC09, Cam12, Dru78, DB01, Gre73, GM05, GVFG09, HS86, HSR98, JGCRC16, Jos08, Kap98, Kri03, KMR01, LS07, MS03, PJH05, Sme99, VG22, DAB$^+$23, NA19]. **Modeling**

[DNM+14, GVFG09, Köv08, Kuk14, MHWvdA97, RMN+14, TL10, HDFT24]. **Models** [Ano04l, BB15, BRL13, GV09, KGW98, KE00, MBO+07, NA04, Nik70, SIY+15, AA19, MK23, SS22]. **Modern** [CTG98, HPL98, KK85, SL20]. **Modified** [DGKCT15, KN01, BGW73]. **Modulators** [ST17]. **Module** [PM16]. **MoF** [MKK+01]. **Molecular** [ÅCL92, Ada97b, ADRAB16, AH19b, AGL05, ALND10, Ave13, AA15, BGG+07, BVHK03, BLC23, BU97, BHV+00, Bas64, Ber03, BWK97, BR05, Bis67, BC80, Brä19, BJV86, CTSO04, CCVB94, CMJR+04, Cio90, CCA13, CS04, CLK15, DB68, Dau64, DNM+14, Dru78, DW98, Fra13, FF72, GP91, GM17, Gil94, GL90, GM91, Hal64, Hal91, HS19, Har67, HZ89, HJ88, HPRR10, Hog13g, HBGvM19, IFAY08, ILS08, Jan97, Jeh65, JH99, JS21, JcH18, KS77, KS88, KSG08, KD11, KTC01, Kry03, Löw80b, LÅJM95, MW08, Mic74, MT04, MWL+05, MKK+00, MP97, MBO+07, Nal09, NM03, ODE75, Ohn67, ÖB81, Öhr15, Oli12, OK11, OBHM17, PTC+13, PWZ+08, Pul77, QGW01, RMN+14, RFG+98, Ray95, Rei73, RM04, Ryc98, SBH+20, Sal11, San98, San92, Sch94, ST78, Sim99, Sjö04]. **Molecular** [Ste73, ST07, Sut97, TAM04, TL10, TM21, Uda00, VWP+98, Yan81, Yas17, dLHD10, Bis19, BSL+19, CAP19, KÖO23, LSC19, MG21, Nal23, NBA20, ÖEO23, PEMC23, RSP21, SBLJ05, SBC10, SM22, SM23, SA23b, Yas23, ŻMM23]. **Molecular-Dynamics** [BHV+00]. **Molecular-Orbital** [MW08, JS21]. **Molecule** [Apo01, Bro98a, Bro98b, CT82, FRM70, FPL97, GM05, JSG+14, Kom05, KMJ97, LKD05, Löw65c, MW98, MCM14, MSM17, OM03, STZY18, Sim05, LMK19, PMK23, SZP21, WLM23]. **Molecule-Ion** [FRM70]. **Molecule-Particle** [GM05]. **Molecules** [ÅVM96, AAE+01, AAM04, ACDK72, BND81, BJMB14, BO86, CE72, Cam12, CL05, CG80, CKC09, Chr72, CLÅ05, Dau70, Del74, EG99, ERC88, FLV99, FVB99, FMA08, GSTvE98, GCAGM17, GNM08, HL97, IBB+19, IS01, Jan97, Kar97, KGW98, KMHL13, Kob97, LR72, LASV18, Lyo08, ML18, Mat96, MFLK11, MKN10, MK18, MTA97, Nal06, Nes67, Nic10, OO05, OBHM17, PB14, PGP17, PBK04, Rei73, RGFC13, RP18, Ser74, Sme92, SSV98, SCTH+07, Sut01, UK05, YTF78, YTC+05, ZDZO11, BLC23, CM24, HO16, MKK+01, QSW20, YMI+21]. **Møller** [GC92, OB23, VI01, GS04a]. **Møller-Plesset** [GS04a]. **Molten** [MKH+97]. **Moment** [RM04, SJO05, YÖ13, PS21]. **Moments** [AB73, BO86, BWK97, Eks98, Glu19, PJH05, Woo98]. **Momentum** [BLKS78, KS77, MTS04, MFLK15, OE17, TM13, WP06, AP03]. **Monoclinic** [DA14]. **Monohydrated** [Tak19]. **Monomer** [PWZ+08]. **monovalent** [FB20]. **Monte** [SH19, AGL05, CCT02, CCM05, CC97, HB14, Hog18e, Hog21, Hog23c, HDFT24, KBH23, MCA+18, NFW+98, RMMP17, RP18, TAU17, vS07]. **Monte-Carlo** [CC97]. **Morse** [Apo01]. **Motion** [Löw85c, Per17, Sch94, Sut97, WN05, YTC+05, MKB04, NBA20]. **Mountains** [Kai15]. **MP2** [JSF08, WmG18]. **muffin** [GWW19]. **muffin-tin** [GWW19]. **Multi** [CLÅ05, MDBM98, PWZ+08, SPD09, LH20, FSP23].

multi-CPU [LH20]. **Multi-electron** [SPD09]. **Multi-Hydrates** [PWZ+08]. **Multi-Photon** [CLÅ05]. **Multi-reference** [MDBM98]. **Multicenter** [ALA21, HPB17]. **Multichannel** [Shi12]. **Multicharged** [BKB+19, Khe19]. **Multiconfiguration** [PGP17, WD70]. **Multiconfigurational** [LJKH13, STZY18, Yea05]. **Multidimensional** [Pol03]. **Multielectron** [KGI+19, OW08]. **Multiphonon** [HK03]. **Multiphoton** [Glu19, VTM98]. **Multiple** [Nal09, SBDD03, ST07]. **Multiplet** [IOI+00, ITI+00, OYI+00]. **Multiply** [AK12, CHR13]. **Multipole** [BO86, Woo98, YÖ13]. **Multireference** [BB99b, EM17, HMW01, LGJP99, LF09, MH98, MSM17, VI01, JMWG19, LH20]. **Multireference-Coupled** [MSM17]. **Multireference-Fock** [BB99b]. **Multiresolution** [DGKCT15, Bis19]. **Multiscale** [TR14]. **Muonium** [Hug98]. **Mutations** [Löw65c]. **myelinated** [JJ20].

N [JMWG19, BMC97, HSR98, Mur03, TBM01]. **N'-Tetramethyldiamide** [HSR98]. **NaEuCl** [APNM03]. **NaH** [LMK19]. **NaK** [MSM17]. **nano** [SBA+03]. **Nanoclusters** [ARS17]. **Nanodosimetry** [Bic04]. **Nanometer** [Ros98]. **Nanoparticles** [GP14, OBHM17, AMAA22]. **Nanoplasmas** [LJ17]. **Nanostructures** [DO09, AGS+19]. **Nanotubes** [AAM04, LYM03, MOB+03]. **nanotubes-gold** [MOB+03]. **NaSmCl** [APNM03]. **native** [YMI+21]. **Natural** [AT91, AAG03, AAAC04, BK70, Dav72, MGAUP23, MPU19]. **Nature** [Brä04, Sjö04, YM97]. **Near** [KsKsN08, MYW00, MYM08, NHYU03, YFK+97]. **Near-Edge** [KsKsN08]. **Nearly** [Lin17a]. **Necessary** [Brä04]. **Negative** [Kom05, SW98]. **Neon** [Sab97]. **Network** [PWZ+08]. **Networks** [SIY+15]. **neural** [MG20, Per20, Rou20]. **Neutral** [DNM+14]. **Neutrino** [KS88]. **neutron** [Kar24]. **Newton** [GDL14, HZ89]. **Next** [SO05a]. **NH** [Sau05b, YTC+05]. **Ni** [SMAS08, Hog23c, HDFT24, KKA97, WHB+24, YKY+00]. **Nitrate** [HBT+00]. **Nitrates** [HTS+00]. **Nitric** [BWH08]. **Nitrides** [TLOK97]. **Nitroaniline** [CCCC15]. **Nitrogen** [RNL14, VI01]. **Nitrones** [RGA99]. **Nitroprusside** [CKRT03]. **NMR** [BB17, BB21, BB22a, CPBS05, PB05, SPAS05]. **NO** [SP99]. **NOCV** [ŻMM23]. **Noise** [DeB09]. **Non** [AHPD+03, AL04, AR03, BVHK03, BS05a, Bis94, KNN17, NBA20, PS05b, Sau05a, Sim99, Sme92, BMR+24, SA23b]. **Non-Adiabatic** [BVHK03, Sim99, BMR+24]. **Non-Born** [NBA20, SA23b]. **Non-Condon** [AHPD+03]. **Non-Coulombic** [KNN17]. **Non-degenerate** [AR03]. **Non-Iterative** [BS05a]. **Non-Linear** [AL04, Bis94, PS05b]. **Non-relativistic** [Sau05a]. **Non-Rigid** [Sme92]. **Nonadditive** [Kap98]. **Nonadditivity** [MS67]. **Nonadiabatic** [Kry03, Nik70, SP99]. **Noncanonical** [LB92]. **Noncovalent** [DSW04]. **Nonempirical** [PB75]. **Nonequilibrium** [KD11, NTT20]. **noninteger** [GJP23]. **nonintegral** [Wen21]. **Nonlinear** [IBB+19, LHL18, MFCT15, MA04, OO82, PGN04, RAR15, BLC23, LCC22].

Nonlocal [LV90, Nes03, Sjö04]. **nonorthogonal** [SKS+19]. **Nonorthogonality** [Löw70b]. **Nonparametrized** [HPRR10]. **Nonrelativistic** [Öhr16, SA23b]. **nonrepresentational** [LT21]. **Nonrigid** [Ser74, SSV98]. **Nonstationary** [Nic17]. **Normality** [IM80]. **Normalizing** [GWW19]. **Notes** [Ano99a]. **Novel** [IFAY08, Mat96, Oli12, LT21]. **Nuclear** [CTSDÖ04b, JcH18, LDB95, Lon99, PSAP10, Ray95, Sab97, SPAS05, SGM+13, Sut97, Vis05]. **Nuclearity** [Bor03]. **Nucleation** [NAY+08]. **Nuclei** [BRL13, DY08, Eks98, Glu19, Bel21, NBA20]. **Nucleic** [CL07, PP68, Tur07]. **nucleosome** [FB20]. **Nucleotide** [ZDZO11]. **nucleus** [LSC19]. **Number** [Ono00, TM13]. **Numbers** [ATL+18, KMR01]. **Numerical** [BS05a, Gut97, Kou15, Lin17b, MK18, Sid18, BG23].

O [CL00, OTA97, SIY+19, YKS+12, ŻM23, CSZ99, BMC97, BRW08, MKK+00, Sau05b]. **o-C** [CSZ99]. **Obituary** [Ano03h, Sab00]. **Objects** [EBR92]. **Observation** [Tos08]. **Observed** [Miy03, SEL01]. **Obtained** [MMM18]. **Obtaining** [HZ89]. **Occupancy** [SBDD03]. **Occurrence** [Löw88b, LFM89]. **Oddershede** [OS05, SO05b]. **OEC** [YKS+12]. **OEP** [BŚG14]. **Off** [DB13]. **Off-Diagonal** [DB13]. **oganesson** [GPEB21]. **OH** [GAI08, PEMC23, RRMAF08]. **Öhrn** [Lin99, LSZ+99b]. **OKa** [MKK+00]. **Oligomers** [CÅ01, PM16]. **Olov** [Bun17, Heh18, Kar02, LÖS02, LÖBS17, SB02]. **On-Line** [Eks98]. **One** [AYÖ17, ARS99, Bel21, BC80, FP06, FCH15, GW18, Kar24, LK13, MM96, OM03, Ort99, SBC09a, SPM09, SAL10, SGK+08, GVFR98]. **One-** [BC80, FP06, LK13, OM03, SGK+08]. **One-Dimensionally** [FCH15]. **One-Electron** [AYÖ17, Ort99, SPM09]. **One-Particle** [GW18]. **One-Photon** [SAL10]. **Ones** [Lin17b]. **Only** [PTC+13]. **Open** [Bad09, Bra77, CG80, Cru09c, FMA08, GC10, GVFR98, LP97, MP89, RTV05, YMI+21]. **Open-Shell** [Bra77, FMA08, GVFR98, LP97, MP89, RTV05, YMI+21]. **Operator** [LMSP01, Löw67c, MT04, Pal04]. **Operators** [FP06, HMC73, Löw96b, MKB04, SS03]. **Oppenheimer** [TA04, NBA20, SZP21, SA23b, Tap01]. **opposite** [SS22]. **Optical** [BMPV99, Bis94, DO09, DA14, HDB03, KsKsN08, MCP12, ML18, PR05, Phi98, RDNFH98, IOA03]. **Optimization** [BHM17, CMDN89, CTG98, HZ89]. **Optimizations** [Hät05]. **Optimized** [GW01, Khe19, KKGG98, WD70, SKGŚ23]. **Orbit** [ÅVM96, ERC88, LF09, RM04]. **Orbital** [Ada97b, AT91, ADRAB16, CTCS05, Cio90, DB68, FF72, GWM+03, Hal91, Har67, IFAY08, KT15, MW08, MNR+98, MKK+00, Nal09, NSM11, ODE75, Ohn67, San92, TSON00, UYT97, Uda00, Yas17, CTSSO19, CTO22, CTC22, JS21, MG21, MGAUP23, MPU19, PEMC23, SCJ+23, Yas23]. **Orbital-Communication** [NSM11]. **Orbital-Free** [KT15]. **Orbital/Plane** [Mon05]. **Orbitals** [AYÖ17, AAG03, AAAC04, AA15, BŚG14, CE78, CB92, CCA13, Dav72, DR90, GM17, Hog13g, HPB17, HM21, KTC01, Lin17b, PTC$^+$13, PTBH13, RP72, Ste73, Yan81, CAP19, KÖO23, LSC19, Rui23]. **Order** [AAM04, BS05a, BB99b, DB13, Hät05, IL98, KB86, KNN17, LDB95, MW98, RR05, SW98, SPH14, VTM98, AHPD$^+$03, Bar23, GJP23, MCC03, VdLCPT98]. **Ordered** [DLMS03]. **Ordering** [CCVB94, GWM$^+$03]. **orders** [Wen21]. **Organic** [BMPV99, Dau70, GAI08, Sey12, GTB23, YMI$^+$21]. **Orientational** [CTSDÖ05]. **Origin** [CKRT03, FRM70, OM03, RGA99]. **Ortho** [DNM$^+$14]. **Ortho-Anisidine** [DNM$^+$14]. **Orthogonal** [DGA18, CAP19]. **Orthogonality** [IM80]. **Orthogonalization** [Sri01]. **Orthogonalizations** [SS17]. **Orthonormal** [CCA13, RP72]. **oscillating** [ALA23]. **Oscillation** [BS72]. **oscillations** [JJ20]. **Oscillator** [BLKS78, CTSOS99, CTSO04, Khe19, KMR01, OOSS17, CTSSO19]. **Oscillator-Strength** [OOSS17]. **Osvaldo** [Ano04i, SBK04]. **Other** [ASGG08, BGG$^+$07, ERC88, Löw92a, Ram08, SBA$^+$03]. **Overlap** [FH65, ÖÖ13]. **Overview** [vS07]. **Oxidation** [SIY$^+$15, ZZ08, YMI$^+$21]. **Oxidation-Theoretical** [SIY$^+$15]. **Oxide** [GP14, SNIM08, YKC$^+$08, CCL03, Fuk03, Sak03b]. **Oxides** [EGCL91, KIT$^+$08, PBOL02]. **Oxonium** [LM97]. **oxy** [RZTSW23, YMI$^+$21]. **oxy-radicals** [YMI$^+$21]. **Oxyanions** [Cse97]. **Oxygen** [Mar08a, MKH$^+$97, NM00, SIY$^+$15, SIY$^+$19, MFMCN01, Sak03a, YMI$^+$21]. **Oxygen-Evolving** [SIY$^+$15]. **Oxygenated** [GAI08]. **oxygenation** [YMI$^+$21]. **Oxynitride** [KsKsN08].

P [CSZ99, Bel19, OM03]. **Packages** [LBH$^+$17]. **Packets** [SAL10]. **Padé** [Bel06, BB13, DeB09]. **Page** [Ano09d, Ano12h, Ano14e, Ano15g, Ano15h, Ano16d, Ano17j, Ano17k, Ano17l, Ano18d, Ano19q, Ano19r, Ano20g, Ano20h, Ano21g, Ano21h, Ano22h, Ano22i, Ano23g, Ano23h, Ano24d, Hog18f, SB13e, Ano64c, Ano65c, Ano67d, Ano68d, Ano70d, Ano72d, Ano73d, Ano74b, Ano75b, Ano77c, Ano78b, Ano80c, Ano81e, Ano81f, Ano82f, Ano82g, Ano85d, Ano86a, Ano88c, Ano89c, Ano90b, Ano91b, Ano92c, Ano92d, Ano94c, Ano95b, Ano96b, Ano97d, Ano97e, Ano98j, Ano98k, Ano98l, Ano99f, Ano99g, Ano99h, Ano08e, Ano08f, Ano09e, Ano09f, Ano12d]. **Pair** [MS65, TM13]. **Pair-Correlated** [MS65]. **Pairs** [AR03, AA03, KN01, AP03]. **Panexperiential** [PB20a]. **Paper** [Hal91]. **Paradigms** [MDBM98]. **Paradox** [McW99]. **Parallel** [HS19, PM16, LH20]. **Parallelization** [TR98]. **Paramagnetic** [Kot68]. **Parameter** [Apo01]. **Parameterization** [AR03]. **Parameters** [GM05]. **Parametric** [Bel11]. **Parametrization** [ACDV01]. **parity** [QSW20]. **Parrinello** [PWZ$^+$08]. **Part** [SBCT04a, SBCT04b, SBC09b, SBC09a, LSZ$^+$98b, LSZ$^+$98c, NBS10, SBM$^+$01a, SBM$^+$01b, Löw88b, LFM89, NBS12, SCT16]. **Partial** [PSS98, SGB16]. **Partial-Wave** [PSS98]. **Participants** [Ano97a, Ano98t, Ano98u, Ano01m, Ano01n]. **Particle** [BGW73, BG73, BC00, CB18, GW18, GSTvE98, Gre73, GM05, IKN$^+$08, KV08, Löw88b, LFM89, SS03, Sig05, Uda00, FB20, GJP23, SA23b]. **Particles** [AJ04, BRL13, Fra13, PGN04, RDNFH98, TTLB04, AGS$^+$19, BKL21, Tők19].

Partition [Nak00]. **Partitioning** [Lar02, Löw98, Mic17]. **Parts** [ÖÖ13]. **Passage** [ML18]. **Passivation** [ARS17]. **Path** [BŚG17, GM91, LPDB03, Nag01]. **paths** [BSL+19]. **Pathway** [HS19]. **Pauli** [LASV18, SO19c]. **Pb** [KIT+08, HHU+21, LvWH+01, MLR+98]. **PbO** [RM04]. **PCM** [Cam12]. **Pd** [CMVPFC16]. **PEDICI** [TR98]. **Peierls** [BE04]. **Pendulum** [PS05b]. **Per-Olov** [Bun17, Heh18, Kar02, LÖS02, LÖBS17, SB02]. **Perchlorate** [Lin05]. **Perform** [PTC+13]. **Performance** [PM14, CCM+19]. **Periodic** [ABB90, FCH15, Gon98, LBV01, Mon05, Ros98]. **Perovskite** [GWM+03, KIT+08, SKT+08]. **Perovskite-Type** [SKT+08]. **Perspectives** [Bel11, CL05, Del74, Nal03, OPPZ06, PTLGOM12, SBG+98, Brä03, SBM+01a, SBM+01b]. **Perturbation** [Bra77, FMA08, GC92, Gon98, GS04a, GS04b, HBE64, HW01, Khe19, KMJ97, KB86, Lau09, LP97, Lin17c, PČ75, RR05, SW98, VI01, KHPP23, LH20, OB23]. **Perturbative** [BE01, BB99b, Bar23]. **PESA** [NHYU03]. **PET** [BWVD+13]. **Pharmacology** [Pul77]. **Phase** [Dah01, DLMS03, GSWW10, HSR98, MRS+99, MCC03, RAR+08, TMN10, TMM03, TSTH03, Yam03, YIYM03]. **Phase-Space** [Dah01]. **Phases** [DA14]. **Phenomena** [ÅVM96, Löw67c, Sri01]. **Phenomenological** [Kar08]. **Phenyloxirane** [JJD05]. **Phonon** [HBKS03, MS03, SHBC19]. **Phonon-assisted** [MS03]. **Phosphorus** [OM03]. **Photobiological** [GBPSR10]. **Photochemical** [Dau70]. **Photodetachment** [HHK+98]. **Photodissociation** [JGNJ08]. **Photodissociations** [LF09]. **Photodynamic** [MM99]. **photoelectrochemical** [PBOL02]. **Photoelectron** [Ada97b, BB99b, Jør74, Jør78, Köv08]. **Photoexcited** [Mic15]. **Photoionization** [Dol09, GCAGM17, MTA00]. **Photolysis** [KLG+08, Lyo08, BTB+20]. **Photon** [CLÅ05, SAL10]. **Photonic** [Tap17]. **Photophysics** [FLV99]. **photosynthesis** [YMI+21]. **Photosystem** [SIY+15, SIY+19]. **Physical** [BS04, Brä12, GM05, LB92, Rei73, SSCL97, BFHS23, PB20a]. **Physically** [SKGŚ23]. **Physicochemical** [TY85]. **Physics** [BVHK03, Bel11, BR20, Cal13, CT82, Dru78, EBR92, Jan65, Nor98, PD10, PR98, SBF+08, SBK15, Sut97, Sut98, Brä03, HPL98, LSZ+98b, LSZ+98c, SBM+01a, SBM+01b, SBC+03, SBSL08, SCT15, SCT16]. **Physisorption** [SH19]. **Pi** [BS72, Lyk64]. **Pi-Electron** [BS72, Lyk64]. **Picture** [GSTvE98, Ort99, ŻMM23]. **Pictures** [Sim99]. **Pionic** [DKV+19]. **planar** [YFK+97]. **Plane** [SED+98, Sla64]. **Plane-Wave** [Mon05]. **Plasma** [SCM09]. **Plasmas** [BKB+19]. **Plasmon** [AGS+19, JJ20, VG22]. **Plasmonic** [ARS17]. **plasticity** [Sak03b]. **Platinum** [HB14, Hog21]. **platinum-doped** [Hog21]. **Plesset** [GS04a, GC92, OB23, VI01]. **Podolsky** [McW99]. **Point** [CCC17, ST17]. **Poisson** [BS05a]. **Polarizabilities** [AB73, AAAC04, BO86, CMFA99, PM16]. **Polarizability** [CCM05, Kom05, PS05a, RM04, PS21]. **Polarizable** [ABC+98, Cam12, JGCRC16, LJKH13, OK11]. **Polarization**

[CTCS05, GEO91, Odd78]. **Polish** [MG23a]. **Polyacetylene** [BE04, För94]. **Polyatomic** [AK12, Rei73]. **Polycrystalline** [HSS^{+}04]. **Polyelectronic** [MKN10]. **Polyenes** [Bas78]. **Polymerization** [MW08]. **Polymers** [And80, CMFA99, DDPC95, DC99, Ker82, LBV01, RPSB00, SD04]. **Polynomial** [Yas17]. **Polynomials** [DGA18, CAP19]. **Polypeptides** [dLHD10]. **Polypyridine** [CÅ01]. **Populating** [Coo18]. **position** [ÖEO23]. **Positron** [BWVD^{+}13, FJS^{+}04, AP03, MAS03, SSK03]. **Positron-Electron** [FJS^{+}04]. **Positron-Emitters** [BWVD^{+}13]. **Positronic** [Shi12]. **Positronium** [Hug98]. **positrons** [AA19, SJAB^{+}22]. **Possible** [Moh08]. **Post** [TA04]. **Post-Born** [TA04]. **Potential** [Apo01, BB99b, Dru78, GMLSC^{+}10, GW18, HBT^{+}00, KSY08, KB98, KKGG98, LBH^{+}17, LRCR98, LMK19, MFCT15, MCM14, MMSK16, MSM17, Nag01, Nes98, Nes03, PTBH13, RFG^{+}98, SJO05, SED^{+}98, Sil14, SM23, ŻM23, LPC24, SKGŚ23, TMK21, ŻMM23]. **potential-based** [ŻMM23]. **Potentials** [Kap98, MMM18, ST78, ŚBG14, GPEB21, KTA03, MMM19, SZP21, SO19c]. **Poul** [Odd05, SBLJ05]. **Power** [McG04, NA04, Pau13, Por04, SO05a, SRZE04, Sva98, Wei04, BG23, MMM22]. **Powers** [AGO07, CTSO04, PGJ07]. **Practical** [GVCN82]. **Precise** [SBF^{+}08]. **Precision** [LJK^{+}08, Hug98, RSP21, San98]. **predicted** [Mur03]. **Prediction** [FU00, IFAY08, KZR86, Tos08, Ort22]. **Predictions** [CO17]. **Predissociative** [Lyo08]. **Preface** [AUS00, AUW03, AH19a, Ano99o, Ano01l, Ano03i, Ano03j, Ano04j, Ano04k, Ano08k, Ano11h, Ano11i, Ano12g, Ano13i, Ano22g, BG01a, BG01b, BS05b, BS06, BS07, Brä21b, BB24b, CTS15, CTS16, Can10, Cru09a, Cru09b, HP98, Hog13f, HO17, Hog18a, Hog23b, JKMB19b, KS97a, Kle08, KOS99, LB99, Löw64b, Löw65b, Löw67b, Löw68b, Löw70c, Löw72b, Löw73b, Löw74b, Löw75b, Löw77b, Löw78b, Löw80c, Löw81c, Löw81d, Löw82c, Löw82d, Löw85b, Löw86b, Löw88c, Löw89, Löw91, Löw92b, Löw92c, Löw94, Löw95, Löw96a, MH21, MG23b, NB10, OB22b, OJ05, PB20b, RB20, SB09b, SB12b, SB13d, Sab14b, SB15, SB17c, SB17d, SB18b, SO19a, Sem98, Wil98a, Wil98b]. **Preliminary** [Gos02a, KGW98]. **Present** [Bun18]. **Preserving** [Lev14]. **Pressure** [GVFG09, MF14, ST17, Yam03]. **pressure-induced** [Yam03]. **Prevention** [MCP12]. **Previous** [Ano67b, Ano68b, Ano70b, Ano72b, Ano73b, Ano74a, Ano75a, Ano77a, Ano78a, Ano80a, Ano81a, Ano81b, Ano82a, Ano82b, Ano85a]. **Primitive** [SW98]. **Primitives** [KGW98]. **Principal** [Öhr17, Tew21]. **Principle** [HPRR10, LFM89, WT99]. **Principles** [Ada97b, Brä12, CCVB94, DA14, Fuk08a, Fuk08b, HBGvM19, IOI^{+}00, KIT^{+}08, KSY08, MTS04, OYI^{+}00, YKC^{+}08, KTA03, Sak03a, Yam03]. **Probabilities** [VI01]. **Probability** [GL68]. **probe** [SM22]. **Probes** [CPBS05]. **Probing** [Nal06]. **Problem** [DSR81, DST^{+}03, HW01, Hyl64, KS88, KO18, Löw70b, Mat78, MP89, Nic17, SB99, Sut97, vL03, BKL21, Lin02]. **Problems**

[AA01, CTCS05, Del74, GAM+13, Har04, Har05, Kar08, Ler85, LB92, Löw65c, OO82, Sut01, YTF78, Gos02b, SSK03]. **Procedure** [CMDN89, PSS98]. **Proceedings** [Hog13g, Hog14]. **Process** [UYT97, AO03, SKS+19]. **Processes** [ALND10, BGG+07, Brä04, CTSDÖ04a, GBPSR10, HL97, LA12, MCG+08, MF04, MM13, MHWvdA97, MA04, Öhr15, OO82, PSAP10, RNL14, Tap01, Tap09, BLC23, Dur20, LSZ+99a, LSZB00, MMM19]. **Processing** [BB11, BB17]. **Produced** [LS07]. **Product** [PTBH13, LPC24]. **production** [Hog21, HDFT24, KBH23]. **products** [SCJ+23]. **Professor** [SBK04]. **Profiles** [KS77, OE17, ÖEO23, VG22]. **Program** [KTC01, Lad73, TR98]. **Progress** [ADRAB16, Ort22, SBC10]. **Projected** [May80, Sme99]. **projectile** [CTO22]. **Projection** [HMC73]. **Projections** [CL05]. **prolate** [MFA21]. **Propagating** [LSZ+99b]. **Propagation** [SGB16]. **Propagator** [CTCS05, CO17, GEO91, Lon99, Löw85c, MM96, Odd78, ÖB81, Yea05, ZDZO11, Lin02, Öhr02, Ort22]. **propensity** [Hes22]. **Properties** [ABB90, BMPV99, BU97, BJMB14, BK70, CTS04, CCCC15, CMVPFC16, DO09, DA14, DST+03, FE97, Fuk00, GVFG09, Hal64, JJD05, KsKsN08, Kla81, Kot68, KKGG98, Kry81, Kry03, KO19, LDB95, LHL18, Lon99, Löw96b, OK11, OBHM17, PV09, Rei73, RM04, She15, TY85, UK05, VWP+98, Wei72, Bis19, RSP21, SBLJ05, TM21]. **Property** [FPL97, MWL+05, Nic11, Nic17, SB99, SYIY03]. **Property-Specific** [Nic11, Nic17]. **Prospects** [WM97]. **Protein** [GBPSR10, FB20, GG20, LL20]. **Proteins** [Kot68]. **Proton** [BWVD+13, Coo18, CS04, DBC+99, HSS+04, McG04, MBM99, Oni15, PBK04, SIY+15]. **Proton-Conductors** [Oni15]. **Protonated** [KKK+97]. **Protonation** [PWZ+08]. **Protons** [AGMdV+13, BRL13, CTSDÖ05, AA19, Kar24]. **Pseudo** [CKRT03, DST+03, GW17, KBS03, TSTH03]. **pseudo-binary** [TSTH03]. **Pseudo-Jahn** [CKRT03, DST+03, KBS03]. **Pseudopotentials** [Gut97]. **PSII** [YKS+12]. **Pt** [SN08, Hog18e, KBH23, KC19, SH19, WHB+24]. **Pt/Al** [KBH23]. **publications** [Ano04i]. **puckering** [MFMCN01]. **Pulse** [VTM98, CM24]. **Pulsed** [BS98]. **Pulses** [MCP12, ML18]. **Pure** [Gal73, LK90, MLR+98]. **Pure-State** [LK90]. **Purine** [PP68]. **purpose** [LH20]. **Pyramidal** [YTC+05]. **Pyrimidine** [PP68].

QED [LT98]. **QM** [BBB10, MC10, SBC10, SIY+15, TL10, ZLC+10]. **QM/MM** [BBB10, SIY+15, MC10, TL10, ZLC+10]. **QSPR** [Sey12]. **Quadratic** [BB13, GC92, LPDB03]. **Quadrature** [Kou15]. **Quadrupole** [PS05a]. **qualitativeness** [PB20a]. **Quantification** [Bel06]. **Quantisation** [PS05b]. **Quantitative** [WD70]. **Quantities** [CH03, KTC01]. **Quantum** [AČP88, AT91, And80, Ano04l, Ano13a, Ano13b, Ano19a, AA01, AGL05, BND81, Bad09, BR82, Bel09, Bel11, BSB13, BB17, BR17, BR65, Brä08, BR20, Brä21a, BB22b, Brä22, BB24a, BKB+19, CCM05, CL05, CD05, CCVB94, CCC17, CS77, CC97, CB18, Cra99, Dau67, Dau70, DO09, Deu99, Dra20, DKV+19, DW98, Fro02, GC10, GG20, GMB04, GSWW10, HPL98, HG17, HPRR10, Hog13a, Hog13b, HB14, Hog18b, Hog18e, Hog21, Hog23a, Hog23c, HDFT24, IBB$^+$19, ILS08, Jan65, JKMB19a, Kar97, KS97b, KBH23, Kla81, KD11, Kra99, Kuk14, KV08, KZR86, Lad73, LBH$^+$17, Lar17, Len68, Löw64a, Löw65a, Löw65c, Löw67a, Löw67c, Löw68a, Löw70a, Löw72a, Löw73a, Löw74a, Löw75a, Löw77a, Löw78a, Löw80a, Löw81a, Löw81b, Löw82a, Löw82b, Löw85a, Löw86a, LSZ88]. **Quantum** [LSZ89, LSZT90, LSZ91, LSZ92a, LSZ92b, Löw92a, LSZ94, LSZ95, LSZ96, LSZ$^+$97b, LSZ$^+$97a, LSZ$^+$98b, LSZ$^+$98c, LSZ$^+$98a, LSZB99, LSZ$^+$99b, LSZ$^+$99a, LSZ$^+$00, LSZB00, LL20, MG21, MCG$^+$08, MS03, MG20, Mat64, McW98, Mez96, MT04, Mic17, Miy03, Moh98, Moh08, MP97, MG23a, NAY$^+$08, NFW$^+$98, NBS10, Nic11, OS05, Öhr17, Oni12, Oni15, PD10, PBOL02, PSAP10, PB20c, Pul77, Pyy78, QSG98, Ray95, Ryc98, SBM$^+$01a, SBM$^+$01b, SB02, SBA$^+$03, SB03, SBC$^+$03, SBCT04a, SBCT04b, SBK04, SO05b, SB05, SBLJ05, SB06, SB07, SBSL08, SBK$^+$08, SBGJ08, SBC09b, SB09a, SBC09a, SBC10, Sab11, SB11, SB12a, SB13a, Sab15, SB17a, SB18a, SPD09, Sal11, SJO05, Sey12, Sig05, SBG$^+$98, SAL10, SGK$^+$08, Sut98, TMN10, Tap09, Tap11, Tap17, TR14, TMMS10, Tos08, TL10, VTM98, Wei72]. **Quantum** [WMM$^+$98, WDD16, vS07, BMR$^+$24, BPK23, BP20, BKL21, CCT02, EW03, HO16, Kar24, LÖS02, LT21, Mic02, MOB$^+$03, NBA20, NTT20, Per20, PMK23, SB17b, SH19]. **Quantum-Chemical** [Kuk14, SJO05, PBOL02]. **Quantum-Classical** [MT04]. **quantum-electrodynamic** [PMK23]. **Quantum-Informed** [TR14]. **Quantum-Mechanical** [BB17, KZR86, Pul77, Wei72, vS07]. **Quantum/Classical** [GMB04, PSAP10, EW03]. **Quarks** [JL03]. **Quartet** [ZBM98]. **Quasi** [GDL14, JSG$^+$14, Shi12]. **Quasi-Bound** [Shi12]. **Quasi-Molecule** [JSG$^+$14]. **Quasi-Newton** [GDL14]. **Quasidegenerate** [BB99b]. **Quasiparticle** [HL90]. **Qubits** [Coo18]. **Quest** [PM14]. **Questions** [DE05].

R [HSR98, JJD05]. **R.** [AGS$^+$19]. **Radial** [ÖÖ13, PS05a, SJO05, ALA23, Lin02]. **Radiation** [BWVD$^+$13, BB13, BB15, Bic13, CL07, CT82, Glu19, LS07, PGJ07, Ram98, Sab07, Sal11, ST07, VTM98, SB07, SS22]. **Radiation-Induced** [Sal11]. **Radiationless** [OO82]. **Radiative** [BS98, BKB$^+$19, DKV$^+$19, KSG08]. **Radical** [ARS99, CL07, EEL96, KBS03, LM97, Lin05, LGK$^+$99, She15, vS07]. **Radicals** [GAI08, LS07, MLPD$^+$98, MVL01, RRMAF08, Tur07, VKI97, YMI$^+$21]. **Radioactive** [Per98b]. **Radiobiological** [BB15]. **Radiobiology** [Fra13]. **Radium** [Bar23]. **Raman** [CM24, MCP12, TP03]. **Ramsey** [PB05]. **Range** [BBB10, Dru78, DB01, DB13, JGCRC16]. **Ranges** [AGO07, Pau13]. **Rare** [BG73, Jan65]. **rate** [SS22]. **Ratios** [MTA00]. **Ratner** [SB17b]. **Ray** [Ada00, CS77, GM17, Kaw97, KsKsN08, KNM$^+$08, MYW00, MW08, MKK$^+$00, MTA97, MTA00, Mur08, Tak19, Uda00, UMD08, YFK$^+$97, Mur03, YKS$^+$12, YNNU03]. **Rayleigh** [BH24, MM99]. **Rays** [AAM04]. **Rb**

[BJMB14]. **Re** [LSZ$^+$99a]. **Reactants** [ASGG08]. **Reaction** [ACC99, ACDV01, ASGG08, BRW08, FHHZ88, Hog18e, JGNJ08, PL98, PTLGOM12, RRMAF08, Saa01]. **Reactions** [BR82, FF72, GAI08, HB14, Kuk14, MÅ01, MM99, MBM99, PSAP10, RAR$^+$08, SW81, Sko12, TMN10, Hes22, PEMC23, YMI$^+$21]. **Reactive** [GSWW10, Nal06]. **Reactivity** [Bro98a, Bro98b, Dau67, Dau70, MF14, MNR$^+$98, Nal03, ST78, SH95]. **Real** [Ste73, Bis19, WLM23]. **real-time** [WLM23]. **realise** [Zap01]. **Rearrangement** [KS88, Mic99, UYT97]. **Reasonable** [WD70]. **Recognition** [Rei73]. **reconstructions** [BB22a]. **Recurrence** [BL18, ÖÖ13]. **Reduced** [BK70, Kry81, LGJP99, PKYM01]. **Reducing** [YÖ13]. **Reduction** [AHPD$^+$03, OO05, OM03]. **Reference** [BŚG14, LT98, MDBM98, OB23, SH19]. **Refined** [YKS$^+$12]. **Reflections** [Noo09]. **Reforming** [Fuk08b]. **Reformulation** [Cio90]. **REG** [FSP23]. **REG-MULTI** [FSP23]. **Region** [BS98, CCC17, GWW19]. **Regioselectivity** [RGA99]. **Regression** [Löw92a]. **Regular** [And80, SR73, YZDM01]. **Regularization** [PSS98]. **Reinvestigation** [PB05]. **Related** [ACDK72, KTC01]. **Relation** [DGA18, Kry03, Sri01, VG22]. **Relations** [BL18, IL98, KNN17, Löw92a, ÖÖ13, SPM09, EW03]. **Relationship** [KB86]. **Relative** [HB14, Kou15]. **Relativistic** [Bar23, Coh04, DKV$^+$19, ERC88, FAS$^+$98, Glu19, HMH$^+$18, HBT$^+$00, Khe19, Ono00, Pyy78, QSG98, SED$^+$98, UK05, VI01, YZDM01, GPEB21, Sau05a, WHB$^+$24]. **Relativity** [Brä08]. **Relaxation** [Jør74, PSAP10, SPG$^+$22]. **Release** [Ber14]. **relevance** [Bel21]. **Relevant** [ILS08, Tur07]. **Remarks** [Die97, Uda97]. **Removing** [Sim05]. **Renner** [BMP03]. **Renormalization** [Kri03, PSS98, RPSB00]. **Reorientations** [YAJHR03]. **Repair** [BB13, BB15]. **Repair-Based** [BB13]. **report** [Gos02a]. **Representability** [LK90]. **Representation** [DGA18, JSG$^+$14, KT98, Per98a, SGB16, JS21]. **Representations** [CTG98]. **Reproduce** [DSW04]. **Reproduction** [KMR01]. **Repulsion** [Ave13, AA18]. **Repulsive** [DB01, DB13]. **Required** [JJD05]. **research** [Gos02a, KÖO23]. **Reservoirs** [Mar08b]. **Residues** [ST17]. **Resolution** [BB11, BB17, Jos08, YKS$^+$12]. **Resolved** [WmG18]. **Resonance** [Bel06, BB11, DeB09, HBE$^+$98, KG12, LA12, Löw88b, LFM89, Ram08, Vis05]. **Resonances** [MM96, Nic17, STZY18, SW81, Sko12, BB21, FCAG19, FTG22]. **Resonant** [AAE$^+$01, GC10, GP04, KO19, PLA01, UYT97]. **Resonant-Coherent** [GP04]. **Response** [ÅVM96, BB13, FPL97, HJ99, JJD05, JH99, Krs16, LV90, LÅJM95, Mic15, MCA$^+$18, PS05a, PM16, RTV05, SBLJ05, Sim05, BLC23, TM21]. **Rest** [KS88]. **Restricted** [FCH15, RTV05]. **resultant** [Nal23]. **Results** [BG23, BH24, Lad73, Miy03, VTPR97, VWOS89, WM97]. **Review** [ASGG08, DB13, Kla81, KHPP23, MK23, Nor98, PMK23, ZZ08, BPK23]. **Revision** [TAM04]. **Revisited** [BND81, BE04, Ran18]. **Revisiting** [LPC24]. **Rh** [GBHM14]. **Rhombohedral** [NP03]. **Rigged** [Tap01]. **Rigid** [Sme92].

Ring [CPBS05, MFMCN01]. **Rings** [FLV99, PWZ$^+$08, BMC97]. **Ritchie** [AGS$^+$19, SO19b]. **Ritz** [BH24, MM99]. **RNA** [AGO07, KN01]. **Robust** [Kou15]. **Role** [GAI08, Kap98, LA12, LASV18, TSON00]. **Root** [MH98]. **Roothaan** [DKMP98, OE17, ÖEO23]. **Rosen** [McW99]. **Rotation** [PR05, SR73, YTC$^+$05]. **Rotation-Vibration** [YTC$^+$05]. **Rotational** [Les75, MWL$^+$05, SJO05, Sau05b]. **Rotations** [CMDN89, MFLK11]. **Rototranslational** [LDB95]. **route** [Hog23c]. **Routes** [BBB10]. **rubrene** [ZLL$^+$20]. **Ruby** [ITI$^+$00, OYI$^+$00]. **Rufus** [SO19b]. **Rule** [CTSOS99, KP77]. **Rules** [CTO18, Coh04, LDB95, OOSS17, Yan81, CTSSO19]. **RuO** [NIO03]. **rutile** [Sak03a]. **Rydberg** [LM97, MLPD$^+$98, MVL01].

S [CSZ99, Miy03, MFMCN01, VT24]. **Sabin** [OB22a]. **Salpeter** [ORL23]. **salt** [MST$^+$03]. **saltatory** [JJ20]. **Sampling** [HS19]. **Sandwiched** [OBHM17]. **Satellite** [Uda00]. **Scalar** [CPBS05]. **Scale** [Fra13, SIY$^+$15]. **Scaled** [STZY18]. **Scaling** [Lev90, Löw88b, LFM89, LLBK$^+$98]. **Scattered** [HL97, Joh73]. **Scattered-Wave** [HL97, Joh73]. **Scattering** [GSWW10, Nes75, Shi12, ST07, TP03, WHB$^+$24, AMAA22, BKL21, HHU$^+$21, HM19, Kar24, SJAB$^+$22]. **ScB** [KM98]. **SCC** [dLHD10]. **SCF** [Ave98, CG80, CDP82, GVFR98, PTC$^+$13]. **SCF-LCAO** [PTC$^+$13]. **Scheme** [DKMP98, LFM89]. **Schemes** [MC10]. **Scholar** [SO19b]. **Schrödinger** [MKN10, BG23, Hyl64, MFCT15, SBK15, VTPR97]. **Science** [JG08, McW01, Odd05, Tan00, AO03, LSZ$^+$00, SBA$^+$03, SBGJ08]. **Sciences** [Löw92a, Ram08]. **Scientific** [Bun17, Kar02]. **Scientist** [Lin99, OB22a, Öhr05]. **Scope** [SIY$^+$19]. **Screening** [HL90, MA04]. **Search** [Kom05, Lev90, Löw92a, Nes98, Zap01]. **Searches** [Kar08]. **Second** [AHPD$^+$03, HJ99, Hät05, IL98, LDB95, MW98, RR05, SW98]. **Second-Order** [Hät05, IL98, LDB95, RR05, SW98, AHPD$^+$03]. **Section** [Jos08]. **Sections** [CTSDÖ04b, CTSDÖ04a, HMH$^+$18, PBK04, RGFC13, MG22]. **Selected** [Bun18, CHSC03, Mar08a, CAG$^+$21, SM22]. **Selection** [CTSOS99, HS19]. **Selective** [AAM04, KKA97, LGK$^+$99, MM99]. **Selectivity** [RGA99]. **Self** [DDPC95, GDL14, HL90, LJKH13, LSC19, Per90, Sla72, WD70, YNNU03, Ort22]. **Self-absorption** [YNNU03]. **Self-Consistent** [GDL14, Sla72, LJKH13, LSC19]. **Self-Consistent-Field** [WD70, Ort22]. **Self-Energy** [DDPC95, HL90]. **Self-Interaction** [Per90]. **selforganization** [Brä02]. **Selftrapping** [MS03]. **Semi** [HSS$^+$04, LK09, Sim99]. **Semi-Classical** [Sim99]. **Semi-empirical** [HSS$^+$04]. **Semi-infinite** [LK09]. **Semiclassical** [HPU$^+$17]. **Semiconductor** [Kra99]. **Semiempirical** [HPU$^+$17]. **Seniority** [ATL$^+$18]. **sensitive** [AMAA22]. **Sensitivity** [PM14]. **sensitized** [GTB23]. **Separability** [McW98]. **Separation** [DeB09, OYI$^+$00]. **Sequence** [CÅ01, VI01, VT24]. **Sequences** [KGW98, KCM70, VT24]. **Sequential** [CCM05, CC97]. **Series** [Ano08l, Ano09i, Ano12h, Ano14e, Ano15g, Ano15h, Ano16d, Ano17j, Ano17k, Ano17l, Ano18d, Ano19q, Ano19r, Ano20g, Ano20h, Ano21g, Ano21h, Ano22h, Ano22i, Ano23g, Ano23h, Ano24d, CB18, Hog18f, Jør78, PB75, SB13e, BG23, SÁ23a]. **Set** [CTSOS99, QGW01, SDGW98, Tap17, VWP+98, RA19, SKGŚ23, Wen21]. **Sets** [AT91, AH19b, GW01, Kla81, MW98, OOSS17, PTC+13, QGW01, SPAS05, SW98, VWP+98, WM97, CCM+19, CAP19, GW23]. **Seven** [HDFT24, LC03]. **Shakeup** [SNMI00]. **Sham** [GV09, KB98, LK90]. **Shape** [AMAA22, MM96]. **Shape-sensitive** [AMAA22]. **Shapes** [BWK97]. **Shell** [Bra77, CG80, DKMP98, FMA08, GVFR98, HUS+11, HL97, JSF08, KS88, LP97, LASV18, MP89, RTV05, MU03, VG22, YMI+21]. **Shielding** [JH99, JcH18, Vis05]. **Shift** [AB73, NA19]. **Shifts** [DY08, HDB03, PGV97]. **Short** [DB01, SGB16]. **Showing** [Jør74]. **SI** [Moh08, CTSSO19, JS21]. **side** [BFHS23]. **Sightseeing** [Ros98]. **Sign** [NA19]. **Signal** [BB11, BB17, DeB09]. **Signal-Noise** [DeB09]. **Signals** [Bel06, Bel11, BB22a]. **SiH** [JSG+14, MVL01]. **Silicate** [KE97, KE00]. **silicates** [NHM03]. **silicide** [TSTH03]. **Silicon** [DO09, HOI+08, KIHA97, EOH03]. **Similarities** [MVL01]. **Similarity** [CCVB94, Löw88b, LFM89, SNM+97, WN05]. **Simple** [AČP88, San98]. **Simplest** [SGM+13]. **Simplest-Level** [SGM+13]. **Simulate** [JJD05]. **Simulation** [Fra13, HB14, MP97, RFG+98, MFMCN01]. **Simulations** [BHV+00, CMJR+04, GBPSR10, HS19, HBGvM19, PWZ+08, TMN10]. **SiN** [Jan97]. **Sinc** [Kou15]. **Single** [BRL13, Bis67, EM17, GWM+03, HBE+98, MH98, Nag01, Tos08]. **Single-** [EM17]. **Single-Center** [Bis67]. **Single-Root** [MH98]. **Singles** [HS86, LGJP99]. **Singlet** [BHM17, GV09, GL68, RLF17, Sme99, SKS+19, VT24]. **Singlet-Triplet** [GL68]. **Singularity** [GS04a]. **SiO** [GP14, MKK+00, OTA97]. **Site** [Bro98a, Chi03, Bro98b, DAB+23]. **Situation** [OW08]. **SIWB** [Fuk15]. **Six** [BH24]. **Size** [CDK15, DDPC95, EM17, IKN+08, Per90]. **Size-Consistency** [DDPC95, Per90]. **Size-Extensivity** [EM17]. **Size-Intensivity** [DDPC95]. **Sizes** [LR72]. **Slag** [MKK+00]. **Slags** [MKH+97]. **Slater** [AYÖ17, HPB17, KÖO23, Mon05, PTC+13, PTBH13, Rui23]. **Slater-Orbital** [Mon05]. **Slater-Orbital/Plane-Wave** [Mon05]. **Slater-Type** [AYÖ17, HPB17, Rui23]. **Slow** [SCTH+07, JS21]. **Small** [HL97, Kap98, Nes67, RK04, UK05]. **SMILETRAP** [SBF+08]. **SnO** [GP14]. **Sodium** [CKRT03, NHM03]. **Soft** [AAM04, KNM+08, Mur08, UMD08, Mur03]. **Software** [KS97b]. **Solar** [KD11, GTB23]. **Solid** [AYÖ17, AJ04, EG99, FAS+98, Löw65c, Miy03, SR73, IOA03, SEL01]. **Solid-State** [EG99, IOA03]. **Solids** [AL04, CMJR+04, DC99, GSTvE98, Gon98, GL90, Köv08, PGN04, AP03, AGS+19, MAS03, SSK03]. **Soliton** [För94]. **Solution** [BH24, BE01, Cam12, CCM05, CB18, JGCRC16, KGW98, MYW00, MFCT15, MKN10, PWZ+08, dLHD10]. **Solutions** [BC09, HPRR10, Kob97, TMN10, MST+03, SKGŚ23]. **Solvation** [KGW98]. **solvatochromism** [CCT02, LCC22]. **Solvent** [AB73, ABC+98, BMPV99, Bas64, CC97, GMLSC+10, MBM99, SS22].

Solvent-Mediated [MBM99]. **Solvent-Shift** [AB73]. **solvents** [CCT02, LCC22]. **Solver** [BS05a]. **Solving** [YÖ13]. **Some** [Ber74, CG80, Dau70, DE05, GEO91, HPB17, HKS90, Ler85, Löw85c, LM92, Löw96b, Löw98, STZY18, SGM+13, Sut98, Sut01, UK05, VTPR97, WM97, YFK+97, SBC10, Löw65c]. **Son** [Heh18]. **Source** [GDL98, Lyo08]. **Sources** [AVB08, BGG+07]. **Space** [BB99b, Dah01, FCH15, GW17, GSWW10, LEK01, MMSK16, Bis19, LMK19, ÖEO23, TMK21]. **Space-Pseudo-Time** [GW17]. **Spaces** [LK09]. **Spatial** [ATL+18, BLC23]. **Special** [Ano12i, Brä08, Löw85c]. **Species** [DNM+14, She15]. **Specific** [Kar24, MDBM98, MKN10, Nic10, Nic11, Nic17]. **Specifics** [Bun17]. **Spectra** [ÅCL92, Ada00, AB73, Bas64, Bas78, Bel11, BB99b, CÅ01, HDB03, JJD05, JGCRC16, Jør74, Jør78, Kaw97, Köv08, Löw88b, LFM89, MVL01, MC10, MHWvdA97, NM00, NBS10, Pet98, RLF17, SJO05, SSV98, Tak19, Uda00, EÜSB21, IOA03, Köv03, Mur03, NBS12, Sak03a, SA23b, YNNU03]. **Spectral** [APNM03, BS98, Mur08, OO05, PB75, UMD08, YKY+00]. **Spectrometer** [KNM+08]. **Spectrometric** [MRS+99]. **Spectrometry** [OO05]. **Spectroscopic** [JJD05, LvWH+01, MW08, RM04]. **Spectroscopy** [BBB10, Bel06, BB11, BB17, BS98, BKB+19, CE78, DKV+19, DeB09, Glu19, HSS+04, Hug98, ILS08, KGI+19, MYM08, Per98b, Ram98, Ray95, SCM09, BB21, BB22a, LSZ+00]. **Spectrum** [Ada97b, CCCC15, CSZ99, MKK+00, SP99]. **Spherical** [Aqu09, Dol09, Lau09, Lin17a, PS05b, SR73]. **Spheroconal** [MFLK15]. **Spheroidal** [KO18, MFA21]. **Spin** [ÅVM96, CAG+21, CHSC03, CCSZ01, DAB+23, DE05, ERC88, Gal73, KKA97, LP97, LF09, Lon99, Mat64, May80, MÅ01, NeMM03, PKYM01, RM04, RP72, Sal74, SPAS05, Sau05a, WmG18, YKS+12, Yea05, Fuk03, VT24]. **Spin-adapted** [CAG+21]. **Spin-constrained** [DAB+23]. **Spin-Coupled** [CCSZ01]. **Spin-Crossover** [NeMM03]. **Spin-Free** [Mat64]. **Spin-Interactions** [Sau05a]. **Spin-Orbit** [ÅVM96, ERC88, LF09, RM04]. **Spin-Projected** [May80]. **Spin-Resolved** [WmG18]. **Spin-Selective** [KKA97]. **Spin-singlet** [VT24]. **Spin-Spin** [DE05, Lon99, PKYM01, SPAS05]. **spin-states** [Fuk03]. **Spin-Tensor** [Yea05]. **Spins** [Eks98]. **Square** [Löw92a, MFCT15, YFK+97]. **Square-planar** [YFK+97]. **Squares** [LJK+08]. **Squeezing** [BR17, Phi98]. **Sr** [GWM+03, KIT+08, GVFG09, NIO03]. **Stability** [Eks98, Jan97, Jan65, MBAPS19, TLOK97, CBSM20, FB20, YIYM03]. **Stabilization** [SSS05]. **Stacking** [FU00, UJYU03]. **Standard** [LBH+17, CCM+19]. **Standpoint** [vS07]. **State** [Ada97a, AdMB99, AB73, AH19b, BS04, CMVPFC16, EG99, Fuk08a, HBKS03, KT15, Kom05, KE97, LT98, LPDB03, Lin98, LK90, MDBM98, MS03, MKN10, MW98, MKK+00, Nag01, Nic10, Nic11, Nic17, RLF17, RT18, Tap17, VWOS89, WMM+98, WN05, CTSSO19, CBSM20, Dur20, Hog21, IOA03, MFMCN01, NHM03, RA19]. **State-** [Nic11, Nic17]. **State-Quantum-Chemistry** [Tap17]. **State-Specific**

[MDBM98, MKN10, Nic10]. **States** [AAE+01, ALND10, AR03, AA05, BR05, BK70, CY00, CKRT03, FE97, GAI08, Gal73, GC10, GV09, Hät05, KM98, KG12, Kom05, KE00, KO19, LMSP01, LP97, LA12, LKD05, Löw88b, LFM89, MKN10, MKH+97, MYM08, MMSK16, Nag97, Nic10, Nic17, Oli90, PD10, PB99, RPSB00, RAR15, RM04, Shi12, Sme99, SBDD03, Tap11, TM13, Wei04, Bel19, BKL21, Fuk03, JMWG19, MFA21, MK23, Nag03, Nal23, NBS10, NBS12, OTA03, OB23, PS21, SZP21, UJYU03, VT24]. **Static** [IS01, PM16]. **Statistical** [Kou15, PD10, Sla72, Spe78]. **Status** [Bun18, KT15, SBG+98]. **Steam** [Fuk08b]. **Steel** [MKH+97]. **Stemming** [YZDM01]. **step** [HDFT24, RZTSW23]. **Stereochemistry** [CH03]. **Stereoregular** [CMFA99]. **Stereoselective** [LDP+04]. **Sternheimer** [FPL97]. **Sternheimer-Like** [FPL97]. **STO** [AA18]. **Stochastics** [Bic13]. **Stoichiometric** [APNM03]. **Stopping** [AGO07, BS04, CTSDÖ04a, CTSO04, CS04, MTS04, McG04, NA04, PGJ07, Pau13, PBK04, Por04, SO05a, SRZE04, Sig05, CTO22, MMM22, MG22, VG22]. **Storage** [PB14, YM97, YM00]. **Stored** [Ber14]. **STOs** [LPC24, ÖÖ13]. **Strand** [Sim07]. **Strategy** [CTG98]. **Strength** [CTSO04, HK03, OOSS17, TLOK97, CTSSO19]. **Strengths** [BLKS78, CTSOS99, Khe19]. **Stretching** [She15]. **Strong** [Chi03, DKV+19, IS01, SBG+98, VTM98]. **Strongly** [DBC17]. **Structural** [DO09, MYW00, SIY+19, VWOS89, YKC+08, Yam03]. **Structure** [ADRAB16, AH19b, Bli65, CL00, DLMS03, EGCL91, EEL96, FP06, FCH15, Fuk00, Fuk15, GSTvE98, GS04a, Gre08, GM91, Har18, Hät05, HJ88, Hog13g, IOI+00, Jan97, KM98, Kat03, Ker82, KsKsN08, KIHA97, KNI+08, KSY08, Kot68, Löw80b, LASV18, MYW00, Nal03, OYI+00, PGN04, PWZ+08, PP68, SS98, SPD09, ST78, SMAS08, TY85, TS10, WD22, YFK+97, BKL21, CTO22, CCL03, EW03, GTB23, Hog14, Ito03, KC19, LSZ+97a, LSZ+99a, LSZB00]. **structure-function** [EW03]. **structured** [Mur03]. **Structures** [BMPV99, CMVPFC16, HOI+08, HTS+00, ITI+00, KIT+08, Köv08, KN01, SNM+97, SIY+19, SSV98, SNIM08, Uda00, YKS+12, YM00, EOH03, KOT+00, KTA03, NHYU03, NIO03, YIYM03]. **Strutinsky** [DKMP98]. **Studied** [BRW08, HSS+04]. **Studies** [AAE+01, AA19, ASGG08, BWH08, Cse97, DY08, Fra13, FHHZ88, Gre73, Les75, LM92, LGK+99, MCG+08, Mar08b, MW98, RAR+08, Sab07, Tur07, MGAUP23, PBOL02, RSP21]. **Study** [ARS17, BJMB14, CTCS05, CCM05, CG80, CL07, CKC09, CPBS05, CS77, CSZ99, Cru09c, DO09, DNM+14, GMLSC+10, GV09, GBHM14, ILS08, JJD05, Jan97, JGCRC16, KIT+08, KGW98, KB98, KKA97, KT98, Lad73, Mam19, MYW00, MW08, MBM99, PSAP10, RMN+14, RRMAF08, RT18, Sab97, SG80, VKI97, YFK+97, ZBM98, BMC97, Bel19, BTB+20, GC01, ORL23, TBM01]. **Sturmian** [AA01, AAG03, AAAC04, GAM+13, GW23, GCAGM17, KO18, MFA21, RA19]. **Sturmians** [Ave98, AA05, Ave13, AA18, CCA13, Gos02b]. **Subject** [Ano64e, Ano65e, Ano67f, Ano68f, Ano70f, Ano72f, Ano73f, Ano74d, Ano75d, Ano77e, Ano78d, Ano08m, Ano12j]. **Subshell** [KRL01]. **Subshells**

[HMH+18]. **Subspace** [GDL14]. **substituents** [GC01]. **Subsystems** [Nal00]. **successive** [PEMC23]. **Sulfur** [SN08, TSON00]. **Sulfuric** [BWH08, KLG+08, KV08]. **Sum** [CTSOS99, CTO18, Coh04, LDB95, OOSS17, CTSSO19]. **Summary** [Lad73]. **Summation** [SÁ23a]. **Summations** [DDPC95]. **Super** [KE98]. **Super-Heavy** [KE98]. **Superconducting** [TMM03]. **Superconductivity** [DB13, DBC17, Kri03]. **Superconductors** [DB01, Lar17]. **Supercritical** [CCCC15, CCC17, Gre08]. **Superexchange** [MCC03]. **Superheavies** [Gre08]. **Superheavy** [FSB+97]. **Superionic** [KTMA08]. **Superposition** [Tap09, VWP+98]. **Support** [Duc97]. **supported** [Hog23c]. **supporting** [Per20]. **Surface** [IKN+08, LC03, PGN04, SN08, VWOS89, Sak03a, SH19, SHBC19, SKK23, ŻM23]. **Surfaces** [AJ04, BB99b, BWH08, LBH+17, SS98, TTLB04, AGS+19, HM19, SCE19, Tők19]. **Surrounding** [Jør74]. **survey** [Ros97]. **Susceptibility** [Laz04]. **Suter** [Miy03]. **Swift** [Sab97, SBCT04a, SBCT04b]. **Switching** [ST17]. **Symbols** [McW01]. **Symmetric** [ACDV01, Col68, Gal73]. **symmetries** [QSW20]. **Symmetry** [AAM04, Ber03, BK70, DST+03, Fow03, Har05, KCM70, KMJ97, Kry81, Ser74, SBDD03, Yan81, KHPP23]. **Symmetry-Adapted** [KMJ97, KHPP23]. **Synthesis** [LDP+04]. **System** [CDK15, GVFR98, Mic15, Moh08, SIY+15, Tos08, ZBM98, Mic22, ŻM23]. **System-Size** [CDK15]. **Systematic** [BJMB14, KGW98]. **Systematically** [SW98]. **Systems** [APNM03, AČP88, ABB90, AGL05, AK12, BGG+07, Bad09, BS72, Ber03, Bra77, BC09, Cal85, CB18, DKV+19, DR90, DBC17, EG99, FIK+03, Fow03, FCH15, Gal73, GC10, HS05, HA13, Har17, HG17, HMW01, IBB+19, KS77, KT98, KTC01, KNN17, KGI+19, LPDB03, LS07, Lin17a, Lin17c, Mar08a, MC10, McW98, MT04, Mon05, MBO+07, Nal06, Nal09, Ohn67, PČ75, PKYM01, Pol03, RTV05, RAR15, RLF17, San98, SRZE04, SPM09, Shi12, SCM09, Sut98, TY85, TAM04, WDD16, BLC23, BPK23, Brä02, KC19, LSZT90, LSZ+98b, LSZ+98c, Min22, SBM+01a, SBM+01b, SBC09b, SBC09a, SPG+22, TSTH03].

T [DB01]. **taa** [NeMM03]. **taatris** [NeMM03]. **Table** [Ros98]. **Target** [CTSO04, CTO22]. **Targets** [CS04, HMH+18, MMM22]. **Tartaric** [HSR98]. **Tautomeric** [KZR86]. **Tautomerism** [KN01, LK14]. **Tautomerization** [HBGvM19]. **Teacher** [Öhr05]. **Teaching** [Deu99]. **Technique** [Löw67c, Löw98, WD70, Lar02, MG21]. **Techniques** [CCVB94, DSR81, Eks98, Mon05, PB75, BPK23]. **Teller** [ABGM03, ADA03, BP82, BO86, Ber03, BMP03, Chi03, CKRT03, DST+03, FIK+03, GWM+03, HBKS03, KH03, KBS03, LPDB03, LC03, LM03, MS03, MCC03, NeMM03, OM03, Pol03, SKT+03, SS03, SIY+19, SCN03, YAJHR03]. **Temperature** [DLMS03, DB13, DBC17, HK03, HBKS03, MF14, WDD16, TMM03, TSTH03, ZLL+20]. **Temperatures** [BB14, Sak03b]. **Tempered** [KGW98]. **Tensor** [MWL+05, Sau05b, Yea05]. **Tensors** [JcH18, Vis05]. **Term** [AHPD+03, VI01, BMR+24]. **Terms**

[BVHK03, Jan65, Kho04, NM03, Öhr16, PKYM01]. **terpenes** [Hes22]. **testing** [PEMC23]. **tetraazacyclotetradecane** [MYW00]. **Tetragonal** [DA14]. **Tetrahedral** [CL05, Cse97]. **Tetramethyldiamide** [HSR98]. **tetraphenylporphyrins** [NHYU03]. **Tetroxide** [RNL14]. **Their** [AČP88, AFE13, BWK97, FE97, GDL98, HM21, KNM+08, LA12, PP68, RK04, Sva98, TY85, dLHD10, Hes22, KOT+00, SYIY03, VG22]. **theorem** [Ort22]. **Theoretic** [Kob68, Nal03, Nal23]. **Theoretical** [Ada97b, Ada00, ASGG08, BWH08, BKC68, BTB+20, CCVB94, CPBS05, CSZ99, DSR81, FHHZ88, GM05, IFAY08, JJD05, JG08, KP77, KKK+97, LK14, Ler85, LGK+99, MG21, MST+03, Miy03, MAS03, MHWvdA97, Pet98, RAR+08, Sab07, STZY18, SIY+15, SIY+19, SG80, Sla81, SSK03, TBM01, ZZ08, ZBM98, Brä03, GC01, SBGJ08, SL20, SEL01]. **Theoretically** [Mur03]. **Theories** [BMM13, Bra67, Cio90, DB68, FH65, GL90, LK13, Nag03, WN05, Bel22, LH20]. **Theorists** [Len68]. **Theory** [ÅVM96, ÅCL92, Ano04l, ARS17, ACDK72, AGL05, BND81, BVHK03, Bas64, Ber74, Bli65, BC00, Brä08, Brä12, Bra77, Bro98a, Bro98b, BŚG17, CTS04, CTCS05, Cam12, CG80, CDP82, CCSZ01, CO17, Dau67, Dau70, Del74, DC99, EG99, EEL96, FP06, FF72, Fuk15, GC10, GC92, GW17, GDL98, GBHM14, Gon98, GS04a, GSWW10, GS04b, GK90, Gut06, Hal91, Har90, Har67, HJ99, HJ88, HBE64, Hog13g, HW01, HMC73, Joh73, Khe19, KMHL13, KMJ97, KK85, KB86, Lad73, Lau09, Lev90, LP97, LS03, Lin17c, LJKH13, LB92, Löw65c, Löw67c, Löw88b, LK90, LLBK+98, LÅJM95, MH98, Mat96, MS65, MFLK15, Mic15, Nag97, Nal09, NSM11, Nes75, Nes03, Nic10, Nik70, Noo09, ODE75, ÖB81, PČ75, Pal04, Per90, PB05, PM16, PGP17, RR05, RTV05]. **Theory** [RC05, SBCT04a, SBCT04b, SB07, SBC09b, SBC09a, SRZE04, SS03, SS90, SW98, Sid18, Sig05, Sme92, SGM+13, TMN10, Tap01, Tap09, VWOS89, VKI97, VRG90, VI01, WT99, Yan81, Yan90, AO03, CTC22, CBSM20, GTB23, HM19, KHPP23, LSZT90, LSZ+98a, MGAUP23, MPU19, MOB+03, MK23, NBS12, OB23, ÖEO23, PEMC23, PMK23, SBLJ05, Tew21, TM21, Zap01]. **Theory-based** [SRZE04]. **Theory-The** [Gut06]. **Therapy** [BWVD+13, Bic13, PGJ07, Pau13, Bel21]. **There** [FCC04]. **Thermal** [MYM08, TLOK97]. **Thermochemistry** [Hur73, Mar08b]. **Thermodynamic** [CCC17]. **Thermodynamics** [HBGvM19, Spe78]. **Thermoelectric** [SNIM08]. **Thickness** [IKN+08]. **Thin** [KsKsN08]. **thiol** [GC01]. **Thiouracils** [KN01]. **Third** [BB99b]. **Third-Order** [BB99b]. **thirty** [Ros97]. **Thomas** [CTC22, Cru09c]. **Thoughts** [Bic04, HKS90]. **Three** [AAE+01, CM24, CB18, GAM+13, HA13, Jan65, Ros98, BKL21]. **Three-** [HA13]. **Three-Atom** [Jan65]. **Three-Body** [AAE+01, GAM+13, BKL21]. **Three-Ion** [Jan65]. **Three-Particle** [CB18]. **Threshold** [MFCT15, AA19]. **thymine** [SS22]. **Ti** [CL00, FU00]. **TiC** [SNM+97]. **Time** [ARS17, BBB10, Bel06, Bel11, GW17, GK90, HG17, JGCRC16, KMHL13, LHL18, Lin17c, Löw67c, MKN10, MCA+18, Öhr15, Öhr17, PČ75, PR98, PS21, SGB16, VTM98, WT99, BB22a, LSZ$^+$99a, LSZB00, NA19, WLM23]. **Time-Dependent** [ARS17, BBB10, GK90, HG17, KMHL13, LHL18, Lin17c, Löw67c, MKN10, MCA$^+$18, Öhr15, Öhr17, VTM98, WT99, PS21, LSZ$^+$99a, LSZB00, NA19, WLM23]. **Time-Independent** [BBB10, PČ75]. **Times** [TMMS10]. **tin** [GWW19]. **TiO** [GP14, Sak03a]. **tissue** [Per20]. **titanium** [TSTH03]. **TKHS** [DLMS03]. **Toluene** [RAR$^+$08]. **Tool** [VKI97]. **Top** [Oli12]. **topics** [SBA$^+$03]. **Topological** [Sjö04, JJ20]. **topological-homotopy** [JJ20]. **Total** [AGO07, CTSSO19, CTC22]. **Tour** [Ros98]. **Tracks** [Fra13]. **tragicomedy** [SL20]. **trail** [AGS$^+$19]. **Trajectories** [GMB04, PSAP10]. **trans** [För94]. **trans-Polyacetylene** [För94]. **Transfer** [BMM13, CHR13, CCSZ01, DBC$^+$99, FLV99, KKA97, LJ17, Les75, MBM99, OYI$^+$00, SIY$^+$15, Lar02, TBM01]. **Transferability** [ODE75, SKK23]. **Transferable** [KTC01]. **Transform** [Bel06, DeB09, HPB17, Mon05, ÖÖ13]. **Transformation** [LLBK$^+$98, PTBH13, RZTSW23, TSTH03]. **Transformations** [CDP82, Löw88b, LFM89]. **Transformed** [WN05]. **Transforms** [AYÖ17]. **Transition** [Ada97a, ARS99, DLMS03, EGCL91, GAI08, HS19, Lin98, MCC03, RR05, SED$^+$98, TLOK97, VI01, AO03, FCAG19, FTG22, MU03, TMM03, Yam03]. **Transitions** [GL68, HK03, LM97, MCP12, MLPD$^+$98, Nik70, BSL$^+$19]. **Translation** [SR73]. **Transmission** [BR05]. **Transport** [BR05, GG20, MOB$^+$03, Rou20]. **Trapped** [WMM$^+$98]. **Trapping** [Phi98, RDNFH98]. **Treated** [Bad09, Löw67c]. **Treating** [NBA20]. **Treatment** [BMPV99, BWVD$^+$13, HL90, Kar97, Kho04, KTC01, LS07, LR72, Lin98, MTS04, Mic99, Nic17, Öhr15, Oli90, PKYM01, VTM98, MKK$^+$01, PMK23]. **Treatments** [ATL$^+$18]. **Trends** [BJMB14, UK05, HPL98, KÖO23, SBSL08]. **Triatomic** [BR82, Pet98]. **Tribute** [SBK04, LSZ$^+$99b, SB02, SBLJ05, SCT15, SCT16]. **Triggered** [Kuk14]. **Trigonal** [ITI$^+$00]. **Trioxide** [SN08]. **Triples** [BB99b, HS86, PJH05]. **Triplet** [GV09, GL68, RLF17]. **Triply** [SBDD03]. **Tropospheric** [AVB08]. **Truncation** [Bun18, SDGW98, Bun23]. **Tumors** [Löw65c]. **Tunneling** [LPDB03, MS03, PLA01, Pol03, FTG22, QSW20, Sak03a]. **Twenty** [Ros97]. **Two** [AR03, BC80, BC00, DE05, FP06, HHK$^+$98, HS05, Hyl64, Kri03, LK13, LR72, MDBM98, OM03, PTBH13, QSG98, RA19, SBC09b, SGK$^+$08, VTM98, WHB$^+$24, YZDM01, ZP17, Bar23, BSL$^+$19, CTC22, LPC24, Rui23]. **Two-Band** [Kri03]. **Two-Body** [FP06]. **Two-Bond** [DE05]. **Two-Center** [ZP17, Rui23]. **Two-Colour** [VTM98]. **Two-Component** [YZDM01, Bar23]. **Two-dimensional** [RA19]. **Two-Electron** [BC80, HS05, Hyl64, LK13, OM03, SGK$^+$08, ZP17]. **Two-Particle** [BC00]. **Type** [AYÖ17, AA15, CB92, DR90, GW01, Hog13g, HPB17, PTBH13, SW98, SKT$^+$08, ALA21, KÖO23, Rui23]. **Types** [KS97b].

U [Miy03]. **UC** [SNM$^+$97]. **UFF** [dLHD10]. **Ultra** [KNM$^+$08, VT24].

Ultra-compact [VT24]. **Ultra-Soft** [KNM+08]. **Ultracold** [ML18]. **Ultrafast** [MCP12]. **Unbounded** [Löw88b, LFM89]. **Uncoupling** [MÅ01]. **underlying** [JJ20]. **Unified** [LR72, LJKH13, SO19c]. **Unique** [Ber03]. **Unit** [NA04]. **Unitary** [CDP82, LHL18, Mat78]. **Units** [Moh08]. **Univariate** [Lev14]. **Unrestricted** [BR65]. **Unstable** [ALND10, KG12, MKN10, NBS10, Nic10, NBS12, PD10]. **Until** [Nor98]. **UO** [MCC03]. **upon** [PGJ07]. **Upper** [Wei72]. **Uranyl** [HBT+00]. **Usage** [SPAS05]. **Use** [FSB+97, GMLSC+10, HM21, McG04, MP89, ALA23]. **Used** [Kla81, MKH+97, Pau13]. **Useful** [VKI97, SH19, Wen21]. **Usefulness** [FP06]. **Using** [AYÖ17, AA05, AA15, BS05a, BC09, CB92, CL00, CTG98, Fuk15, GMB04, HJ99, HL90, ILS08, KGW98, KSY08, KB98, KMR01, KV08, LHL18, MCP12, MM96, Mur08, OE17, PJH05, PB75, QGW01, STZY18, SED+98, SGB16, SW98, SYM+08, Uda00, UMD08, VTM98, dLHD10, AA19, BH24, BB22a, Bis19, CCM+19, GDL14, HDFT24, JMWG19, LPC24, MMM19, SA23b, SKS+19, SYIY03]. **Utilization** [ODE75, GG20]. **UV** [BS98]. **UV/VUV** [BS98].

V [TMM03, YIYM03]. **vacancies** [EOH03, Sak03a]. **Vacancy** [NM00]. **Vacuum** [Gre98, Gre08]. **Valence** [CCSZ01, Cse97, FVB99, GVCN82, SH95, SIY+19, WD70]. **Valence-Bond** [GVCN82]. **Valency** [San92]. **Validation** [DSW04, MG21]. **Validity** [Per17]. **Values** [AHPD+03, BKC68]. **Vanadium** [YKC+08, YIYM03]. **Variable** [SGB16]. **Variation** [BLC23, Kar08]. **Variational** [ADRAB16, CTG98, EG99, IM80, LFM89, MM99, MCA+18, OW08, Öhr17, TAU17, WT99, SYIY03, VT24]. **variational-X** [SYIY03]. **Variationally** [GW01, MRHdCK15]. **Various** [JJD05, Kar08, KB86]. **VB** [CTG98, RFG+98]. **Vectors** [GDL14, IM80, Sri01]. **veil** [FSP23]. **Verifying** [BWVD+13]. **Version** [LLBK+98]. **versions** [LH20]. **Vertical** [MLPD+98]. **Very** [Sim07]. **via** [BWVD+13, Gre08, ML18, MCM14, OPPZ06, ÖÖ13, ÖEO23, SIY+19]. **Vibration** [YTC+05]. **Vibrational** [BR17, ILS08, JJD05, Les75, PSAP10, SJO05, SSV98, Tak19]. **Vibronic** [AR03, BP82, Bor03, Chi03, CH03, CHSC03, HDB03, KH03, Kri03, SBC+03]. **Vibronic-induced** [HDB03]. **Vicinal** [SPAS05]. **Vicinity** [MYM08]. **View** [Löw65c]. **VII** [QGW01]. **vinyl** [GC01]. **Violation** [Kar08, QSW20]. **Virial** [LDB95]. **Visualization** [CCVB94]. **vivo** [BB17]. **Volatile** [GAI08]. **Volum** [Ano98f]. **Volume** [Ano64b, Ano65b, Ano67c, Ano68c, Ano70c, Ano72c, Ano73c, Ano77b, Ano80b, Ano81c, Ano81d, Ano82e, Ano85c, Ano98g, Ano98b, Ano98h, Ano98c, Ano98i, Ano01g, Ano01b, Ano01f, Ano08n, Ano09j, Ano10g, Ano10h, SBK04, Ano01d, Ano01a, Ano01e, Ano01h, Ano01c, LSZ+99a, SB17a, SB17b]. **Volumes** [Ano67b, Ano68b, Ano70b, Ano72b, Ano73b, Ano74a, Ano75a, Ano77a, Ano78a, Ano80a, Ano81a, Ano81b, Ano82a, Ano82b, Ano85a]. **vs** [BFHS23, MS03]. **VUV** [BS98].

Waals [LR72]. **wagging** [MFMCN01]. **Was** [Miy03, SEL01]. **Water** [BRL13, CTSDÖ05, CCCC15, CHR13, FCC04, GP14, KBH23, KMHL13, KN01, KV08, RFG+98, RGFC13, SOS13, SIY+15, SCTH+07, SKK23, YMI+21]. **Wave** [BRL13, Bis67, CTG98, Dau64, DB01, FP06, GM17, Har17, Har18, HL97, Joh73, KNN17, LK13, MDÖ05, MS65, Mon05, PSS98, RGFC13, RMMP17, SAL10, Bel22, VT24, SED+98, Sla64]. **Wavefunctions** [HS05, HA13, Sal74, GWW19]. **Wavelengths** [Khe19]. **Wavepackets** [ILS08]. **Way** [PB14]. **Weakly** [KT98, MHWvdA97]. **Weizsäcker** [Cru09c]. **Well** [BRW08, MFCT15]. **wetting** [SYIY03]. **WF** [MKK+01]. **Which** [BR65, GVFR98]. **Wigner** [HW01, HMW01, MH98]. **Wires** [KD11]. **Within** [JGCRC16, Lau09, LJKH13, GWW19, Gut97, SKGŚ23, TM21]. **without** [Ber02]. **WKB** [Pol03]. **WO** [HSS+04]. **Wolniewicz** [PMK23]. **Work** [FU00, KKK+97, SB02]. **Workshop** [Ano98t, Ano98u, Ano01m, Ano01n]. **World** [Ros98]. **Worst** [PS05b].

X [Ada97b, BJMB14, FSB+97, Fuk03, Gut97, IFAY08, Kaw97, KNM+08, MW08, Mur08, NHYU03, OTA97, Ros97, SBA+03, UMD08, YFK+97, Ada00, AAM04, BMC97, CL00, CS77, GM17, HOI+08, Kaw97, KsKsN08, KNM+08, LSZ+00, MYW00, MW08, MKK+00, MTA97, MTA00, Mur03, Mur08, Nak00, SBK+08, SNMI00, SYIY03, Tak19, Tan00, Uda00, UMD08, YKS+12, YFK+97, YNNU03]. **X-Ray** [Ada00, CS77, GM17, Kaw97, KsKsN08, KNM+08, MYW00, MW08, MKK+00, MTA97, MTA00, Mur08, Tak19, Uda00, UMD08, YFK+97, Mur03, YKS+12, YNNU03]. **X-Rays** [AAM04]. **XANES** [KNM+08, MST+03, NM00, YKY+00]. **XHY** [DE05]. **XY** [YTC+05].

years [Cra99, Ros97]. **yl** [NeMM03]. **Yngve** [Lin99, LSZ+99b]. **Young** [Sal74].

Zerner [Sab00]. **Zero** [Dru78, FH65, HBKS03, MYM08]. **Zero-Phonon** [HBKS03]. **Zero-Range** [Dru78]. **Zinc** [MYM08]. **Zn** [FU00, NHYU03]. **Zn-tetraphenylporphyrins** [NHYU03]. **ZnI** [BKC68]. **ZnO** [KNI+08, OTA03]. **Zr** [SMAS08, TMM03].

References

Aquilanti:2001:SEQ

[AA01] Vincenzo Aquilanti and John Avery. Sturmian expansions for quantum mechanical many-body problems and hyperspherical harmonics. *Advances in Quantum Chemistry*, 39:71–102, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760539006X.

Avery:2003:KPC

[AA03] John Avery and James Avery. Kramers pairs in configuration interaction. *Advances in Quantum Chemistry*, 43:185–206, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603430050`.

Avery:2005:ASA

[AA05] James Avery and John Avery. Autoionizing states of atoms calculated using generalized Sturmians. *Advances in Quantum Chemistry*, 49:103–119, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605490024`.

Avery:2015:MIE

[AA15] James Emil Avery and John Scales Avery. Molecular integrals for exponential-type orbitals using hyperspherical harmonics. *Advances in Quantum Chemistry*, 70:265–324, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327614000057`.

Avery:2018:CSI

[AA18] James E. Avery and John S. Avery. 4-center STO interelectron repulsion integrals with Coulomb Sturmians. *Advances in Quantum Chemistry*, 76:133–146, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327617300710`.

Archubi:2019:STE

[AA19] Claudio D. Archubi and Néstor R. Arista. Studies of threshold effects in the interaction of protons, electrons, and positrons in matter using dielectric models. *Advances in Quantum Chemistry*, 80:247–269, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300322`.

Avery:2004:ADP

[AAAC04] John Avery, James Avery, Vincenzo Aquilanti, and Andrea Caligiana. Atomic densities, polarizabilities, and natural orbitals derived from generalized Sturmian calculations. *Advances in Quantum Chemistry*, 47:157–176, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604470099`.

Alferova:2001:FET

[AAE+01] T. Alferova, S. Andersson, N. Elander, S. Levin, and E. Yarevsky. Finite-element three-body studies of bound and resonant states in atoms and molecules. *Advances in Quantum Chemistry*, 40:323–344, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400232`.

Avery:2003:NOG

[AAG03] John Avery, James Avery, and Osvaldo Goscinski. Natural orbitals from generalized Sturmian calculations. *Advances in Quantum Chemistry*, 43:207–216, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603430062`.

Alon:2004:AMC

[AAM04] Ofir E. Alon, Vitali Averbukh, and Nimrod Moiseyev. Atoms, molecules, crystals and nanotubes in laser fields: From dynamical symmetry to selective high-order harmonic generation of soft X-rays. *Advances in Quantum Chemistry*, 47:393–421, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604470221`.

Amos:1973:SSE

[AB73] A. T. Amos and B. L. Burrows. Solvent-shift effects on electronic spectra and excited-state dipole moments and polarizabilities. *Advances in Quantum Chemistry*, 7:289–313, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605663`.

Albers:1990:LAP

[ABB90] R. C. Albers, A. M. Boring, and J. C. Boettger. LDA applications to the properties of periodic systems. *Advances in Quantum Chemistry*, 21:365–398, 1990. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860605X`.

Amovilli:1998:RAD

[ABC+98] Claudio Amovilli, Vincenzo Barone, Roberto Cammi, Eric Cancès, Maurizio Cossi, Benedetta Mennucci, Christian S. Pomelli, and Jacopo Tomasi. Recent advances in the description of solvent effects with the polarizable continuum model. *Advances* *in Quantum Chemistry*, 32:227–261, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604165.

Aramburu:2003:JTI

[ABGM03] J. A. Aramburu, M. T. Barriuso, P. García Fernández, and M. Moreno. Jahn–Teller ions in cubic crystals explored through DFT calculations. *Advances in Quantum Chemistry*, 44:445–459, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760344029X.

Aquilanti:1999:HCC

[ACC99] Vincenzo Aquilanti, Gabriella Capecchi, and Simonetta Cavalli. Hyperspherical coordinates for chemical reaction dynamics. *Advances in Quantum Chemistry*, 36:341–363, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604918.

Aslangul:1972:ALE

[ACDK72] Claude Aslangul, Raymond Constanciel, Raymond Daudel, and Philemon Kottis. Aspects of the localizability of electrons in atoms and molecules: Loge theory and related methods. *Advances in Quantum Chemistry*, 6:93–141, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605420.

Aquilanti:2001:ARH

[ACDV01] Vincenzo Aquilanti, Simonetta Cavalli, Dario De Fazio, and Alessandro Volpi. The A + BC reaction by the hyperquantization algorithm: The symmetric hyperspherical parametrization for $J > 0$. *Advances in Quantum Chemistry*, 39:103–121, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390071.

Aagren:1992:TMA

[ÅCL92] Hans Ågren, Amary Cesar, and Christoph-Maria Liegener. Theory of molecular Auger spectra. *Advances in Quantum Chemistry*, 23:1–82, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600283.

Adams:1988:LAM

[AČP88] B. G. Adams, J. Čížek, and J. Paldus. Lie algebraic methods and their applications to simple quantum systems. *Advances in Quantum Chemistry*, 19:1–85, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606139.

Adachi:1997:ESC

[Ada97a] Hirohiko Adachi. Electronic state calculation of transition metal cluster. *Advances in Quantum Chemistry*, 29:49–81, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602634.

Adachi:1997:TCM

[Ada97b] Hirohiko Adachi. Theoretical calculation of molecular photoelectron spectrum by the first-principles DV–Xα molecular orbital method. *Advances in Quantum Chemistry*, 29:179–192, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602695.

Adachi:2000:TAX

[Ada00] Hirohiko Adachi. Theoretical analysis of X-ray and electron spectra by DV-Xα method. *Advances in Quantum Chemistry*, 37: 1–29, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370022.

Avram:2003:JTE

[ADA03] C. N. Avram, Gh. E. Draganescu, and N. M. Avram. Jahn–Teller effect in laser crystal $LiCaAlF_6 : Cr^{3+}$. *Advances in Quantum Chemistry*, 44:527–534, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440343.

Adamo:1999:CDF

[AdMB99] Carlo Adamo, Andrea di Matteo, and Vincenzo Barone. From classical density functionals to adiabatic connection methods. the state of the art. *Advances in Quantum Chemistry*, 36:45–75, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604785.

Almora-Diaz:2016:RPV

[ADRAB16] César X. Almora-Díaz, Herzain I. Rivera-Arrieta, and Carlos F. Bunge. Recent progress in the variational orbital approach to atomic and molecular electronic structure. *Advances in Quantum Chemistry*, 72:129–176, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000325.

Aksoy:2013:FIE

[AFE13] S. Aksoy, S. Firat, and M. Ertürk. Further improvements on $\psi^{(\alpha*)}$-etos with hyperbolic cosine functions and their effectiveness in atomic calculations. *Advances in Quantum Chemistry*, 67:217–230, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012411544600008X.

Aspuru-Guzik:2005:QMC

[AGL05] Alán Aspuru-Guzik and William A. Lester, Jr. Quantum Monte Carlo: Theory and application to molecular systems. *Advances in Quantum Chemistry*, 49:209–226, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490048.

Abril:2013:ICE

[AGMdV+13] Isabel Abril, Rafael Garcia-Molina, Pablo de Vera, Ioanna Kyriakou, and Dimitris Emfietzoglou. Inelastic collisions of energetic protons in biological media. *Advances in Quantum Chemistry*, 65:129–164, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000066.

Akar:2007:TES

[AGO07] A. Akar, H. Gümüs, and N. T. Okumuşoğlu. Total electron stopping powers and CSDA-ranges from 20 eV to 10 MeV electron energies for components of DNA and RNA. *Advances in Quantum Chemistry*, 52:277–288, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760652012X.

Arista:2019:PEC

[AGS+19] Néstor R. Arista, Juana L. Gervasoni, Silvina Segui, Isidro Villó-Pérez, and Raúl O. Barrachina. Plasmon excitation by charged particles in solids, surfaces, and nanostructures: Following the trail of R. H. Ritchie. *Advances in Quantum Chemistry*, 80:271–317, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300334.

Ancarani:2019:P

[AH19a] Lorenzo Ugo Ancarani and Philip E. Hoggan. Preface. *Advances in Quantum Chemistry*, 79:xv–xvii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300498.

Ancarani:2019:SAM

[AH19b] Lorenzo Ugo Ancarani and Philip E. Hoggan, editors. *State of The Art of Molecular Electronic Structure Computations: Correlation Methods, Basis Sets and More*, volume 79 of *Advances in quantum chemistry*. Elsevier, Amsterdam, The Netherlands, 2019. CODEN AQCHA9. ISBN 0-12-816174-4, 0-12-816175-2 (e-book). ISSN 0065-3276. xvii + 341 pp. LCCN QD453 .A28 79; QC462. URL https://www.sciencedirect.com/science/journal/00653276/78.

Al-Hazmi:2003:NCC

[AHPD+03] Faten Al-Hazmi, Victor Z. Polinger, Janette L. Dunn, Colin A. Bates, Elie A. Moujaes, and Michel Abou-Ghantous. Non-condon correction to Franck–Condon values of second-order reduction factors: The cubic T term. *Advances in Quantum Chemistry*, 44:169–182, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440112.

Alducin:2004:ELI

[AJ04] M. Alducin and J. I. Juaristi. Energy loss in the interaction of atomic particles with solid surfaces. *Advances in Quantum Chemistry*, 45 (part 1):223–245, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450102.

Averbukh:2012:EDM

[AK12] Vitali Averbukh and Premysl Kolorenc. Electronic decay in multiply charged polyatomic systems. *Advances in Quantum Chemistry*, 63:309–342, 2012. CODEN AQCHA9. ISBN 0-12-397009-

1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000060.

Arista:2004:NLA

[AL04] Néstor R. Arista and Agustín F. Lifschitz. Non-linear approach to the energy loss of ions in solids. *Advances in Quantum Chemistry*, 45 (part 1):47–77, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450035.

Ammar:2021:CFM

[ALA21] Abdallah Ammar, Arnaud Leclerc, and Lorenzo Ugo Ancarani. Multicenter integrals involving complex Gaussian-type functions. *Advances in Quantum Chemistry*, 83:287–304, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000083.

Ammar:2023:UCG

[ALA23] Abdallah Ammar, Arnaud Leclerc, and Lorenzo Ugo Ancarani. On the use of complex GTOs for the evaluation of radial integrals involving oscillating functions. *Advances in Quantum Chemistry*, 88:133–149, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000242.

Atabek:2010:USL

[ALND10] O. Atabek, R. Lefebvre, and T. T. Nguyen-Dang. Unstable states in laser assisted and controlled molecular processes. *Advances in Quantum Chemistry*, 60:51–104, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600020.

Apell:2022:SSI

[AMAA22] S. Peter Apell, Gautam Mukhopadhyay, Tomasz J. Antosiewicz, and Javier Aizpurua. Shape-sensitive inelastic scattering from metallic nanoparticles. *Advances in Quantum Chemistry*, 85:??, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000053.

Andre:1980:QMM

[And80] Jean-Marie André. Quantum mechanical methods for regular polymers. *Advances in Quantum Chemistry*, 12:65–102,

1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603147.

Anonymous:1964:AI

[Ano64a] Anonymous. Author index. *Advances in Quantum Chemistry*, 1: 375–381, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603822.

Anonymous:1964:CV

[Ano64b] Anonymous. Contributors to the volume. *Advances in Quantum Chemistry*, 1:??, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603688.

Anonymous:1964:CP

[Ano64c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 1:iv, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603706.

Anonymous:1964:LC

[Ano64d] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 1:v–vi, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603718.

Anonymous:1964:SI

[Ano64e] Anonymous. Subject index. *Advances in Quantum Chemistry*, 1:382–385, 1964. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1965:AI

[Ano65a] Anonymous. Author index. *Advances in Quantum Chemistry*, 2: 361–368, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600775.

Anonymous:1965:CV

[Ano65b] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 2:??, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600659.

Anonymous:1965:CP

[Ano65c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 2:iv, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600672.

Anonymous:1965:LC

[Ano65d] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 2:v–vi, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600684.

Anonymous:1965:SI

[Ano65e] Anonymous. Subject index. *Advances in Quantum Chemistry*, 2:369–372, 1965. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1967:AI

[Ano67a] Anonymous. Author index. *Advances in Quantum Chemistry*, 3:383–388, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600933.

Anonymous:1967:CPV

[Ano67b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 3:xiii–xvi, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600842.

Anonymous:1967:CV

[Ano67c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 3:??, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600799.

Anonymous:1967:CP

[Ano67d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 3:iv, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600817.

Anonymous:1967:LC

[Ano67e] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 3:v–vi, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600829.

Anonymous:1967:SI

[Ano67f] Anonymous. Subject index. *Advances in Quantum Chemistry*, 3:389–392, 1967. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1968:AI

[Ano68a] Anonymous. Author index. *Advances in Quantum Chemistry*, 4: 327–331, 1968. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603974`.

Anonymous:1968:CPV

[Ano68b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 4:xiii–xiv, 1968. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1968:CV

[Ano68c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 4:??, 1968. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603846`.

Anonymous:1968:CP

[Ano68d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 4:iv, 1968. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860386X`.

Anonymous:1968:LC

[Ano68e] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 4:v–vi, 1968. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603871`.

Anonymous:1968:SI

[Ano68f] Anonymous. Subject index. *Advances in Quantum Chemistry*, 4:332–334, 1968. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1970:AI

[Ano70a] Anonymous. Author index. *Advances in Quantum Chemistry*, 5: 297–301, 1970. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603433`.

Anonymous:1970:CPV

[Ano70b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 5:xiii–xv, 1970. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1970:CV

[Ano70c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 5:??, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603305.

Anonymous:1970:CP

[Ano70d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 5:iv, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603329.

Anonymous:1970:LC

[Ano70e] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 5:ix–x, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603330.

Anonymous:1970:SI

[Ano70f] Anonymous. Subject index. *Advances in Quantum Chemistry*, 5:302–303, 1970. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1972:AI

[Ano72a] Anonymous. Author index. *Advances in Quantum Chemistry*, 6:395–408, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605511.

Anonymous:1972:CPV

[Ano72b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 6:xii–xvi, 1972. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1972:CV

[Ano72c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 6:??, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605365.

Anonymous:1972:CP

[Ano72d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 6:iv, 1972. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605389`.

Anonymous:1972:LC

[Ano72e] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 6:ix–x, 1972. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605390`.

Anonymous:1972:SI

[Ano72f] Anonymous. Subject index. *Advances in Quantum Chemistry*, 6:409–413, 1972. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1973:AI

[Ano73a] Anonymous. Author index. *Advances in Quantum Chemistry*, 7:447–454, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605705`.

Anonymous:1973:CPV

[Ano73b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 7:xiii–xvi, 1973. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1973:CV

[Ano73c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 7:??, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605535`.

Anonymous:1973:CP

[Ano73d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 7:iv, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605559`.

Anonymous:1973:LC

[Ano73e] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 7:ix–x, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605560`.

Anonymous:1973:SI

[Ano73f] Anonymous. Subject index. *Advances in Quantum Chemistry*, 7:455–457, 1973. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1974:CPV

[Ano74a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 8:xiii–xvii, 1974. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1974:CP

[Ano74b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 8:iv, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600544.

Anonymous:1974:LC

[Ano74c] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 8:ix, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600556.

Anonymous:1974:SI

[Ano74d] Anonymous. Subject index. *Advances in Quantum Chemistry*, 8:289–291, 1974. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1975:CPV

[Ano75a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 9:301–304, 1975. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1975:CP

[Ano75b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 9:iv, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600350.

Anonymous:1975:LC

[Ano75c] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 9:vii–viii, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600362.

Anonymous:1975:SI

[Ano75d] Anonymous. Subject index. *Advances in Quantum Chemistry*, 9:299–300, 1975. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1977:CPV

[Ano77a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 10:335–338, 1977. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1977:CV

[Ano77b] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 10:??, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605729.

Anonymous:1977:CP

[Ano77c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 10:iv, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605742.

Anonymous:1977:LC

[Ano77d] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 10:ix, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605754.

Anonymous:1977:SI

[Ano77e] Anonymous. Subject index. *Advances in Quantum Chemistry*, 10:329–333, 1977. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1978:CPV

[Ano78a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 11:483–487, 1978. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1978:CP

[Ano78b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 11:iv, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602294.

Anonymous:1978:LC

[Ano78c] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 11:ix–x, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602300.

Anonymous:1978:SI

[Ano78d] Anonymous. Subject index. *Advances in Quantum Chemistry*, 11:479–482, 1978. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1980:CPV

[Ano80a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 12:321–325, 1980. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1980:CV

[Ano80b] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 12:??, 1980. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860307X`.

Anonymous:1980:CP

[Ano80c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 12:iv, 1980. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603093`.

Anonymous:1980:I

[Ano80d] Anonymous. Index. *Advances in Quantum Chemistry*, 12:317–320, 1980. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1980:LC

[Ano80e] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 12:vii, 1980. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860310X`.

Anonymous:1981:CPVa

[Ano81a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 13:246–251, 1981. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1981:CPVb

[Ano81b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 14:243–248, 1981. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1981:CVa

[Ano81c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 13:??, 1981. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602865.

Anonymous:1981:CVb

[Ano81d] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 14:??, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603202.

Anonymous:1981:CPa

[Ano81e] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 13:iv, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602889.

Anonymous:1981:CPb

[Ano81f] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 14:iv, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603226.

Anonymous:1981:Ia

[Ano81g] Anonymous. Index. *Advances in Quantum Chemistry*, 13:243–245, 1981. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1981:Ib

[Ano81h] Anonymous. Index. *Advances in Quantum Chemistry*, 14:241–242, 1981. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1981:LCa

[Ano81i] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 13:vii, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602890.

Anonymous:1981:LCb

[Ano81j] Anonymous. List of contributors. *Advances in Quantum Chemistry*, 14:vii, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603238.

Anonymous:1982:CPVa

[Ano82a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 15:273–277, 1982. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1982:CPVb

[Ano82b] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 16:281–285, 1982. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1982:Ca

[Ano82c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 15: vii, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601197.

Anonymous:1982:Cb

[Ano82d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 16: vii–viii, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603482.

Anonymous:1982:CV

[Ano82e] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 16:??, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603457.

Anonymous:1982:CPa

[Ano82f] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 15:iv, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601185.

Anonymous:1982:CPb

[Ano82g] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 16:iv, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603470.

Anonymous:1982:Ea

[Ano82h] Anonymous. Editors. *Advances in Quantum Chemistry*, 15:??, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601161.

Anonymous:1982:Ia

[Ano82i] Anonymous. Index. *Advances in Quantum Chemistry*, 15:267–272, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601252.

Anonymous:1982:Ib

[Ano82j] Anonymous. Index. *Advances in Quantum Chemistry*, 16:273–280, 1982. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1985:CPV

[Ano85a] Anonymous. Contents of previous volumes. *Advances in Quantum Chemistry*, 17:339–344, 1985. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1985:C

[Ano85b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 17:vii, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602993.

Anonymous:1985:CV

[Ano85c] Anonymous. Contributors to this volume. *Advances in Quantum Chemistry*, 17:??, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602968.

Anonymous:1985:CP

[Ano85d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 17:iv, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602981.

Anonymous:1985:I

[Ano85e] Anonymous. Index. *Advances in Quantum Chemistry*, 17:335–338, 1985. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1986:CP

[Ano86a] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 18:iv, 1986. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600453.

Anonymous:1986:I

[Ano86b] Anonymous. Index. *Advances in Quantum Chemistry*, 18:345–350, 1986. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1988:ANF

[Ano88a] Anonymous. Announcement of new format. *Advances in Quantum Chemistry*, 19:xiii, 1988. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1988:C

[Ano88b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 19: ix–x, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606103.

Anonymous:1988:CP

[Ano88c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 19:iv, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606097.

Anonymous:1988:EB

[Ano88d] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 19:??, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606073.

Anonymous:1988:I

[Ano88e] Anonymous. Index. *Advances in Quantum Chemistry*, 19:349–365, 1988. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1989:ANF

[Ano89a] Anonymous. Announcement of new format. *Advances in Quantum Chemistry*, 20:xiii, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606255.

Anonymous:1989:C

[Ano89b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 20: ix–x, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606231.

Anonymous:1989:CP

[Ano89c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 20:iv, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860622X.

Anonymous:1989:EB

[Ano89d] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 20:??, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606206.

Anonymous:1989:I

[Ano89e] Anonymous. Index. *Advances in Quantum Chemistry*, 20:443–453, 1989. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1990:C

[Ano90a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 21:xi–xii, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605870.

Anonymous:1990:CP

[Ano90b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 21:iv, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605869.

Anonymous:1990:EB

[Ano90c] Anonymous. Edited board. *Advances in Quantum Chemistry*, 21:??, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605845.

Anonymous:1990:I

[Ano90d] Anonymous. Index. *Advances in Quantum Chemistry*, 21:399–405, 1990. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1991:C

[Ano91a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 22:vii, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603597.

Anonymous:1991:CP

[Ano91b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 22:iv, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603585.

Anonymous:1991:EB

[Ano91c] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 22:??, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603561.

Anonymous:1991:I

[Ano91d] Anonymous. Index. *Advances in Quantum Chemistry*, 22:375–385, 1991. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1992:Ca

[Ano92a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 23: vii, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860026X`.

Anonymous:1992:Cb

[Ano92b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 24: vii, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600982`.

Anonymous:1992:CPa

[Ano92c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 23:iv, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600258`.

Anonymous:1992:CPb

[Ano92d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 24:iv, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600970`.

Anonymous:1992:EBa

[Ano92e] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 23:??, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600234`.

Anonymous:1992:EBb

[Ano92f] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 24:??, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600957`.

Anonymous:1992:Ia

[Ano92g] Anonymous. Index. *Advances in Quantum Chemistry*, 23:353–363, 1992. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1992:Ib

[Ano92h] Anonymous. Index. *Advances in Quantum Chemistry*, 24:291–298, 1992. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1994:AE

[Ano94a] Anonymous. Advisory editors. *Advances in Quantum Chemistry*, 25:??, 1994. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860012X`.

Anonymous:1994:C

[Ano94b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 25: vii, 1994. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600155`.

Anonymous:1994:CP

[Ano94c] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 25:iv, 1994. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600143`.

Anonymous:1994:I

[Ano94d] Anonymous. Index. *Advances in Quantum Chemistry*, 25:315–320, 1994. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1995:C

[Ano95a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 26: vii, 1995. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601082`.

Anonymous:1995:CP

[Ano95b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 26:iv, 1995. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601070`.

Anonymous:1995:EB

[Ano95c] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 26:??, 1995. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601057`.

Anonymous:1995:I

[Ano95d] Anonymous. Index. *Advances in Quantum Chemistry*, 26:359–367, 1995. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1996:C

[Ano96a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 27: ix, 1996. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602488`.

Anonymous:1996:CP

[Ano96b] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 27:iv, 1996. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602464`.

Anonymous:1996:D

[Ano96c] Anonymous. Dedication. *Advances in Quantum Chemistry*, 27: viii, 1996. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602476`.

Anonymous:1996:EB

[Ano96d] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 27:??, 1996. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602440`.

Anonymous:1996:I

[Ano96e] Anonymous. Index. *Advances in Quantum Chemistry*, 27:399–407, 1996. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1997:CPc

[Ano97a] Anonymous. Conference participants. *Advances in Quantum Chemistry*, 28:xvii–xviii, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602014`.

Anonymous:1997:Ca

[Ano97b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 28: xii–xiv, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601999`.

Anonymous:1997:Cb

[Ano97c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 29: xi–xiii, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602609`.

Anonymous:1997:CPa

[Ano97d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 28:iv, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601987`.

Anonymous:1997:CPb

[Ano97e] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 29:iv, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602592`.

Anonymous:1997:EBa

[Ano97f] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 28:??, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601963`.

Anonymous:1997:EBb

[Ano97g] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 29:??, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602579`.

Anonymous:1997:Ia

[Ano97h] Anonymous. Index. *Advances in Quantum Chemistry*, 28:361–370, 1997. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1997:Ib

[Ano97i] Anonymous. Index. *Advances in Quantum Chemistry*, 29:471–481, 1997. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:AE

[Ano98a] Anonymous. Advisory editors. *Advances in Quantum Chemistry*, 31:??, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601732`.

Anonymous:1998:CVb

[Ano98b] Anonymous. Contents volume 31. *Advances in Quantum Chemistry*, 31:ix–x, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:CVd

[Ano98c] Anonymous. Contents volume 31. *Advances in Quantum Chemistry*, 32:xi–xii, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:Cb

[Ano98d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 30:ix–xii, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604979`.

Anonymous:1998:Cc

[Ano98e] Anonymous. Contributors. *Advances in Quantum Chemistry*, 33:xi–xiv, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:CVf

[Ano98f] Anonymous. Contributors volum 33. *Advances in Quantum Chemistry*, 33:xi–xiv, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604244.

Anonymous:1998:CVa

[Ano98g] Anonymous. Contributors volume 31. *Advances in Quantum Chemistry*, 31:xi–xiii, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601768.

Anonymous:1998:CVc

[Ano98h] Anonymous. Contributors volume 32. *Advances in Quantum Chemistry*, 31:xi–xiii, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860177X.

Anonymous:1998:CVe

[Ano98i] Anonymous. Contributors volume 32. *Advances in Quantum Chemistry*, 32:vii–ix, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604025.

Anonymous:1998:CPb

[Ano98j] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 30:iv, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604967.

Anonymous:1998:CPc

[Ano98k] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 32:iv, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604013.

Anonymous:1998:CPd

[Ano98l] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 33:iv, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604232.

Anonymous:1998:EBb

[Ano98m] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 30:??, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604943.

Anonymous:1998:EBc

[Ano98n] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 32:??, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603998.

Anonymous:1998:EBd

[Ano98o] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 33:??, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604219.

Anonymous:1998:Ia

[Ano98p] Anonymous. Index. *Advances in Quantum Chemistry*, 30:493–506, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:Ib

[Ano98q] Anonymous. Index. *Advances in Quantum Chemistry*, 31:337–345, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:Ic

[Ano98r] Anonymous. Index. *Advances in Quantum Chemistry*, 32:331–338, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:Id

[Ano98s] Anonymous. Index. *Advances in Quantum Chemistry*, 33:389–398, 1998. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1998:WPa

[Ano98t] Anonymous. Workshop participants. *Advances in Quantum Chemistry*, 31:xvii–xix, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601793.

Anonymous:1998:WPb

[Ano98u] Anonymous. Workshop participants. *Advances in Quantum Chemistry*, 32:xvii–xix, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604049.

Anonymous:1999:BN

[Ano99a] Anonymous. Biographic notes. *Advances in Quantum Chemistry*, 36:xix–xxii, 1999. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860475X.

Anonymous:1999:Ca

[Ano99b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 34: vii, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605286.

Anonymous:1999:Cb

[Ano99c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 35: vii–viii, 1999. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1999:Cc

[Ano99d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 35: vii–viii, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604505.

Anonymous:1999:Cd

[Ano99e] Anonymous. Contributors. *Advances in Quantum Chemistry*, 36: xi–xiv, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604736.

Anonymous:1999:CPa

[Ano99f] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 34:iv, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605274.

Anonymous:1999:CPb

[Ano99g] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 35:iv, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604499.

Anonymous:1999:CPc

[Ano99h] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 36:iv, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604724.

Anonymous:1999:EBa

[Ano99i] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 34:??, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605250.

Anonymous:1999:EBb

[Ano99j] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 35:??, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604475`.

Anonymous:1999:EBc

[Ano99k] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 36:??, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604700`.

Anonymous:1999:Ia

[Ano99l] Anonymous. Index. *Advances in Quantum Chemistry*, 34:381–388, 1999. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1999:Ib

[Ano99m] Anonymous. Index. *Advances in Quantum Chemistry*, 35:371–380, 1999. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1999:Ic

[Ano99n] Anonymous. Index. *Advances in Quantum Chemistry*, 36:385–394, 1999. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:1999:P

[Ano99o] Anonymous. Preface. *Advances in Quantum Chemistry*, 34:ix–x, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605298`.

Anonymous:2000:Ca

[Ano00a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 37:xi–xiii, 2000. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327600370009`.

Anonymous:2000:Cb

[Ano00b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 38:vii, 2000. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327600380005`.

Anonymous:2000:Ia

[Ano00c] Anonymous. Index. *Advances in Quantum Chemistry*, 37:385–393, 2000. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2000:Ib

[Ano00d] Anonymous. Index. *Advances in Quantum Chemistry*, 38:279–287, 2000. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2001:CVb

[Ano01a] Anonymous. Contents volume 39. *Advances in Quantum Chemistry*, 40:xv–xx, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400025.

Anonymous:2001:CVe

[Ano01b] Anonymous. Contents volume 39. *Advances in Quantum Chemistry*, 40:xv–xx, 2001. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2001:CVh

[Ano01c] Anonymous. Contents volume 40. *Advances in Quantum Chemistry*, 39:xv–xx, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390228.

Anonymous:2001:CVa

[Ano01d] Anonymous. Contributors volume 39. *Advances in Quantum Chemistry*, 39:xi–xiii, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390216.

Anonymous:2001:CVc

[Ano01e] Anonymous. Contributors volume 39. *Advances in Quantum Chemistry*, 39:xxi–xxiii, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760539023X.

Anonymous:2001:CVf

[Ano01f] Anonymous. Contributors volume 39. *Advances in Quantum Chemistry*, 40:xxi–xxiii, 2001. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2001:CVd

[Ano01g] Anonymous. Contributors volume 40. *Advances in Quantum Chemistry*, 40:xi–xiii, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400013.

Anonymous:2001:CVg

[Ano01h] Anonymous. Contributors volume 40. *Advances in Quantum Chemistry*, 40:xxi–xxv, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400037.

Anonymous:2001:EB

[Ano01i] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 40:ii–iii, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400001.

Anonymous:2001:Ia

[Ano01j] Anonymous. Index. *Advances in Quantum Chemistry*, 39:367–381, 2001. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2001:Ib

[Ano01k] Anonymous. Index. *Advances in Quantum Chemistry*, 40:381–395, 2001. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2001:P

[Ano01l] Anonymous. Preface. *Advances in Quantum Chemistry*, 39:xxv–xxvi, 2001. CODEN AQCHA9. ISSN 0065-3276.

Anonymous:2001:WPc

[Ano01m] Anonymous. Workshop participants. *Advances in Quantum Chemistry*, 39:xxvii–xxxi, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390253.

Anonymous:2001:WPd

[Ano01n] Anonymous. Workshop participants. *Advances in Quantum Chemistry*, 40:xxvii–xxxi, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400050.

Anonymous:2002:C

[Ano02] Anonymous. Contributors. *Advances in Quantum Chemistry*, 41:ix, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410416.

Anonymous:2003:AIB

[Ano03a] Anonymous. Anniversary Isaac Bersuker 75. *Advances in Quantum Chemistry*, 44:xxxiii–xxxvi, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440483.

Anonymous:2003:Cc

[Ano03b] Anonymous. Contents. *Advances in Quantum Chemistry*, 43: v–vii, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430104.

Anonymous:2003:Ce

[Ano03c] Anonymous. Contents. *Advances in Quantum Chemistry*, 44: v–xvi, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440458.

Anonymous:2003:Cb

[Ano03d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 42: xiii–xvi, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420364.

Anonymous:2003:Cd

[Ano03e] Anonymous. Contributors. *Advances in Quantum Chemistry*, 43: ix, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430086.

Anonymous:2003:Cf

[Ano03f] Anonymous. Contributors. *Advances in Quantum Chemistry*, 44:xvii–xxii, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760344046X.

Anonymous:2003:EB

[Ano03g] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 42:ii–iii, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420352.

Anonymous:2003:OFH

[Ano03h] Anonymous. Obituary Frank Ham (1928–2002). *Advances in Quantum Chemistry*, 44:xxvii–xxxi, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440471.

Anonymous:2003:Pa

[Ano03i] Anonymous. Preface. *Advances in Quantum Chemistry*, 43:xi–xii, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430098.

Anonymous:2003:Pb

[Ano03j] Anonymous. Preface. *Advances in Quantum Chemistry*, 44:xxiii–xxv, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440495.

Anonymous:2004:A

[Ano04a] Anonymous. Acknowledgement. *Advances in Quantum Chemistry*, 47:xix, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470294.

Anonymous:2004:Ca

[Ano04b] Anonymous. Contents. *Advances in Quantum Chemistry*, 45 (part 1):v–viii, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450138.

Anonymous:2004:Cc

[Ano04c] Anonymous. Contents. *Advances in Quantum Chemistry*, 46 (part 2):v–viii, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460146.

Anonymous:2004:Ce

[Ano04d] Anonymous. Contents. *Advances in Quantum Chemistry*, 47:v–xi, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470257.

Anonymous:2004:Cb

[Ano04e] Anonymous. Contributors. *Advances in Quantum Chemistry*, 45 (part 1):ix–x, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760445014X.

Anonymous:2004:Cd

[Ano04f] Anonymous. Contributors. *Advances in Quantum Chemistry*, 46 (part 2):ix–x, 2004. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460158.

Anonymous:2004:Cf

[Ano04g] Anonymous. Contributors. *Advances in Quantum Chemistry*, 47: xiii–xvi, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470270.

Anonymous:2004:I

[Ano04h] Anonymous. Index. *Advances in Quantum Chemistry*, 46 (part 2):xi, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760446016X.

Anonymous:2004:LPO

[Ano04i] Anonymous. List of publications of osvaldo goscinski. *Advances in Quantum Chemistry*, 47:xxiii–xxx, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470312.

Anonymous:2004:Pa

[Ano04j] Anonymous. Preface. *Advances in Quantum Chemistry*, 45 (part 1):xi, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450151.

Anonymous:2004:Pb

[Ano04k] Anonymous. Preface. *Advances in Quantum Chemistry*, 47:xvii–xviii, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470269.

Anonymous:2004:QCT

[Ano04l] Anonymous. Quantum chemistry — theory, models, and computations. *Advances in Quantum Chemistry*, 47:xxi–xxii, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470300.

Anonymous:2005:Ca

[Ano05a] Anonymous. Contents. *Advances in Quantum Chemistry*, 48: v–xi, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480259.

Anonymous:2005:Cb

[Ano05b] Anonymous. Contents. *Advances in Quantum Chemistry*, 49: v–vii, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490103.

Anonymous:2005:Cc

[Ano05c] Anonymous. Contents. *Advances in Quantum Chemistry*, 50: v–viii, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500157.

Anonymous:2005:Cd

[Ano05d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 48: xiii–xv, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480260.

Anonymous:2005:Ce

[Ano05e] Anonymous. Contributors. *Advances in Quantum Chemistry*, 49: ix, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490085.

Anonymous:2005:Cf

[Ano05f] Anonymous. Contributors. *Advances in Quantum Chemistry*, 50: ix–x, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500212.

Anonymous:2006:Ca

[Ano06a] Anonymous. Contents. *Advances in Quantum Chemistry*, 51: v–vi, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760651007X.

Anonymous:2006:Cb

[Ano06b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 51: vii, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500169.

Anonymous:2007:Ca

[Ano07a] Anonymous. Contents. *Advances in Quantum Chemistry*, 52: v–viii, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520143.

Anonymous:2007:Cb

[Ano07b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 52: ix–x, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520155.

Anonymous:2008:Cb

[Ano08a] Anonymous. Contents. *Advances in Quantum Chemistry*, 55:v–x, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002250.

Anonymous:2008:Ca

[Ano08b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 53: ix–xiv, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530145.

Anonymous:2008:Cc

[Ano08c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 54: xi–xvii, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000287.

Anonymous:2008:Cd

[Ano08d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 55: xi–xvi, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002237.

Anonymous:2008:CPa

[Ano08e] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 54:iv, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000330.

Anonymous:2008:CPb

[Ano08f] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 55:iv, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002274.

Anonymous:2008:EB

[Ano08g] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 54:??, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000317.

Anonymous:2008:EHC

[Ano08h] Anonymous. Experiments on highly charged heavy ions in conjunction with exotic atoms. *Advances in Quantum Chemistry*, 53:217–235, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760753011X.

Anonymous:2008:F

[Ano08i] Anonymous. Foreword. *Advances in Quantum Chemistry*, 54:xix–xx, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000263.

Anonymous:2008:HFG

[Ano08j] Anonymous. HITRAP: a facility at GSI for highly charged ions. *Advances in Quantum Chemistry*, 53:83–98, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530078.

Anonymous:2008:P

[Ano08k] Anonymous. Preface. *Advances in Quantum Chemistry*, 54:xxi–xxviii, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000275.

Anonymous:2008:SE

[Ano08l] Anonymous. Series editors. *Advances in Quantum Chemistry*, 55:??, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002262.

Anonymous:2008:SI

[Ano08m] Anonymous. Subject index. *Advances in Quantum Chemistry*, 54:361–363, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000299.

Anonymous:2008:VE

[Ano08n] Anonymous. Volume editors. *Advances in Quantum Chemistry*, 55:??, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002286.

Anonymous:2009:Ca

[Ano09a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 56:xi, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004115.

Anonymous:2009:Cb

[Ano09b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 57: xi–xii, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006042.

Anonymous:2009:Cc

[Ano09c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 58: ix–x, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007047.

Anonymous:2009:CPa

[Ano09d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 56:iv, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004097.

Anonymous:2009:CPb

[Ano09e] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 57:iv, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006029.

Anonymous:2009:CPc

[Ano09f] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 58:iv, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007023.

Anonymous:2009:EBa

[Ano09g] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 57:??, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006017.

Anonymous:2009:EBb

[Ano09h] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 58:??, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007011.

Anonymous:2009:SE

[Ano09i] Anonymous. Series editors. *Advances in Quantum Chemistry*, 56:??, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004073.

Anonymous:2009:VE

[Ano09j] Anonymous. Volume editors. *Advances in Quantum Chemistry*, 56:??, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004085.

Anonymous:2010:Cb

[Ano10a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 59: xiii–xvi, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590154.

Anonymous:2010:Cd

[Ano10b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 60: xi–xiii, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600147.

Anonymous:2010:Ca

[Ano10c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 59:iv, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590130.

Anonymous:2010:Cc

[Ano10d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 60:iv, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600123.

Anonymous:2010:EBa

[Ano10e] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 59:??, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590117.

Anonymous:2010:EBb

[Ano10f] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 60:??, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761060010X.

Anonymous:2010:VEa

[Ano10g] Anonymous. Volume editors. *Advances in Quantum Chemistry*, 59:??, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590129.

Anonymous:2010:VEb

[Ano10h] Anonymous. Volume editors. *Advances in Quantum Chemistry*, 60:??, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600111.

Anonymous:2011:Cb

[Ano11a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 61: xiii–xiv, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000115.

Anonymous:2011:Cd

[Ano11b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 62: xiii–xiv, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012386013200019X.

Anonymous:2011:Ca

[Ano11c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 61: iv, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000097.

Anonymous:2011:Cc

[Ano11d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 62:iv, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000188.

Anonymous:2011:EB

[Ano11e] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 62:??, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000176.

Anonymous:2011:Ea

[Ano11f] Anonymous. Editors. *Advances in Quantum Chemistry*, 61: ??, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000073.

Anonymous:2011:Ec

[Ano11g] Anonymous. Editors. *Advances in Quantum Chemistry*, 62:??, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000164.

Anonymous:2011:Pa

[Ano11h] Anonymous. Preface. *Advances in Quantum Chemistry*, 61:ix–xi, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000140.

Anonymous:2011:Pb

[Ano11i] Anonymous. Preface. *Advances in Quantum Chemistry*, 62:ix–xi, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000103.

Anonymous:2012:Ca

[Ano12a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 63:ix, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000175.

Anonymous:2012:Cc

[Ano12b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 64:xi–xii, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000107.

Anonymous:2012:Cb

[Ano12c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 64:iv, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000089.

Anonymous:2012:CP

[Ano12d] Anonymous. Copyright page. *Advances in Quantum Chemistry*, 63:iv, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000151.

Anonymous:2012:EB

[Ano12e] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 63:??, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012397009100014X.

Anonymous:2012:I

[Ano12f] Anonymous. Index. *Advances in Quantum Chemistry*, 63:343–348, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000072.

Anonymous:2012:P

[Ano12g] Anonymous. Preface. *Advances in Quantum Chemistry*, 63: vii–viii, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000163.

Anonymous:2012:SP

[Ano12h] Anonymous. Series page. *Advances in Quantum Chemistry*, 64:??, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000120.

Anonymous:2012:SE

[Ano12i] Anonymous. Special editors. *Advances in Quantum Chemistry*, 63:??, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000138.

Anonymous:2012:SI

[Ano12j] Anonymous. Subject index. *Advances in Quantum Chemistry*, 64:259–266, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984099920.

Anonymous:2013:AQCa

[Ano13a] Anonymous. Advances in quantum chemistry. *Advances in Quantum Chemistry*, 65:??, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000157.

Anonymous:2013:AQCb

[Ano13b] Anonymous. Advances in quantum chemistry. *Advances in Quantum Chemistry*, 65:??, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000170.

Anonymous:2013:Cb

[Ano13c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 65: xvii–xix, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000212.

Anonymous:2013:Ca

[Ano13d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 65:iv, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000182.

Anonymous:2013:EB

[Ano13e] Anonymous. Editorial Board. *Advances in Quantum Chemistry*, 65:??, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000169.

Anonymous:2013:Ia

[Ano13f] Anonymous. Index. *Advances in Quantum Chemistry*, 65:451–461, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000224.

Anonymous:2013:Ib

[Ano13g] Anonymous. Index. *Advances in Quantum Chemistry*, 66:239–248, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012408099709989X.

Anonymous:2013:Ic

[Ano13h] Anonymous. Index. *Advances in Quantum Chemistry*, 67:291–296, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000352.

Anonymous:2013:P

[Ano13i] Anonymous. Preface. *Advances in Quantum Chemistry*, 65: xiii–xv, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000200.

Anonymous:2014:Cb

[Ano14a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 69: xi–xii, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012800345909992X.

Anonymous:2014:Ca

[Ano14b] Anonymous. Copyright. *Advances in Quantum Chemistry*, 69:iv, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012800345909989X.

Anonymous:2014:Ia

[Ano14c] Anonymous. Index. *Advances in Quantum Chemistry*, 68:315–320, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000241.

Anonymous:2014:Ib

[Ano14d] Anonymous. Index. *Advances in Quantum Chemistry*, 69:333–344, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459099918.

Anonymous:2014:SP

[Ano14e] Anonymous. Series page. *Advances in Quantum Chemistry*, 69:ii, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459099931.

Anonymous:2015:Cb

[Ano15a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 70: xiii–xiv, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327614000173.

Anonymous:2015:Cd

[Ano15b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 71: xiii–xv, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000489.

Anonymous:2015:Ca

[Ano15c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 70:iv, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327614000148`.

Anonymous:2015:Cc

[Ano15d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 71:iv, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000453`.

Anonymous:2015:Ia

[Ano15e] Anonymous. Index. *Advances in Quantum Chemistry*, 70:415–425, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327614000185`.

Anonymous:2015:Ib

[Ano15f] Anonymous. Index. *Advances in Quantum Chemistry*, 71:373–382, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000490`.

Anonymous:2015:SPa

[Ano15g] Anonymous. Series page. *Advances in Quantum Chemistry*, 70:ii, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327614000124`.

Anonymous:2015:SPb

[Ano15h] Anonymous. Series page. *Advances in Quantum Chemistry*, 71:ii, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000441`.

Anonymous:2016:Cb

[Ano16a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 72:xi–xii, 2016. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300090`.

Anonymous:2016:Ca

[Ano16b] Anonymous. Copyright. *Advances in Quantum Chemistry*, 72:iv, 2016. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300065`.

Anonymous:2016:I

[Ano16c] Anonymous. Index. *Advances in Quantum Chemistry*, 72:229–235, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300107.

Anonymous:2016:SP

[Ano16d] Anonymous. Series page. *Advances in Quantum Chemistry*, 72:ii, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300041.

Anonymous:2017:Cb

[Ano17a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 73:xiii–xvi, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300259.

Anonymous:2017:Cd

[Ano17b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 74:xi–xii, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300175.

Anonymous:2017:Cf

[Ano17c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 75:ix–x, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300503.

Anonymous:2017:Ca

[Ano17d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 73:iv, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300223.

Anonymous:2017:Cc

[Ano17e] Anonymous. Copyright. *Advances in Quantum Chemistry*, 74:iv, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300151.

Anonymous:2017:Ce

[Ano17f] Anonymous. Copyright. *Advances in Quantum Chemistry*, 75:iv, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300485.

Anonymous:2017:Ia

[Ano17g] Anonymous. Index. *Advances in Quantum Chemistry*, 73:415–423, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300260.

Anonymous:2017:Ib

[Ano17h] Anonymous. Index. *Advances in Quantum Chemistry*, 74:381–392, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300199.

Anonymous:2017:Ic

[Ano17i] Anonymous. Index. *Advances in Quantum Chemistry*, 75:267–272, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300527.

Anonymous:2017:SPa

[Ano17j] Anonymous. Series page. *Advances in Quantum Chemistry*, 73:ii, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761630020X.

Anonymous:2017:SPb

[Ano17k] Anonymous. Series page. *Advances in Quantum Chemistry*, 74:ii, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300138.

Anonymous:2017:SPc

[Ano17l] Anonymous. Series page. *Advances in Quantum Chemistry*, 75:ii, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300461.

Anonymous:2018:Cb

[Ano18a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 77:ix–x, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300121.

Anonymous:2018:Ca

[Ano18b] Anonymous. Copyright. *Advances in Quantum Chemistry*, 77:iv, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300108.

Anonymous:2018:I

[Ano18c] Anonymous. Index. *Advances in Quantum Chemistry*, 77:423–432, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300170.

Anonymous:2018:SP

[Ano18d] Anonymous. Series page. *Advances in Quantum Chemistry*, 77:ii, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761830008X.

Anonymous:2019:AQC

[Ano19a] Anonymous. Advances in quantum chemistry. *Advances in Quantum Chemistry*, 78:i, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300036.

Anonymous:2019:AJM

[Ano19b] Anonymous. Anniversary Jean Maruani. *Advances in Quantum Chemistry*, 78:xvii–xix, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300103.

Anonymous:2019:Cb

[Ano19c] Anonymous. Contributors. *Advances in Quantum Chemistry*, 78:xi–xii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300085.

Anonymous:2019:Cd

[Ano19d] Anonymous. Contributors. *Advances in Quantum Chemistry*, 79:xi–xiii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300486.

Anonymous:2019:Cf

[Ano19e] Anonymous. Contributors. *Advances in Quantum Chemistry*, 80:ix–xi, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300759.

Anonymous:2019:Ca

[Ano19f] Anonymous. Copyright. *Advances in Quantum Chemistry*, 78:iv, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300061.

Anonymous:2019:Cc

[Ano19g] Anonymous. Copyright. *Advances in Quantum Chemistry*, 79:iv, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300462`.

Anonymous:2019:Ce

[Ano19h] Anonymous. Copyright. *Advances in Quantum Chemistry*, 80:iv, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300735`.

Anonymous:2019:EB

[Ano19i] Anonymous. Editorial board. *Advances in Quantum Chemistry*, 78:ii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300048`.

Anonymous:2019:FM

[Ano19j] Anonymous. Front matter. *Advances in Quantum Chemistry*, 78:iii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532761930005X`.

Anonymous:2019:Ia

[Ano19k] Anonymous. Index. *Advances in Quantum Chemistry*, 78:453–465, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300115`.

Anonymous:2019:Ie

[Ano19l] Anonymous. Index. *Advances in Quantum Chemistry*, 79:337–341, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300644`.

Anonymous:2019:If

[Ano19m] Anonymous. Index. *Advances in Quantum Chemistry*, 80:361–366, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300772`.

Anonymous:2019:Ib

[Ano19n] Anonymous. Introduction. *Advances in Quantum Chemistry*, 79:53, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300590`.

Anonymous:2019:Ic

[Ano19o] Anonymous. Introduction. *Advances in Quantum Chemistry*, 79: 133, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300619`.

Anonymous:2019:Id

[Ano19p] Anonymous. Introduction. *Advances in Quantum Chemistry*, 79: 239, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300632`.

Anonymous:2019:SPa

[Ano19q] Anonymous. Series page. *Advances in Quantum Chemistry*, 79:ii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300449`.

Anonymous:2019:SPb

[Ano19r] Anonymous. Series page. *Advances in Quantum Chemistry*, 80:ii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300711`.

Anonymous:2020:Cb

[Ano20a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 81: ix–xi, 2020. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327620300289`.

Anonymous:2020:Cd

[Ano20b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 82: ix, 2020. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532762030040X`.

Anonymous:2020:Ca

[Ano20c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 81:iv, 2020. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327620300265`.

Anonymous:2020:Cc

[Ano20d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 82:iv, 2020. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327620300381`.

Anonymous:2020:Ia

[Ano20e] Anonymous. Index. *Advances in Quantum Chemistry*, 81:325–329, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300320.

Anonymous:2020:Ib

[Ano20f] Anonymous. Index. *Advances in Quantum Chemistry*, 82:369–378, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300423.

Anonymous:2020:SPa

[Ano20g] Anonymous. Series page. *Advances in Quantum Chemistry*, 81:ii, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300241.

Anonymous:2020:SPb

[Ano20h] Anonymous. Series page. *Advances in Quantum Chemistry*, 82:ii, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300368.

Anonymous:2021:Cb

[Ano21a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 83:xi–xiii, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000277.

Anonymous:2021:Cd

[Ano21b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 84:ix–x, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000411.

Anonymous:2021:Ca

[Ano21c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 83:iv–vi, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000253.

Anonymous:2021:Cc

[Ano21d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 84:iv, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000393.

Anonymous:2021:Ia

[Ano21e] Anonymous. Index. *Advances in Quantum Chemistry*, 83:329–334, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000290.

Anonymous:2021:Ib

[Ano21f] Anonymous. Index. *Advances in Quantum Chemistry*, 84:565–574, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000435.

Anonymous:2021:SPa

[Ano21g] Anonymous. Series page. *Advances in Quantum Chemistry*, 83:ii, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762100023X.

Anonymous:2021:SPb

[Ano21h] Anonymous. Series page. *Advances in Quantum Chemistry*, 84:ii, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762100037X.

Anonymous:2022:Cb

[Ano22a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 85:xi–xiii, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000272.

Anonymous:2022:Cd

[Ano22b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 86:vii, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000405.

Anonymous:2022:Ca

[Ano22c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 85:iv, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000259.

Anonymous:2022:Cc

[Ano22d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 86:iv, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000387.

Anonymous:2022:Ia

[Ano22e] Anonymous. Index. *Advances in Quantum Chemistry*, 85:377–387, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000302.

Anonymous:2022:Ib

[Ano22f] Anonymous. Index. *Advances in Quantum Chemistry*, 86:323–327, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000454.

Anonymous:2022:P

[Ano22g] Anonymous. Preface. *Advances in Quantum Chemistry*, 86:ix–xi, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000417.

Anonymous:2022:SPa

[Ano22h] Anonymous. Series page. *Advances in Quantum Chemistry*, 85:ii, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000235.

Anonymous:2022:SPb

[Ano22i] Anonymous. Series page. *Advances in Quantum Chemistry*, 86:ii, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000363.

Anonymous:2023:Cb

[Ano23a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 87:xi–xiii, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000461.

Anonymous:2023:Cd

[Ano23b] Anonymous. Contributors. *Advances in Quantum Chemistry*, 88:xi–xiv, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S006532762300062X.

Anonymous:2023:Ca

[Ano23c] Anonymous. Copyright. *Advances in Quantum Chemistry*, 87:iv, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000448.

Anonymous:2023:Cc

[Ano23d] Anonymous. Copyright. *Advances in Quantum Chemistry*, 88: iv, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000606`.

Anonymous:2023:Ia

[Ano23e] Anonymous. Index. *Advances in Quantum Chemistry*, 87:415–420, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327623000497`.

Anonymous:2023:Ib

[Ano23f] Anonymous. Index. *Advances in Quantum Chemistry*, 88:373–379, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000643`.

Anonymous:2023:SPa

[Ano23g] Anonymous. Series page. *Advances in Quantum Chemistry*, 87:ii, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327623000424`.

Anonymous:2023:SPb

[Ano23h] Anonymous. Series page. *Advances in Quantum Chemistry*, 88: ii, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000588`.

Anonymous:2024:Cb

[Ano24a] Anonymous. Contributors. *Advances in Quantum Chemistry*, 89: ix–x, 2024. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S006532762400008X`.

Anonymous:2024:Ca

[Ano24b] Anonymous. Copyright. *Advances in Quantum Chemistry*, 89: iv, 2024. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327624000066`.

Anonymous:2024:I

[Ano24c] Anonymous. Index. *Advances in Quantum Chemistry*, 89:383–391, 2024. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327624000121`.

Anonymous:2024:SP

[Ano24d] Anonymous. Series page. *Advances in Quantum Chemistry*, 89: ii, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327624000042.

Adachi:2003:MET

[AO03] Hirohiko Adachi and Kazuyoshi Ogasawara. Many-electron theory for electronic transition process — its importance in materials science. *Advances in Quantum Chemistry*, 42:1–22, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420388.

Alatalo:2003:RAC

[AP03] M. Alatalo and M. J. Puska. Recent advances in the calculations for momentum distributions of annihilating electron-positron pairs in solids. *Advances in Quantum Chemistry*, 42:127–143, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420443.

Acevedo:2003:SIC

[APNM03] R. Acevedo, C. Portillo, G. Navarro, and T. Meruane. Spectral intensities in cubic stoichiometric elpasolites: The $Cs_2NaSmCl_6$ and $Cs_2NaEuCl_6$ systems. *Advances in Quantum Chemistry*, 44:509–525, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440331.

Apostolova:2001:PMP

[Apo01] Elena S. Apostolova. *D*-parameter of the Morse potential as a new bond index for estimating bond breaking energy in a molecule. *Advances in Quantum Chemistry*, 40:143–159, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760140013X.

Aquino:2009:HHA

[Aqu09] N. Aquino. The hydrogen and helium atoms confined in spherical boxes. *Advances in Quantum Chemistry*, 57:123–171, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760900608X.

Atanasov:2003:DBP

[AR03] M. Atanasov and D. Reinen. A DFT based parameterization of the vibronic mixing between two non-degenerate electronic states and the application to s^2-lone pairs. *Advances in Quantum Chemistry*, 44:355–368, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440239.

Angeli:1999:CTM

[ARS99] Celestino Angeli, Christian Rolando, and Michèle Suard. Complexation of transition metal cations (Sc^+, Fe^+, Cu^+) by one cyanide radical. *Advances in Quantum Chemistry*, 36:271–282, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604876.

Ashwell:2017:TDD

[ARS17] Adam P. Ashwell, Mark A. Ratner, and George C. Schatz. A time-dependent density functional theory study of the impact of ligand passivation on the plasmonic behavior of Ag nanoclusters. *Advances in Quantum Chemistry*, 75:117–145, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300011.

Ariya:2008:GEM

[ASGG08] Parisa A. Ariya, Henrik Skov, Mette M.-L. Grage, and Michael Evan Goodsite. Gaseous elemental mercury in the ambient atmosphere: Review of the application of theoretical calculations and experimental studies for determination of reaction coefficients and mechanisms with halogens and other reactants. *Advances in Quantum Chemistry*, 55:43–55, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002043.

Almlof:1991:ANO

[AT91] Jan Almlöf and Peter R. Taylor. Atomic natural orbital (ANO) basis sets for quantum chemical calculations. *Advances in Quantum Chemistry*, 22:301–373, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603664.

Alcoba:2018:HTB

[ATL+18] Diego R. Alcoba, Alicia Torre, Luis Lain, Ofelia B. Oña, Gustavo E. Massaccesi, and Pablo Capuzzi. Hybrid treatments based on determinant seniority numbers and spatial excitation levels in the configuration interaction framework. *Advances in Quantum Chemistry*, 76:315–332, 2018. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300400.

Adachi:2000:P

[AUS00] H. Adachi, M. Uda, and R. Sekine. Preface. *Advances in Quantum Chemistry*, 37:xv–xvi, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370010.

Adachi:2003:P

[AUW03] H. Adachi, M. Uda, and H. Wakita. Preface. *Advances in Quantum Chemistry*, 42:xvii, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420376.

Andino:2008:TCA

[AVB08] Jean M. Andino and Annik Vivier-Bunge. Tropospheric chemistry of aromatic compounds emitted from anthropogenic sources. *Advances in Quantum Chemistry*, 55:297–310, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002146.

Avery:1998:MES

[Ave98] John Avery. Many-electron Sturmians as an alternative to the SCF–CI method. *Advances in Quantum Chemistry*, 31:201–229, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601896.

Avery:2013:FER

[Ave13] J. E. Avery. Fast electron repulsion integrals for molecular Coulomb Sturmians. *Advances in Quantum Chemistry*, 67:129–151, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000066.

AAgren:1996:RTC

[ÅVM96] Hans Ågren, Olav Vahtras, and Boris Minaev. Response theory and calculations of spin-orbit coupling phenomena in molecules. *Advances in Quantum Chemistry*, 27:71–162, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602518.

Akdemir:2017:EOE

[AYÖ17] Selda Akdemir, Niyazi Yükçü, and Emin Öztekin. Evaluation of one-electron basic integrals of irregular solid harmonics and Slater-type orbitals using Fourier transforms. *Advances in Quantum Chemistry*, 73:183–195, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000301.

Bader:2009:CAT

[Bad09] Richard F. W. Bader. Confined atoms treated as open quantum systems. *Advances in Quantum Chemistry*, 57:285–318, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006133.

Barysz:2023:RPI

[Bar23] Maria Barysz. Relativistic perturbative and infinite-order two-component methods for heavy elements: Radium atom. *Advances in Quantum Chemistry*, 87:281–295, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762300014X.

Basu:1964:TSE

[Bas64] Sadhan Basu. Theory of solvent effects on molecular electronic spectra. *Advances in Quantum Chemistry*, 1:145–169, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603779.

Basu:1978:CLE

[Bas78] Sadhan Basu. Convergence limit in the electronic spectra of linear polyenes. *Advances in Quantum Chemistry*, 11:33–49, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602336.

Barbier:1999:HCH

[BB99a] C. Barbier and Gaston Berthier. Half a century of hybridization. *Advances in Quantum Chemistry*, 36:1–25, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604761.

Bernholdt:1999:CAM

[BB99b] David E. Bernholdt and Rodney J. Bartlett. A critical assessment of multireference-fock space CCSD and perturbative third-order triples approximations for photoelectron spectra and quasidegenerate potential energy surfaces. *Advances in Quantum Chemistry*, 34:271–293, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860533X.

Belkic:2011:HRS

[BB11] Dževad Belkić and Karen Belkić. High-resolution signal processing in magnetic resonance spectroscopy for early cancer diagnostics. *Advances in Quantum Chemistry*, 62:243–347, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000061.

Belkic:2013:MRB

[BB13] Dzevad Belkić and Karen Belkić. Mechanistic repair-based Padé linear–quadratic model for cell response to radiation damage. *Advances in Quantum Chemistry*, 65:407–449, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000145.

Bouchelaghem:2014:IEL

[BB14] F. Bouchelaghem and M. Bouledroua. Isotopic effects in the Li^+–Li collisions at lower and higher temperatures. *Advances in Quantum Chemistry*, 68:239–255, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000125.

Belkic:2015:MRM

[BB15] Dzevad Belkić and Karen Belkić. Mechanistic radiobiological models for repair of cellular radiation damage. *Advances in Quantum Chemistry*, 70:163–263, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327614000045.

Belkic:2017:HRQ

[BB17] Dzevad Belkić and Karen Belkić. High-resolution quantum-mechanical signal processing for in vivo NMR spectroscopy. *Advances in Quantum Chemistry*, 74:347–379, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300399.

Belkic:2021:CTD

[BB21] Dževad Belkić and Karen Belkić. Derivative NMR spectroscopy for j-coupled resonances in analytical chemistry and medical diagnostics. *Advances in Quantum Chemistry*, 84:95–265, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000034.

Belkic:2022:NSH

[BB22a] Dževad Belkić and Karen Belkić. NMR spectroscopy at high magnetic fields: Derivative reconstructions of components from envelopes using encoded time signals. *Advances in Quantum Chemistry*, 86:151–221, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000181.

Brandas:2022:AQC

[BB22b] Erkki Brändas and Rodney J. Bartlett, editors. *Advances in Quantum Chemistry*, volume 86. Elsevier Academic Press, Amsterdam, The Netherlands, 2022. ISBN 0-443-18665-0 (hardcover), 0-443-18666-9 (ePub). ISSN 0065-3276. xi + 327 pp. LCCN QD462.

Brandas:2024:AQC

[BB24a] Erkki J. Brändas and Rodney J. Bartlett, editors. *Advances in Quantum Chemistry*, volume 89 of *Advances in quantum chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2024. ISBN 0-443-24121-X. ISSN 0065-3276. 391 pp. LCCN QD462.

Brandas:2024:P

[BB24b] Erkki J. Brändas and Rodney J. Bartlett. Preface. *Advances in Quantum Chemistry*, 89:xi–xii, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327624000091.

Barone:2010:ERC

[BBB10] Vincenzo Barone, Małgorzata Biczysko, and Giuseppe Brancato. Extending the range of computational spectroscopy by QM/MM approaches: Time-dependent and time-independent routes. *Advances in Quantum Chemistry*, 59:17–57, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590026.

Bishop:1980:AOT

[BC80] David M. Bishop and Lap M. Cheung. Accurate one- and two-electron diatomic molecular calculations. *Advances in Quantum Chemistry*, 12:1–42, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603123.

Brand:2000:TET

[BC00] Joachim Brand and Lorenz S. Cederbaum. Theory of extended two-particle Green's functions. *Advances in Quantum Chemistry*, 38:65–120, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600380030.

Burrows:2009:ESC

[BC09] B. L. Burrows and M. Cohen. Exact solutions for confined model systems using Kummer functions. *Advances in Quantum Chemistry*, 57:173–201, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006091.

Bendazzoli:2001:FCS

[BE01] Gian Luigi Bendazzoli and Stefano Evangelisti. Full CI solution of perturbative equations. *Advances in Quantum Chemistry*, 39:189–207, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390125.

Bendazzoli:2004:HMP

[BE04] Gian Luigi Bendazzoli and Stefano Evangelisti. The Hückel model of polyacetylene revisited: Asymptotic analysis of Peierls instability. *Advances in Quantum Chemistry*, 47:347–368, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470208.

Belkic:2006:FPT

[Bel06] Dževad Belkić. Fast padé transform for exact quantification of time signals in magnetic resonance spectroscopy. *Advances in Quantum Chemistry*, 51:157–233, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510056.

Belkic:2009:QMM

[Bel09] Dževad Belkić. Quantum mechanical methods for loss-excitation and loss-ionization in fast ion-atom collisions. *Advances in Quantum Chemistry*, 56:251–321, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004061.

Belkic:2011:PAT

[Bel11] Dževad Belkić. Parametric analysis of time signals and spectra from perspectives of quantum physics and chemistry. *Advances in Quantum Chemistry*, 61:145–260, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000048.

BelenRuiz:2019:CIS

[Bel19] María Belén Ruiz. Configuration interaction study of the ^{3}P ground and low-lying states of the boron anion. The boron electron affinity. *Advances in Quantum Chemistry*, 79:135–153, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761930022X.

Belkic:2021:CFO

[Bel21] Dževad Belkić. One electron-capture in collisions of fast nuclei with biomolecules of relevance to ion therapy. *Advances in Quantum Chemistry*, 84:267–345, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000010.

Belkic:2022:DWT

[Bel22] Dževad Belkić. Distorted wave theories with correct boundary conditions for double charge exchange in ion-atom collisions at intermediate and high energies. *Advances in Quantum Chemistry*, 86:223–296, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762200017X.

Berthier:1974:SRD

[Ber74] G. Berthier. Some recent developments in the theory of coordination compounds of metals. *Advances in Quantum Chemistry*, 8:183–230, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600623.

Berrondo:2002:LDC

[Ber02] M. Berrondo. Learning differential calculus without limits. *Advances in Quantum Chemistry*, 41:107–120, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410490.

Bersuker:2003:UJT

[Ber03] Isaac B. Bersuker. A unique Jahn–Teller mechanism of all the symmetry breakings in molecular systems and condensed matter. *Advances in Quantum Chemistry*, 44:1–12, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760344001X.

Bernstein:2014:RSE

[Ber14] Elliot R. Bernstein. On the release of stored energy from energetic materials. *Advances in Quantum Chemistry*, 69:31–69, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459000027.

Broclawik:2023:ICC

[BFHS23] Ewa Brocławik, Maciej Fidrysiak, Maciej Hendzel, and Józef Spałek. Interparticle correlations and chemical bonding from physical side: Covalency vs atomicity and ionicity. *Advances in Quantum Chemistry*, 87:351–373, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000151.

Berg:1973:AIP

[BG73] R. A. Berg and A. E. S. Green. An analytic independent particle model for atoms. III. Ionization of rare gas atoms by electrons in the Born approximation. *Advances in Quantum Chemistry*, 7:277–288, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605651.

Brandas:2001:Pa

[BG01a] E. Brändas and O. Goscinski. Preface. *Advances in Quantum Chemistry*, 39:xxv–xxvi, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390241.

Brandas:2001:Pb

[BG01b] E. Brändas and O. Goscinski. Preface. *Advances in Quantum Chemistry*, 40:xxv–xxvi, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400049.

Bagci:2023:EAA

[BG23] Ali Bağcı and Z. Güneş. An efficient approximation for accelerating convergence of numerical power series: Results for the 1*D*-Schrödinger equation. *Advances in Quantum Chemistry*, 88:35–55, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327622000491.

Baccarelli:2007:EDM

[BGG+07] I. Baccarelli, F. A. Gianturco, A. Grandi, R. R. Lucchese, and N. Sanna. Electron-driven molecular processes induced in biological systems by electromagnetic and other ionizing sources. *Advances in Quantum Chemistry*, 52:189–230, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760652009X.

Bass:1973:AIP

[BGW73] J. N. Bass, A. E. S. Green, and J. H. Wood. An analytic independent particle model for atoms. II. Modified Hartree–Fock calculations for atoms. *Advances in Quantum Chemistry*, 7:263–275, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860564X.

Bagci:2024:CSS

[BH24] A. Bağcı and Philip E. Hoggan. Chapter six — solution of the Dirac–Coulomb equation using the Rayleigh–Ritz method: Results for He-like atoms. *Advances in Quantum Chemistry*, 89:339–357, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000709.

Buchanan:2017:SFO

[BHM17] Eric A. Buchanan, Zdenek Havlas, and Josef Michl. Singlet fission: Optimization of chromophore dimer geometry. *Advances in Quantum Chemistry*, 75:175–227, 2017. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300321.

Bastug:2000:MDS

[BHV+00] Turgut Bastug, Masaru Hirata, Sven Varga, Burkhard Fricke, Sakir Erkoç, and Takeshi Mukoyama. Molecular-dynamics simulations of gold clusters. *Advances in Quantum Chemistry*, 37:353–364, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370253.

Bichsel:2004:TAN

[Bic04] Hans Bichsel. Thoughts about nanodosimetry. *Advances in Quantum Chemistry*, 46 (part 2):329–338, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460134.

Bichsel:2013:SEL

[Bic13] Hans Bichsel. Stochastics of energy loss and biological effects of heavy ions in radiation therapy. *Advances in Quantum Chemistry*, 65:1–38, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000017.

Bishop:1967:SCM

[Bis67] David M. Bishop. Single-center molecular wave functions. *Advances in Quantum Chemistry*, 3:25–59, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600866.

Bishop:1994:ANL

[Bis94] David M. Bishop. Aspects of non-linear optical calculations. *Advances in Quantum Chemistry*, 25:1–45, 1994. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600179.

Bischoff:2019:CAM

[Bis19] Florian A. Bischoff. Computing accurate molecular properties in real space using multiresolution analysis. *Advances in Quantum Chemistry*, 79:3–52, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761930019X.

Bellayouni:2014:SSE

[BJMB14] S. Bellayouni, I. Jendoubi, N. Mabrouk, and H. Berriche. Systematic study of the electronic properties and trends in the LiX (X = Na, K, Rb, Cs and Fr) molecules. *Advances in Quantum Chemistry*, 68:203–238, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128005361000113`.

Briels:1986:DMC

[BJV86] W. J. Briels, A. P. J. Jansen, and A. Van Der Avoird. Dynamics of molecular crystals. *Advances in Quantum Chemistry*, 18:131–206, 1986. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600490`.

Bingel:1970:SPR

[BK70] W. A. Bingel and W. Kutzelnigg. Symmetry properties of reduced density matrices and natural p-states. *Advances in Quantum Chemistry*, 5:201–218, 1970. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603408`.

Buyadzhi:2019:AQA

[BKB$^+$19] Vasily V. Buyadzhi, Anna A. Kuznetsova, Anna A. Buyadzhi, Eugeny V. Ternovsky, and Tatyana B. Tkach. Advanced quantum approach in radiative and collisional spectroscopy of multicharged ions in plasmas. *Advances in Quantum Chemistry*, 78:171–191, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327618300261`.

Bieniewski:1968:AIC

[BKC68] T. M. Bieniewski, T. K. Krueger, and S. J. Czyzak. Atomic intensities: a comparison of theoretical and experimental f-values for ZnI, CdI and HgI. *Advances in Quantum Chemistry*, 4:141–152, 1968. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603925`.

Budylin:2021:CFA

[BKL21] A. M. Budylin, Ya. Yu. Koptelov, and S. B. Levin. On asymptotic structure of three-body scattering states for the scattering problem of charged quantum particles. *Advances in Quantum Chemistry*, 84:347–424, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000186.

Barca:2018:RRF

[BL18] Giuseppe M. J. Barca and Pierre-François Loos. Recurrence relations for four-electron integrals over Gaussian basis functions. *Advances in Quantum Chemistry*, 76:147–165, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761730031X.

Bartkowiak:2023:MSS

[BLC23] Wojciech Bartkowiak, Paweł Lipkowski, and Marta Chołuj. Molecular systems in spatial confinement: Variation of linear and nonlinear electrical response of molecules in the bond dissociation processes. *Advances in Quantum Chemistry*, 87:335–350, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000096.

Blinder:1965:TAH

[Bli65] S. M. Blinder. Theory of atomic hyperfine structure. *Advances in Quantum Chemistry*, 2:47–91, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600726.

Bonham:1978:EMC

[BLKS78] R. A. Bonham, J. S. Lee, R. Kennerly, and W. St. John. Experimental measurements of charge and momentum densities, generalized oscillator strengths, and excitation frequencies. *Advances in Quantum Chemistry*, 11:1–32, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602324.

Batandjieva:1997:ISF

[BMC97] Borislava Batandjieva, Ingrid Miadoková, and Ivan Cernušák. An *ab initio* study of four-membered rings. boranes HBXYBH; (X, Y = C, N, O). *Advances in Quantum Chemistry*, 28:219–234, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602178.

Belkic:2013:FBT

[BMM13] Dzevad Belkić, Ivan Mancev, and Nenad Milojević. Four-body theories for transfer ionization in fast ion-atom collisions. *Advances in Quantum Chemistry*, 65:339–362, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000121.

Bevilacqua:2003:RTI

[BMP03] Giuseppe Bevilacqua, Liana Martinelli, and Giuseppe Pastori Parravicini. Renner–Teller interaction matrices and Green's function formalism. *Advances in Quantum Chemistry*, 44:45–57, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440045.

Baraldi:1999:RDC

[BMPV99] I. Baraldi, Fabio Momicchioli, G. Ponterini, and D. Vanossi. A recent development of the CS INDO model: Treatment of solvent effects on structures and optical properties of organic dyes. *Advances in Quantum Chemistry*, 36:121–150, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604815.

Baer:2024:CFQ

[BMR+24] Michael Baer, Soumya Mukherjee, Satyam Ravi, Satrajit Adhikari, and Narayanasami Sathyamurthy. Chapter four — the quantum mechanical non-adiabatic coupling term as friction in the formation of DH_2^+. *Advances in Quantum Chemistry*, 89:291–304, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000540.

Bader:1981:QTA

[BND81] R. F. W. Bader and T. T. Nguyen-Dang. Quantum theory of atoms in molecules — Dalton revisited. *Advances in Quantum Chemistry*, 14:63–124, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603263.

Bersuker:1986:JTE

[BO86] I. B. Bersuker and I. Ya. Ogurtsov. The Jahn–Teller effect in dipole (multipole) moments and polarizabilities of molecules. *Advances in Quantum Chemistry*, 18:1–84, 1986. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600477.

Borshch:2003:VIH

[Bor03] Serguei A. Borshch. Vibronic interactions in high nuclearity clusters. *Advances in Quantum Chemistry*, 44:389–400, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440252.

Bersuker:1982:VIJ

[BP82] I. B. Bersuker and V. Z. Polinger. Vibronic interactions and the Jahn–Teller effect. *Advances in Quantum Chemistry*, 15:85–160, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601227.

Brandas:2020:LQD

[BP20] Erkki J. Brändas and Roman R. Poznański. Is life quantum Darwinian? *Advances in Quantum Chemistry*, 82:1–11, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300204.

Bauman:2023:CCD

[BPK23] Nicholas P. Bauman, Bo Peng, and Karol Kowalski. Coupled-cluster downfolding techniques: a review of existing applications in classical and quantum computing for chemical systems. *Advances in Quantum Chemistry*, 87:141–166, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762300028X.

Boys:1965:QCW

[BR65] S. F. Boys and P. Rajagopal. Quantum calculations: Which are accumulative in accuracy, unrestricted in expansion functions, and economical in computation. *Advances in Quantum Chemistry*, 2:1–24, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600702.

Basilevsky:1982:QDL

[BR82] M. V. Basilevsky and V. M. Ryaboy. Quantum dynamics of linear triatomic reactions. *Advances in Quantum Chemistry*, 15:1–83, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601215.

Bihary:2005:DST

[BR05] Zsolt Bihary and Mark A. Ratner. Density of states and transmission in molecular transport junctions. *Advances in Quantum Chemistry*, 48:23–34, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760548003X.

Berrondo:2017:VQS

[BR17] Manuel Berrondo and Jose Récamier. Vibrational quantum squeezing induced by inelastic collisions. *Advances in Quantum Chemistry*, 74:129–147, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300351.

Brandas:2020:CPQ

[BR20] Erkki Brändas and Kenneth Ruud, editors. *Chemical Physics and Quantum Chemistry*, volume 81 of *Advances in quantum chemistry*. Academic Press Inc., New York, USA, 2020. CODEN AQCHA9. ISBN 0-12-819757-9 (hardcover), 0-12-819758-7 (e-book). ISSN 0065-3276. LCCN QD462.

Bratoz:1967:ETH

[Bra67] S. Bratož. Electronic theories of hydrogen bonding. *Advances in Quantum Chemistry*, 3:209–237, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600908.

Brandow:1977:LCP

[Bra77] B. H. Brandow. Linked-cluster perturbation theory for closed- and open-shell systems. *Advances in Quantum Chemistry*, 10: 187–249, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860581X.

Brandas:2002:DSM

[Brä02] Erkki J. Brändas. Dissipative systems and microscopic self-organization. *Advances in Quantum Chemistry*, 41:121–138, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410507.

Brandas:2003:NPT

[Brä03] Erkki J. Brändas. New perspectives in theoretical chemical physics. *Advances in Quantum Chemistry*, 42:383–397, 2003.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420625.

Brandas:2004:JBN

[Brä04] Erkki J. Brändas. Are Jordan blocks necessary for the interpretation of dynamical processes in nature? *Advances in Quantum Chemistry*, 47:93–106, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470063.

Brandas:2008:QMS

[Brä08] Erkki J. Brändas. Quantum mechanics and the special and general theory of relativity. *Advances in Quantum Chemistry*, 54:115–132, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760700010X.

Brandas:2012:ELP

[Brä12] Erkki J. Brändas. Examining the limits of physical theory: Analytical principles and logical implications. *Advances in Quantum Chemistry*, 63:33–117, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000023.

Brandas:2019:MFE

[Brä19] Erkki J. Brändas. Molecular foundation of evolution. *Advances in Quantum Chemistry*, 78:1–30, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300327.

Brandas:2021:AQC

[Brä21a] Erkki Brändas, editor. *Advances in Quantum Chemistry*, volume 84. Academic Press Inc., New York, USA, 2021. ISBN 0-12-823877-1 (hardcover), 0-12-823878-X (ePub ebook). ISSN 0065-3276. xiii + 574 pp. LCCN QD462.

Brandas:2021:P

[Brä21b] Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 84: xi–xiii, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000423.

Brandas:2022:QDE

[Brä22] Erkki J. Brändas. Quantum Darwinism and entropy. *Advances in Quantum Chemistry*, 86:297–321, 2022. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327622000193`.

Bernal-Rodriguez:2013:SIL

[BRL13] Mario A. Bernal-Rodríguez and Jacinto A. Liendo. Single ionization of liquid water by protons, alpha particles, and carbon nuclei: Comparative analysis of the continuum distorted wave methodologies and empirical models. *Advances in Quantum Chemistry*, 65:203–229, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B978012396455700008X`.

Broclawik:1998:DFT

[Bro98a] Ewa Brocławik. Density functional theory in catalysis: Activation and reactivity of a hydrocarbon molecule on a metallic active site. *Advances in Quantum Chemistry*, 33:349–367, 1998. CODEN AQCHA9. ISSN 0065-3276.

Broctawik:1998:DFT

[Bro98b] Ewa Broctawik. Density functional theory in catalysis: Activation and reactivity of a hydrocarbon molecule on a metallic active site. *Advances in Quantum Chemistry*, 33:349–367, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860444X`.

Brandao:2008:IWS

[BRW08] João Brandão, Carolina M. A. Rio, and Wenli Wang. An important well studied atmospheric reaction, $O(^1D) + H_2$. *Advances in Quantum Chemistry*, 55:21–41, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327607002031`.

Basu:1972:CEO

[BS72] Sadhan Basu and Purnendranath Sen. Collective electron oscillation in pi-electron systems. *Advances in Quantum Chemistry*, 6:159–175, 1972. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605444`.

Berzinsh:1998:ARL

[BS98] U. Berzinsh and S. Svanberg. Atomic radiative lifetimes measured by pulsed laser spectroscopy in the UV/VUV spectral region. *Advances in Quantum Chemistry*, 30:283–299, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605122.

Bauer:2004:CPS

[BS04] Peter Bauer and Dieter Semrad. Chemical and physical state effects in electronic stopping. *Advances in Quantum Chemistry*, 46 (part 2):153–163, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460067.

Berger:2005:NIN

[BS05a] Raphael J. F. Berger and Dage Sundholm. A non-iterative numerical solver of Poisson and Helmholtz equations using high-order finite-element functions. *Advances in Quantum Chemistry*, 50:235–247, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760550011X.

Brandas:2005:P

[BS05b] Erkki Brändas and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 49:xi–xii, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490097.

Brandas:2006:P

[BS06] Erkki J. Brändas and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 51:ix–x, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510093.

Brandas:2007:P

[BS07] Erkki Brändas and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 52:xi–xii, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520167.

Belkic:2013:AQC

[BSB13] Dževad Belkić, John R. Sabin, and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 65 of *Advances in Quan-*

tum Chemistry. Elsevier Academic Press, Amsterdam, The Netherlands, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. ???? pp. LCCN QC451 .U57 2012 .v65. Founding editor Per-Olov Löwdin (1916–2000).

Buksztel:2014:OOR

[BŚG14] A. Buksztel, S. Śmiga, and I. Grabowski. OEP orbitals as a reference for ab initio many-body calculations. *Advances in Quantum Chemistry*, 68:105–123, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012800536100006X.

Buksztel:2017:CED

[BŚG17] Adam Buksztel, Szymon Śmiga, and Ireneusz Grabowski. The correlation effects in density functional theory along the dissociation path. *Advances in Quantum Chemistry*, 73:263–283, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000374.

Breuil:2019:DTE

[BSL+19] Gabriel Breuil, Kaltrina Shehu, Elise Lognon, Sylvain Pitié, Benjamin Lasorne, and Thibaud Etienne. Diagnosis of two evaluation paths to density-based descriptors of molecular electronic transitions. *Advances in Quantum Chemistry*, 79:289–310, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300206.

Bocharnikova:2020:TSB

[BTB+20] Elena N. Bocharnikova, Olga N. Tchaikovskaya, Olga K. Bazyl, Viktor Ya. Artyukhov, and George V. Mayer. Theoretical study of bisphenol A photolysis. *Advances in Quantum Chemistry*, 81:191–217, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300802.

Barysz:1997:MPB

[BU97] Maria Barysz and Miroslav Urban. Molecular properties of boron-coinage metal dimers: BCu, BAg, BAu. *Advances in Quantum Chemistry*, 28:257–272, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602208.

Bunge:2017:SSL

[Bun17] Carlos F. Bunge. Specifics on the scientific legacy of Per-Olov Löwdin. *Advances in Quantum Chemistry*, 74:53–82, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300338`.

Bunge:2018:PSS

[Bun18] Carlos F. Bunge. Present status of selected configuration interaction with truncation energy error. *Advances in Quantum Chemistry*, 76:3–34, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327617300357`.

Bunge:2023:FAC

[Bun23] Carlos F. Bunge. Fully automatic calculations of atomic energy levels with truncation energy errors. *Advances in Quantum Chemistry*, 88:3–27, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000333`.

Baer:2003:ENA

[BVHK03] M. Baer, Á. Vibók, G. J. Halász, and D. J. Kouri. The electronic non-adiabatic coupling terms: On the connection between molecular physics and field theory. *Advances in Quantum Chemistry*, 44:103–118, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440070`.

Bianco:2008:TSD

[BWH08] Roberto Bianco, Shuzhi Wang, and James T. Hynes. Theoretical studies of the dissociation of sulfuric acid and nitric acid at model aqueous surfaces. *Advances in Quantum Chemistry*, 55:387–405, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327607002183`.

Bielinska-Waz:1997:DSM

[BWK97] Dorota Bielińska-Wąż and Jacek Karwowski. Determining the shapes of molecular electronic bands from their intensity distribution moments. *Advances in Quantum Chemistry*, 28:159–169, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602130`.

Beebe-Wang:2013:VRT

[BWVD+13] Joanne Beebe-Wang, Paul Vaska, F. Avraham Dilmanian, Stephen G. Peggs, and David J. Schlyer. Verifying radiation treatment in proton therapy via PET imaging of the induced positron-emitters. *Advances in Quantum Chemistry*, 65:111–127, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000054.

Bylicki:1998:MIC

[Byl98] Miroslaw Bylicki. Methods involving complex coordinates applied to atoms. *Advances in Quantum Chemistry*, 32:207–226, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604153.

Cronstrand:2001:ACI

[CÅ01] Peter Cronstrand and Hans Ågren. Assignment and convergence of IR spectra for a sequence of polypyridine oligomers. *Advances in Quantum Chemistry*, 40:213–223, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400177.

Chilkuri:2021:CTS

[CAG+21] Vijay Gopal Chilkuri, Thomas Applencourt, Kevin Gasperich, Pierre-François Loos, and Anthony Scemama. Spin-adapted selected configuration interaction in a determinant basis. *Advances in Quantum Chemistry*, 83:65–81, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000022.

Calais:1985:GEI

[Cal85] Jean-Louis Calais. Gap equations and instabilities for extended systems. *Advances in Quantum Chemistry*, 17:225–250, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603032.

Caldwell:2013:CCP

[Cal13] Dennis Caldwell. Conundrums in chemical physics. *Advances in Quantum Chemistry*, 66:31–111, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124080997000027.

Cammi:2012:RAC

[Cam12] Roberto Cammi. Recent advances in the coupled-cluster analytical derivatives theory for molecules in solution described with the polarizable continuum model (PCM). *Advances in Quantum Chemistry*, 64:1–29, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000016.

Canuto:2010:P

[Can10] Sylvio Canuto. Preface. *Advances in Quantum Chemistry*, 59: ix–xi, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590142.

Coletti:2019:HOP

[CAP19] Cecilia Coletti, Vincenzo Aquilanti, and Federico Palazzetti. Hypergeometric orthogonal polynomials as expansion basis sets for atomic and molecular orbitals: the Jacobi ladder. *Advances in Quantum Chemistry*, 79:55–77, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300255.

Carbo:1992:MCA

[CB92] Ramon Carbó and Emili Besalú. Many center AO integral evaluation using cartesian exponential type orbitals (CETO'S). *Advances in Quantum Chemistry*, 24:115–237, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601021.

Cox:2018:SSM

[CB18] Hazel Cox and Adam L. Baskerville. The series solution method in quantum chemistry for three-particle systems. *Advances in Quantum Chemistry*, 77:201–240, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300042.

Cox:2020:BSS

[CBSM20] Hazel Cox, Adam L. Baskerville, Ville J. J. Syrjanen, and Michael Melgaard. The bound state stability of the hydride ion in Hartree–Fock theory. *Advances in Quantum Chemistry*, 81:167–189, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762030006X.

Coutinho:1997:SES

[CC97] Kaline Coutinho and Sylvio Canuto. Solvent effects from a sequential Monte-Carlo — quantum mechanical approach. *Advances in Quantum Chemistry*, 28:89–105, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602099`.

Coletti:2013:DKC

[CCA13] C. Coletti, D. Calderini, and V. Aquilanti. d-dimensional Kepler–Coulomb Sturmians and hyperspherical harmonics as complete orthonormal atomic and molecular orbitals. *Advances in Quantum Chemistry*, 67:73–127, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780124115446000054`.

Cardenuto:2017:QCT

[CCC17] Marcelo Hidalgo Cardenuto, Kaline Coutinho, and Sylvio Canuto. Quantum chemistry with thermodynamic condition. a journey into the supercritical region and approaching the critical point. *Advances in Quantum Chemistry*, 74:253–265, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300417`.

Cardenuto:2015:EPS

[CCCC15] Marcelo Hidalgo Cardenuto, Kaline Coutinho, Benedito J. C. Cabral, and Sylvio Canuto. Electronic properties in supercritical fluids: the absorption spectrum of p-nitroaniline in supercritical water. *Advances in Quantum Chemistry*, 71:323–339, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000131`.

Chang:2003:ESC

[CCL03] Jyunju Chang, Youngmin Choi, and Jae Do Lee. Electronic structure of chromium aluminum oxide. *Advances in Quantum Chemistry*, 42:163–173, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603420467`.

Canuto:2005:DPF

[CCM05] Sylvio Canuto, Kaline Coutinho, and Prasanta K. Mukherjee. The dipole polarizability of F^- in aqueous solution. A sequential Monte Carlo/quantum mechanics study. *Advances in Quantum Chemistry*, 48:141–150, 2005. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480107.

Carbone:2019:APC

[CCM+19] Johanna P. Carbone, Lan Cheng, Rolf H. Myhre, Devin Matthews, Henrik Koch, and Sonia Coriani. An analysis of the performance of coupled cluster methods for K-edge core excitations and ionizations using standard basis sets. *Advances in Quantum Chemistry*, 79:241–261, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300280.

Cooper:2001:RAS

[CCSZ01] David L. Cooper, Nick J. Clarke, Phillip C. Stancil, and Bernard Zygelman. Recent applications of spin-coupled valence bond theory to charge transfer collisions. *Advances in Quantum Chemistry*, 40:37–48, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400086.

Canuto:2002:NDM

[CCT02] Sylvio Canuto, Kaline Coutinho, and Daniel Trzesniak. New developments in Monte Carlo/quantum mechanics methodology. the solvatochromism of β-carotene in different solvents. *Advances in Quantum Chemistry*, 41:161–183, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410520.

Carbo:1994:MQS

[CCVB94] Ramon Carbó, Blanca Calabuig, Leonel Vera, and Emili Besalú. Molecular quantum similarity: Theoretical framework, ordering principles, and visualization techniques. *Advances in Quantum Chemistry*, 25:253–313, 1994. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600210.

Carbo-Dorca:2005:MEQ

[CD05] Ramon Carbó-Dorca. Mathematical elements of quantum electronic density functions. *Advances in Quantum Chemistry*, 49: 121–207, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490036.

Carbo-Dorca:2000:EDF

[CDBG00] Ramon Carbó-Dorca, Emili Besalú, and Xavier Gironés. Extended density functions. *Advances in Quantum Chemistry*, 38: 1–63, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600380029.

Chakraborty:2015:SSD

[CDK15] Debajit Chakraborty, James Dufty, and Valentin V. Karasiev. System-size dependence in grand canonical and canonical ensembles. *Advances in Quantum Chemistry*, 71:11–27, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761500009X.

Carbo:1982:EUM

[CDP82] Ramon Carbó, Llorenç Domingo, and Josep-Jordi Peris. Elementary unitary MO transformations and SCF theory. *Advances in Quantum Chemistry*, 15:215–265, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601240.

Caldwell:1972:MCD

[CE72] Dennis J. Caldwell and Henry Eyring. Magnetic circular dichroism and diamagnetic molecules. *Advances in Quantum Chemistry*, 6:143–158, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605432.

Caldwell:1978:LOS

[CE78] Dennis Caldwell and Henry Eyring. Localized orbitals in spectroscopy. *Advances in Quantum Chemistry*, 11:93–114, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860235X.

Carbo:1980:OSS

[CG80] Ramon Carbó and Odd Gropen. Open shell SCF theory: An *ab Initio* study of some interstellar molecules. *Advances in Quantum Chemistry*, 12:159–187, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603160.

Cimpoesu:2003:IAA

[CH03] F. Cimpoesu and K. Hirao. The ab initio analytical approach of vibronic quantities: Application to inorganic stereochemistry. *Advances in Quantum Chemistry*, 44:369–387, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440240.

Chibotaru:2003:MAC

[Chi03] L. F. Chibotaru. Microscopic approach to cooperative Jahn–Teller effect in crystals with strong intra-site vibronic coupling. *Advances in Quantum Chemistry*, 44:649–667, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440434.

Christoffersen:1972:ICL

[Chr72] Ralph E. Christoffersen. *Ab Initio* calculations on large molecules. *Advances in Quantum Chemistry*, 6:333–393, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860550X.

Champion:2013:FBA

[CHR13] Christophe Champion, Jocelyn Hanssen, and Roberto D. Rivarola. The first Born approximation for ionization and charge transfer in energetic collisions of multiply charged ions with water. *Advances in Quantum Chemistry*, 65:269–313, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000108.

Cimpoesu:2003:SHE

[CHSC03] F. Cimpoesu, K. Hirao, N. Stanica, and V. Chihaia. The spin Hamiltonian effective approach to the vibronic effects-selected cases. *Advances in Quantum Chemistry*, 44:273–288, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440173.

Cioslowski:1990:DFR

[Cio90] Jerzy Cioslowski. Density functional reformulation of molecular orbital theories. *Advances in Quantum Chemistry*, 21:303–316, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606024.

Charkin:2009:DSM

[CKC09] O. P. Charkin, N. M. Klimenko, and D. O. Charkin. DFT study of molecules confined inside fullerene and fullerene-like cages. *Advances in Quantum Chemistry*, 58:69–114, 2009.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007072.

Coronado:2003:PJT

[CKRT03] E. Coronado, S. Klokishner, O. Reu, and B. Tsukerblat. Pseudo-Jahn–Teller origin of the metastable states in sodium nitroprusside. *Advances in Quantum Chemistry*, 44:429–444, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440288.

Chang:2000:EST

[CL00] Hyunju Chang and Jae Do Lee. Electronic structure of Ti_4O_7 using DV-Xα cluster calculation method. *Advances in Quantum Chemistry*, 37:291–300, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370204.

Capozziello:2005:FPQ

[CL05] Salvatore Capozziello and Alessandra Lattanzi. From Fischer projections to quantum mechanics of tetrahedral molecules: New perspectives in chirality. *Advances in Quantum Chemistry*, 49:227–247, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760549005X.

Cauet:2007:RCN

[CL07] Emilie Cauët and Jacques Liévin. Radical cations of the nucleic bases and radiation damage to DNA: Ab initio study. *Advances in Quantum Chemistry*, 52:121–147, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520064.

Cronstrand:2005:MPA

[CLÅ05] Peter Cronstrand, Yi Luo, and Hans Ågren. Multi-photon absorption of molecules. *Advances in Quantum Chemistry*, 50:1–21, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500017.

Cruz:2015:HHH

[CLK15] Salvador A. Cruz and Eugenio Ley-Koo. The hydrogen H_2^+ and HeH^{2+} molecular ions confined in dihedral angles. *Advances in Quantum Chemistry*, 71:69–113, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000088.

Chathanathil:2024:CTC

[CM24] Jabir Chathanathil and Svetlana A. Malinovskaya. Chapter three — chirped pulse control of Raman coherence in atoms and molecules. *Advances in Quantum Chemistry*, 89:225–289, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000539.

Carbo:1989:JRG

[CMDN89] Ramon Carbó, Joan Miró, Llorenç Domingo, and Juan J. Novoa. Jacobi rotations: a general procedure for electronic energy optimization. *Advances in Quantum Chemistry*, 20:375–441, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606309.

Champagne:1999:TCP

[CMFA99] Benoît Champagne, David H. Mosley, Joseph G. Fripiat, and Jean-Marie AndrÉ. Towards the calculations of polarizabilities of stereoregular polymers. *Advances in Quantum Chemistry*, 35:95–110, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604578.

Caturla:2004:MDS

[CMJR+04] M. J. Caturla, A. Gras Martí, J. J. Jiménez-Rodríguez, J.-C. Jiménez Saez, and M.-C. Pérez-Martín. Molecular dynamics simulations of energy deposition in solids. *Advances in Quantum Chemistry*, 45 (part 1):79–98, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450047.

Cruz-Martinez:2016:GSS

[CMVPFC16] Heriberto Cruz-Martínez, José Manuel Vásquez-Pérez, Omar Solorza Feria, and Patrizia Calaminici. On the ground state structures and energy properties of $\mathrm{Co}_n\ \mathrm{Pd}_n$ ($n = 1$–10) clusters. *Advances in Quantum Chemistry*, 72:177–199, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000246.

Corzo:2017:EPT

[CO17] Héctor H. Corzo and J. Vince Ortiz. Electron propagator theory: Foundations and predictions. *Advances in Quantum Chemistry*, 74:267–298, 2017. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761630034X.

Cohen:2004:ARS

[Coh04] Scott M. Cohen. Aspects of relativistic sum rules. *Advances in Quantum Chemistry*, 46 (part 2):241–265, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460092.

Coleman:1968:SGM

[Col68] A. J. Coleman. The symmetric group made easy. *Advances in Quantum Chemistry*, 4:83–108, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603901.

Cooper:2018:CEP

[Coo18] W. Grant Cooper. Consequences of EPR–proton qubits populating DNA. *Advances in Quantum Chemistry*, 77:19–120, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300746.

Contreras:2005:TNS

[CPBS05] Rubén H. Contreras, Juan E. Peralta, Verónica Barone, and Gustavo E. Scuseria. Theoretical NMR ^{n}J(^{13}C, ^{13}C) scalar couplings as probes to study diamagnetic ring currents in fullerenes. *Advances in Quantum Chemistry*, 48:127–139, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480090.

Craig:1999:JGC

[Cra99] David Craig. A journey with good companions. fifty years of quantum chemistry. *Advances in Quantum Chemistry*, 34:1–50, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605304.

Cruz:2009:Pa

[Cru09a] Salvador A. Cruz. Preface. *Advances in Quantum Chemistry*, 57: ix, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006030.

Cruz:2009:Pb

[Cru09b] Salvador A. Cruz. Preface. *Advances in Quantum Chemistry*, 58: vii, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007035.

Cruz:2009:TFD

[Cru09c] Salvador A. Cruz. Thomas–Fermi–Dirac-Weizsäcker density functional formalism applied to the study of many-electron atom confinement by open and closed boundaries. *Advances in Quantum Chemistry*, 57:255–283, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006121.

Coppens:1977:AXR

[CS77] Philip Coppens and Edwin D. Stevens. Accurate X-ray diffraction and quantum chemistry: The study of charge density distributions. *Advances in Quantum Chemistry*, 10:1–35, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605778.

Cruz:2004:ACB

[CS04] Salvador A. Cruz and Jacques Soullard. Advances in the core-and-bond formalism for proton stopping in molecular targets. *Advances in Quantum Chemistry*, 46 (part 2):195–239, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460080.

Cserny:1997:SVB

[Cse97] I. Cserny. Studies of the valence band of tetrahedral oxyanions. *Advances in Quantum Chemistry*, 29:207–232, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602713.

Cory:1999:TSF

[CSZ99] Marshall G. Cory, Krassimir K. Stavrev, and Michael C. Zerner. A theoretical study of the (Fe_2 $(\mu - S_2)(P(o\text{-}C_6H_4S)_3)_2)^{2-}$ electronic spectrum. *Advances in Quantum Chemistry*, 35:357–369, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604682.

Craig:1982:RMI

[CT82] D. P. Craig and T. Thirunamachandran. Radiation molecule interactions in chemical physics. *Advances in Quantum Chemistry*, 16:97–160, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603524.

Cabrera-Trujillo:2022:CSM

[CTC22] Remigio Cabrera-Trujillo and Salvador A. Cruz. Mean total and orbital excitation energies of atomic ions in two approaches of the Thomas–Fermi theory. *Advances in Quantum Chemistry*, 85:81–108, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762200003X.

Cabrera-Trujillo:2005:OIK

[CTCS05] R. Cabrera-Trujillo, S. A. Cruz, and J. Soullard. From the orbital implementation of the kinetic theory to the polarization propagator method in the study of energy deposition problems. *Advances in Quantum Chemistry*, 48:335–367, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480181.

Cooper:1998:MVR

[CTG98] David L. Cooper, Thorstein Thorsteinsson, and Joseph Gerratt. Modern VB representations of CASSCF wave functions and the fully variational optimization of modern VB wave functions using the CASVB strategy. *Advances in Quantum Chemistry*, 32:51–67, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604062.

Cabrera-Trujillo:2018:DSR

[CTO18] Remigio Cabrera-Trujillo and Jens Oddershede. Dipole sum rules of an endohedral confined hydrogen atom: Effects of the cavity discontinuity. *Advances in Quantum Chemistry*, 77:295–315, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300017.

Cabrera-Trujillo:2022:CFE

[CTO22] Remigio Cabrera-Trujillo and Jens Oddershede. Electronic stopping from orbital mean excitation energies including both projectile and target electronic structure. *Advances in Quantum Chemistry*, 85:327–342, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000144.

Cabrera-Trujillo:2004:TCE

[CTS04] Remigio Cabrera-Trujillo and John R. Sabin. The theory and computation of energy deposition properties. *Advances in Quantum Chemistry*, 45 (part 1):1–5, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450011.

Cabrera-Trujillo:2015:P

[CTS15] Remigio Cabrera-Trujillo and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 71:xi–xii, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000477.

Cabrera-Trujillo:2016:P

[CTS16] Remigio Cabrera-Trujillo and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 72:ix, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300089.

Cabrera-Trujillo:2004:DPS

[CTSDÖ04a] R. Cabrera-Trujillo, J. R. Sabin, E. Deumens, and Y. Öhrn. Dynamical processes in stopping cross sections. *Advances in Quantum Chemistry*, 45 (part 1):99–124, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450059.

Cabrera-Trujillo:2004:CCS

[CTSDÖ04b] R. Cabrera-Trujillo, John R. Sabin, E. Deumens, and Y. Öhrn. Calculation of cross sections in electron-nuclear dynamics. *Advances in Quantum Chemistry*, 47:253–274, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470154.

Cabrera-Trujillo:2005:OEE

[CTSDÖ05] Remigio Cabrera-Trujillo, John R. Sabin, Erik Deumens, and Yngve Öhrn. Orientational effects in energy deposition by protons in water. *Advances in Quantum Chemistry*, 48:47–57,

2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480053.

Cabrera-Trujillo:2004:MSP

[CTSO04] Remigio Cabrera-Trujillo, John R. Sabin, and Jens Oddershede. Molecular stopping powers from the target oscillator strength distribution. *Advances in Quantum Chemistry*, 46 (part 2):121–151, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460055.

Cabrera-Trujillo:1999:BSR

[CTSOS99] R. Cabrera-Trujillo, John R. Sabin, J. Oddershede, and Stephan P. A. Sauer. The Bethe sum rule and basis set selection in the calculation of generalized oscillator strengths. *Advances in Quantum Chemistry*, 35:175–192, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604608.

Cabrera-Trujillo:2019:BCS

[CTSSO19] Remigio Cabrera-Trujillo, Stephan P. A. Sauer, John R. Sabin, and Jens Oddershede. Bound and continuum state contributions to dipole oscillator strength sum rules: Total and orbital mean excitation energies for cations of C, F, Si, and Cl. *Advances in Quantum Chemistry*, 80:127–146, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300309.

Chang:2000:ESC

[CY00] Myung Chul Chang and Soo-Chang Yu. The electronic states in Ca-doped $BaTiO_3$ ceramics. *Advances in Quantum Chemistry*, 37:179–191, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370137.

Djeroud:2014:FPC

[DA14] S. Djeroud and F. Adjailia. First-principles calculations of electronic and optical properties of $LiAlH_4$ in its monoclinic and tetragonal phases. *Advances in Quantum Chemistry*, 68:293–313, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000162.

DeBaerdemacker:2023:SCH

[DAB+23] Stijn De Baerdemacker, Amir Ayati, Hugh G. A. Burton, Xeno De Vriendt, Patrick Bultinck, and Guillaume Acke. Spin-constrained Hartree–Fock and the generator coordinate method for the 2-site Hubbard model. *Advances in Quantum Chemistry*, 88:161–182, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000369.

Dahl:2001:DMP

[Dah01] Jens Peder Dahl. Density matrices and phase-space functions. *Advances in Quantum Chemistry*, 39:1–18, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390010.

Daudel:1964:BMM

[Dau64] R. Daudel. On the basis of the main methods of calculating molecular electronic wave functions. *Advances in Quantum Chemistry*, 1:115–143, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603767.

Daudel:1967:QTC

[Dau67] R. Daudel. Quantum theory of chemical reactivity. *Advances in Quantum Chemistry*, 3:161–208, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600891.

Daudel:1970:SAQ

[Dau70] R. Daudel. Some aspects of the quantum theory of photochemical reactivity of organic molecules. *Advances in Quantum Chemistry*, 5:1–26, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603354.

Davidson:1972:NO

[Dav72] Ernest R. Davidson. Natural orbitals. *Advances in Quantum Chemistry*, 6:235–266, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860547X.

Dahl:1968:MOT

[DB68] J. P. Dahl and C. J. Ballhausen. Molecular orbital theories of inorganic complexes. *Advances in Quantum Chemistry*, 4:170–226, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603949.

Dunne:2001:WBC

[DB01] L. J. Dunne and E. J. Brändas. *D*-wave bipolaronic condensate with short range repulsive electronic correlations in an extended Hubbard model of high-T_c cuprate superconductors. *Advances in Quantum Chemistry*, 40:225–247, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400189.

Dunne:2013:RDL

[DB13] Lawrence J. Dunne and Erkki J. Brändas. Review of off-diagonal long-range order and high-temperature superconductivity from repulsive electronic correlations. *Advances in Quantum Chemistry*, 66:1–30, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124080997000015.

DiDonato:1999:PAE

[DBC+99] Mariangela Di Donato, Raffaele Borrelli, Amedeo Capobianco, Guglielmo Monaco, Roberto Improta, Meziane Brahimi, and Andrea Peluso. Proton assisted electron transfer. *Advances in Quantum Chemistry*, 36:301–322, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860489X.

Dunne:2017:HTS

[DBC17] Lawrence J. Dunne, Erkki J. Brändas, and Hazel Cox. High-temperature superconductivity in strongly correlated electronic systems. *Advances in Quantum Chemistry*, 74:183–208, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300387.

Deleuze:1999:NCT

[DC99] M. S. Deleuze and L. S. Cederbaum. The new challenges of the theory of ionization for polymers and solids. *Advances in Quantum Chemistry*, 35:77–94, 1999. CODEN AQCHA9. ISSN

0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604566`.

Deleuze:1995:SCS

[DDPC95] Michaël Deleuze, Joseph Delhalle, Barry T. Pickup, and Jean-Louis Calais. Size-consistency and size-intensivity aspects of many-body Green's-function calculations on polymers: Characterization of the convergence of direct lattice self-energy summations. *Advances in Quantum Chemistry*, 26:35–98, 1995. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601112`.

DelBene:2005:TBS

[DE05] Janet E. Del Bene and José Elguero. Two-bond spin-spin coupling constants $({}^{2h}\mathrm{J}_{X\,\text{—}\,Y})$ across X — H — Y hydrogen bonds: Some fundamental questions. *Advances in Quantum Chemistry*, 50:23–35, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605500029`.

Dz:2009:ESN

[DeB09] Dz and evad Belkić. Exact signal-noise separation by Froissart doublets in fast Padé transform for magnetic resonance spectroscopy. *Advances in Quantum Chemistry*, 56:95–179, 2009. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608004036`.

DelRe:1974:CPP

[Del74] Giuseppe Del Re. Current problems and perspectives in the MO–LCAO theory of molecules. *Advances in Quantum Chemistry*, 8:95–136, 1974. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860060X`.

Deumens:1999:TQM

[Deu99] Erik Deumens. Teaching quantum mechanics. *Advances in Quantum Chemistry*, 35:21–31, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604530`.

DelPunta:2018:LRC

[DGA18] Jessica A. Del Punta, Gustavo Gasaneo, and Lorenzo U. Ancarani. On the Laguerre representation of Coulomb functions and the relation to orthogonal polynomials. *Advances in Quantum Chemistry*, 76:79–101, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300643.

Dominguez-Gutierrez:2015:MAL

[DGKCT15] Fco. Javier Domínguez-Gutiérrez, Predrag S. Krstić, and Remigio Cabrera-Trujillo. Multiresolution approach for laser-modified collisions of atoms and ions. *Advances in Quantum Chemistry*, 71:353–371, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000155.

Diercksen:1997:IR

[Die97] Geerd H. F. Diercksen. Introductory remarks. *Advances in Quantum Chemistry*, 28:xix, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602026.

Delchev:1998:CCA

[DKMP98] Ya. I. Delchev, A. I. Kuleff, Jean Maruani, and R. L. Pavlov. A consistent calculation of atomic energy shell corrections: Strutinsky's method in the Hartree–Fock–Roothaan scheme. *Advances in Quantum Chemistry*, 31:53–73, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601835.

Dubrovskaya:2019:QCS

[DKV$^+$19] Yuliya V. Dubrovskaya, Olga Yu Khetselius, Larisa A. Vitavetskaya, Valentin B. Ternovsky, and Inga N. Serga. Quantum chemistry and spectroscopy of pionic atomic systems with accounting for relativistic, radiative, and strong interaction effects. *Advances in Quantum Chemistry*, 78:193–222, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300273.

deLima:2010:MDP

[dLHD10] Guilherme Ferreira de Lima, Thomas Heine, and Hélio Anderson Duarte. Molecular dynamics of polypeptides and their inclusion compounds with β-cyclodextrin in aqueous solution using DC–SCC–DFTB/UFF approach. *Advances in Quantum Chemistry*, 59:145–180, 2010. CODEN AQCHA9. ISSN

0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327610590051`.

Dolin:2003:LTP

[DLMS03] S. P. Dolin, A. A. Levin, T. Yu Mikhailova, and M. V. Solin. Low-temperature phase transition and structure of ordered phase in $K_3H(SO_4)_2$ (TKHS)-family materials. *Advances in Quantum Chemistry*, 44:579–586, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440380`.

Djilani:2014:MMS

[DNM$^+$14] I. Djilani, L. Nouar, F. Madi, S. Haiahem, A. Bouhadiba, and D. Khatmi. Molecular modeling study of neutral and cationic species of ortho-anisidine by β-cyclodextrin. *Advances in Quantum Chemistry*, 68:279–291, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128005361000150`.

Degoli:2009:EQC

[DO09] Elena Degoli and Stefano Ossicini. Engineering quantum confined silicon nanostructures: Ab-initio study of the structural, electronic and optical properties. *Advances in Quantum Chemistry*, 58:203–279, 2009. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327609007102`.

Dolmatov:2009:PAE

[Dol09] V. K. Dolmatov. Photoionization of atoms encaged in spherical fullerenes. *Advances in Quantum Chemistry*, 58:13–68, 2009. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327609007060`.

Dunlap:1990:GTO

[DR90] B. I. Dunlap and N. Rösch. The Gaussian-type orbitals density functional approach to finite systems. *Advances in Quantum Chemistry*, 21:317–339, 1990. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608606036`.

Dral:2020:QCA

[Dra20] Pavlo O. Dral. Quantum chemistry assisted by machine learning. *Advances in Quantum Chemistry*, 81:291–324, 2020.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300125.

Drukarev:1978:ZRP

[Dru78] G. Drukarev. The zero-range potential model and its application in atomic and molecular physics. *Advances in Quantum Chemistry*, 11:251–274, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602397.

Dedieu:1982:ICM

[DRV82] A. Dedieu, M.-M. Rohmer, and A. Veillard. Ab initio calculations of metalloporphyrins. *Advances in Quantum Chemistry*, 16:43–95, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603512.

Dinesha:1981:GTT

[DSR81] K. V. Dinesha, C. R. Sarma, and S. Rettrup. Group theoretical techniques and the many-electron problem. *Advances in Quantum Chemistry*, 14:125–168, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603275.

Dunbar:2003:MPL

[DST$^+$03] Kim R. Dunbar, Eric J. Schelter, Boris S. Tsukerblat, Andrei V. Palii, Sergei M. Ostrovsky, Vadim Yu. Mirovitskii, and Sophia I. Klokishner. Magnetic properties of a low symmetry d^5 complex: An adiabatic pseudo-Jahn–Teller problem. *Advances in Quantum Chemistry*, 44:413–428, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440276.

Duan:2004:VAF

[DSW04] Guilin Duan, Vedene H. Smith, Jr., and Donald F. Weaver. Validation of the applicability of force fields to reproduce ab initio noncovalent interactions involving aromatic groups. *Advances in Quantum Chemistry*, 47:65–92, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470051.

Dufty:2004:HIH

[DTC04] James W. Dufty, Bernard Talin, and Annette Calisti. High Z ions in hot, dense matter. *Advances in Quantum Chemistry*, 46 (part 2):293–305, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460110.

Duch:1997:AIS

[Duc97] Włodzisław Duch. Artificial intelligence support for computational chemistry. *Advances in Quantum Chemistry*, 28:329–343, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602257.

Durbeej:2020:CES

[Dur20] Bo Durbeej. Competing excited-state deactivation processes in bacteriophytochromes. *Advances in Quantum Chemistry*, 81: 243–268, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300137.

Dunlap:1998:QCM

[DW98] Brett I. Dunlap and Robert W. Warren. Quantum chemical molecular dynamics. *Advances in Quantum Chemistry*, 33:167–187, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604359.

Drake:2008:SLH

[DY08] G. W. F. Drake and Z.-C. Yan. Studies of light halo nuclei from atomic isotope shifts. *Advances in Quantum Chemistry*, 53:37–56, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530042.

El-Basil:1992:EMO

[EBR92] Sherif El-Basil and Milan Randić. Equivalence of mathematical objects of interest in chemistry and physics. *Advances in Quantum Chemistry*, 24:239–290, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601033.

Engels:1996:RDC

[EEL96] Bernd Engels, Leif A. Eriksson, and Sten Lunell. Recent developments in configuration interaction and density functional theory calculations of radical hyperfine structure. *Advances in Quantum Chemistry*, 27:297–369, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602543.

Ellis:1999:DVM

[EG99] D. E. Ellis and Diana Guenzburger. The discrete variational method in density-functional theory and its applications to large molecules and solid-state systems. *Advances in Quantum Chemistry*, 34:51–141, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605316.

Ellis:1991:TMC

[EGCL91] D. E. Ellis, J. Guo, H.-P. Cheng, and J. J. Low. Transition metal clusters: Electronic structure and interaction with hydrogen and oxides. *Advances in Quantum Chemistry*, 22:125–165, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603639.

Ekstrom:1998:SMN

[Eks98] Curt Ekström. Spins and moments of nuclei far from stability determined by on-line atomic-beam techniques. *Advances in Quantum Chemistry*, 30:361–378, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605171.

Erturk:2017:SEC

[EM17] Murat Erturk and Leszek Meissner. Size-extensivity corrections in single- and multireference configuration interaction calculations. *Advances in Quantum Chemistry*, 73:145–160, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000362.

Esashi:2003:ESS

[EOH03] Noboru Esashi, Yasuhiko Ohama, and Yoshinori Hayafuji. Electronic structures of silicon clusters with vacancies. *Advances in Quantum Chemistry*, 42:439–451, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420674.

Ermler:1988:SOC

[ERC88] Walter C. Ermler, Richard B. Ross, and Phillip A. Christiansen. Spin-orbit coupling and other relativistic effects in atoms and molecules. *Advances in Quantum Chemistry*, 19:139–182, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606152.

Ermis:2021:CSA

[EÜSB21] Betül Ermiş, Aslı Ünal, Emine Soydaş, and Uğur Bozkaya. Anharmonic force field from coupled-cluster methods and accurate computation of infrared spectra. *Advances in Quantum Chemistry*, 83:139–153, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000058.

Ellis:2003:TSF

[EW03] D. E. Ellis and O. Warschkow. Toward structure-function relations — a hybrid quantum/classical approach. *Advances in Quantum Chemistry*, 42:35–66, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420406.

Fricke:1998:RDC

[FAS+98] B. Fricke, J. Anton, K. Schulze, W.-D. Sepp, and P. Kürpick. Relativistic and dynamic contributions in ion-atom and ion-solid collisions. *Advances in Quantum Chemistry*, 30:273–282, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605110.

Farcau:2020:IMD

[FB20] Alex-Adrian Farcaş and Attila Bende. The influence of monovalent and divalent metal cations on the stability of the DNA–protein interaction in the nucleosome core particle. *Advances in Quantum Chemistry*, 81:269–290, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300113.

Flores:2019:IEE

[FCAG19] Fernando Flores, Guillermo Chiappe, Enrique V. Anda, and Edith C. Goldberg. Inelastic electron excitation of transition metal atoms and Kondo resonances. *Advances in Quantum Chemistry*, 80:1–22, 2019. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300292.

Fileti:2004:TFI

[FCC04] Eudes E. Fileti, Kaline Coutinho, and Sylvio Canuto. Is there a favorite isomer for hydrogen-bonded methanol in water? *Advances in Quantum Chemistry*, 47:51–63, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760447004X.

Fripiat:2015:FSR

[FCH15] Joseph G. Fripiat, Benoît Champagne, and Frank E. Harris. The Fourier space restricted Hartree–Fock method for the electronic structure calculation of one-dimensionally periodic systems. *Advances in Quantum Chemistry*, 71:153–194, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000106.

Fukushima:1997:ESI

[FE97] Kimichika Fukushima and Hiroshi Endo. Electronic states of impurities and their effect on material properties. *Advances in Quantum Chemistry*, 29:269–283, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602749.

Fujimoto:1972:MOT

[FF72] Hiroshi Fujimoto and Kenichi Fukui. Molecular orbital theory of chemical reactions. *Advances in Quantum Chemistry*, 6:177–201, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605456.

Fischer-Hjalmars:1965:ZDO

[FH65] Inga Fischer-Hjalmars. Zero differential overlap in π-electron theories. *Advances in Quantum Chemistry*, 2:25–46, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600714.

Fischer-Hjalmars:1982:MBA

[FHHE82] Inga Fischer-Hjalmars and Anita Henriksson-Enflo. Metals in biology: An attempt at classification. *Advances in Quantum Chemistry*, 16:1–41, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603500.

Friedrich:1988:TSR

[FHHZ88] Břetislav Friedrich, Zdeněk Havlas, Zdeněk Herman, and Rudolf Zahradník. Theoretical studies of reaction mechanisms in chemistry. *Advances in Quantum Chemistry*, 19:247–288, 1988. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608606176`.

Fishman:2003:DCJ

[FIK+03] A. Ya Fishman, M. A. Ivanov, T. E. Kurennykh, A. S. Lahtin, L. L. Surat, and V. B. Vykhodets. Diffusion in concentrated Jahn–Teller systems. *Advances in Quantum Chemistry*, 44:497–508, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760344032X`.

Froelich:2004:PEA

[FJS+04] P. Froelich, S. Jonsell, A. Saenz, S. Eriksson, B. Zygelman, and A. Dalgarno. Positron-electron annihilation in hydrogen-antihydrogen collisions. *Advances in Quantum Chemistry*, 47:465–480, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604470245`.

Ferretti:1999:PMC

[FLV99] Alessandro Ferretti, Alessandro Lami, and Giovanni Villani. On the photophysics of molecules with charge-transfer excitations between aromatic rings. *Advances in Quantum Chemistry*, 36:283–300, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604888`.

Fritzsche:2008:CAA

[FMA08] Stephan Fritzsche, Brajesh K. Mani, and Dilip Angom. A computer-algebraic approach to the derivation of Feynman–Goldstone perturbation expansions for open-shell atoms and molecules. *Advances in Quantum Chemistry*, 53:177–215, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327607530108`.

Forner:1994:SDT

[För94] Wolfgang Förner. Soliton dynamics in trans-polyacetylene. *Advances in Quantum Chemistry*, 25:207–252, 1994. CO-

DEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600209.

Fowler:2003:SAD

[Fow03] P. W. Fowler. Symmetry aspects of distortivity in π systems. *Advances in Quantum Chemistry*, 44:219–237, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440148.

Fan:2006:UEW

[FP06] Peng-Dong Fan and Piotr Piecuch. The usefulness of exponential wave function expansions employing one- and two-body cluster operators in electronic structure theory: The extended and generalized coupled-cluster methods. *Advances in Quantum Chemistry*, 51:1–57, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510019.

Fowler:1997:SLR

[FPL97] P. W. Fowler, S. A. Peebles, and A. C. Legon. A Sternheimer-like response property of the bromine molecule: Electric field dependence of the Br field gradient. *Advances in Quantum Chemistry*, 28:247–256, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602191.

Francis:2013:MSS

[Fra13] Ziad Francis. Molecular scale simulation of ionizing particles tracks for radiobiology and hadrontherapy studies. *Advances in Quantum Chemistry*, 65:79–110, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000042.

Feinberg:1970:OBA

[FRM70] M. J. Feinberg, Klaus Ruedenberg, and Ernest L. Mehler. The origin of binding and antibinding in the hydrogen molecule-ion. *Advances in Quantum Chemistry*, 5:27–98, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603366.

Froelich:2002:QCA

[Fro02] Piotr Froelich. Quantum chemistry of antimatter. *Advances in Quantum Chemistry*, 41:185–202, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410532.

Fricke:1997:UDX

[FSB+97] B. Fricke, W.-D. Sepp, T. Bastug, S. Varga, K. Schulze, J. Anton, and V. Pershina. Use of the DV–Xα-method in the field of superheavy atoms. *Advances in Quantum Chemistry*, 29:109–121, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602658.

Falcioni:2023:RML

[FSP23] Fabio Falcioni, Benjamin C. B. Symons, and Paul L. A. Popelier. REG-MULTI: Lifting the veil on electrostatic interactions. *Advances in Quantum Chemistry*, 88:305–328, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000230.

Flores:2022:CSI

[FTG22] F. Flores, M. S. Tacca, and E. C. Goldberg. An ionic Hamiltonian for transition metal atoms: Kondo resonances and tunneling currents. *Advances in Quantum Chemistry*, 85:353–375, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000132.

Fujimoto:2000:PCW

[FU00] Yasunari Fujimoto and Masayuki Uda. Prediction of change in the work functions due to stacking faults in Mg, Ti, Co, Cu, and Zn. *Advances in Quantum Chemistry*, 37:229–235, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370162.

Fukushima:2000:ESC

[Fuk00] Kimichika Fukushima. Electronic structure calculations to determine the effects of impurities on ceramic properties. *Advances in Quantum Chemistry*, 37:255–270, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370186.

Fukushima:2003:DXC

[Fuk03] Kimichika Fukushima. DV–Xα cluster calculations of spin-states in hydrogen and Cu oxide clusters. *Advances in Quantum Chemistry*, 42:223–238, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420522.

Fukushima:2008:FPA

[Fuk08a] Kimichika Fukushima. First-principles analysis of the antiferromagnetic state. *Advances in Quantum Chemistry*, 54:47–60, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000056.

Fukushima:2008:FPI

[Fuk08b] Kimichika Fukushima. First-principles investigation of dimethyl ether steam reforming. *Advances in Quantum Chemistry*, 54:341–359, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000251.

Fukushima:2015:ESC

[Fuk15] Kimichika Fukushima. Electronic structure calculations for antiferromagnetism of cuprates using SIWB method for anions in DV and a density functional theory confirming from finite element method. *Advances in Quantum Chemistry*, 70:1–29, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327614000021.

Fliszar:1999:CVE

[FVB99] Sándor Fliszár, Edouard C. Vauthier, and Vincenzo Barone. Core and valence electrons in atom-by-atom descriptions of molecules. *Advances in Quantum Chemistry*, 36:27–44, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604773.

Galano:2008:ARO

[GAI08] Annia Galano and J. Raúl Alvarez-Idaboy. Atmospheric reactions of oxygenated volatile organic compounds + OH radicals: Role of hydrogen-bonded intermediates and transition states. *Advances in Quantum Chemistry*, 55:245–274, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002122.

Gallup:1973:SGC

[Gal73] G. A. Gallup. The symmetric groups and calculation of energies of n-electron systems in pure spin states. *Advances in Quantum Chemistry*, 7:113–141, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605602.

Gasaneo:2013:TBC

[GAM+13] G. Gasaneo, L. U. Ancarani, D. M. Mitnik, J. M. Randazzo, A. L. Frapiccini, and F. D. Colavecchia. Three-body Coulomb problems with generalized Sturmian functions. *Advances in Quantum Chemistry*, 67:153–216, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000078.

Ghomari:2014:DFT

[GBHM14] R. Ghomari, A. Bouferguene, P. E. Hoggan, and S. M. Mekelleche. A density functional theory study of the adsorption of 2-cyclohexenone on Rh(111). *Advances in Quantum Chemistry*, 68:175–190, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000095.

Groenhof:2010:CSP

[GBPSR10] Gerrit Groenhof, Martial Boggio-Pasqua, Lars V. Schäfer, and Michael A. Robb. Computer simulations of photobiological processes: The effect of the protein environment. *Advances in Quantum Chemistry*, 59:181–212, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590063.

Gauss:1992:AEG

[GC92] Jürgen Gauss and Dieter Cremer. Analytical energy gradients in Møller–Plesset perturbation and quadratic configuration interaction methods: Theory and application. *Advances in Quantum Chemistry*, 23:205–299, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600313.

Girard:2001:EHS

[GC01] Y. Girard and P. Chaquin. Effects of halogen substituents on the conformations of vinyl alcohol and vinyl thiol: a theoretical study. *Advances in Quantum Chemistry*, 40:161–177,

2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400141.

Garcia-Calderon:2010:TRS

[GC10] Gastón García-Calderón. Theory of resonant states: An exact analytical approach for open quantum systems. *Advances in Quantum Chemistry*, 60:407–455, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761060007X.

Granados-Castro:2017:SAP

[GCAGM17] Carlos Mario Granados-Castro, Lorenzo Ugo Ancarani, Gustavo Gasaneo, and Dario M. Mitnik. A Sturmian approach to photoionization of molecules. *Advances in Quantum Chemistry*, 73:3–57, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000295.

Geerlings:1998:DFT

[GDL98] P. Geerlings, F. De Proft, and W. Langenaeker. Density functional theory: a source of chemical concepts and a cost-effective methodology for their calculation. *Advances in Quantum Chemistry*, 33:303–328, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604426.

Goings:2014:SCF

[GDL14] J. J. Goings, F. Ding, and X. Li. Self-consistent field using direct inversion in iterative subspace method and quasi-Newton vectors. *Advances in Quantum Chemistry*, 68:77–86, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000046.

Geertsen:1991:SAC

[GEO91] Jan Geertsen, Steffen Eriksen, and Jens Oddershede. Some aspects of the coupled cluster based polarization propagator method. *Advances in Quantum Chemistry*, 22:167–209, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603640.

Georgiev:2020:QTU

[GG20] Danko D. Georgiev and James F. Glazebrook. Quantum transport and utilization of free energy in protein α-helices. *Advances in Quantum Chemistry*, 82:253–300, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300022.

Gill:1994:MIG

[Gil94] Peter M. W. Gill. Molecular integrals over Gaussian basis functions. *Advances in Quantum Chemistry*, 25:141–205, 1994. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600192.

Gritsenko:2023:GEN

[GJP23] Oleg V. Gritsenko, Mohammad Reza Jangrouei, and Katarzyna Pernal. Generalized exciton with a noninteger particle and hole charge as an excitation order. *Advances in Quantum Chemistry*, 87:191–207, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000047.

Gross:1990:TDD

[GK90] E. K. U. Gross and W. Kohn. Time-dependent density functional theory. *Advances in Quantum Chemistry*, 21:255–291, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606000.

Goodman:1968:PST

[GL68] Lionel Goodman and Bernard J. Laurenzi. Probability of singlet-triplet transitions. *Advances in Quantum Chemistry*, 4:153–169, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603937.

Gordon:1990:LDF

[GL90] Roy G. Gordon and Richard LeSar. Local density functional theories of ionic and molecular solids. *Advances in Quantum Chemistry*, 21:341–363, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606048.

Glushkov:2019:MSA

[Glu19] Alexander V. Glushkov. Multiphoton spectroscopy of atoms and nuclei in a laser field: Relativistic energy approach and radiation atomic lines moments method. *Advances in Quantum Chemistry*, 78:253–285, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327618300285`.

Grinberg:1991:FPI

[GM91] Horacio Grinberg and Julio Marañon. The Feynman path integral formalism: Atomic and molecular electronic structure. *Advances in Quantum Chemistry*, 22:7–123, 1991. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603627`.

Gross:2005:TMC

[GM05] Allan Gross and Kurt V. Mikkelsen. A theoretical model to calculate fundamental physical parameters for molecule-particle interactions. *Advances in Quantum Chemistry*, 50:125–142, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605500078`.

Genoni:2017:XRC

[GM17] Alessandro Genoni and Benjamin Meyer. X-ray constrained wave functions: Fundamentals and effects of the molecular orbitals localization. *Advances in Quantum Chemistry*, 73:333–362, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000271`.

Gindensperger:2004:HQC

[GMB04] E. Gindensperger, C. Meier, and J. A. Beswick. Hybrid quantum/classical dynamics using Bohmian trajectories. *Advances in Quantum Chemistry*, 47:331–346, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604470191`.

Galvan:2010:UAS

[GMLSC$^+$10] Ignacio Fdez. Galván, Aurora Muñoz-Losa, Catalina Soriano-Correa, M. Luz Sánchez, M. Elena Martín, and Manuel A. Aguilar. Use of the average solvent potential approach in the study of solvent effects. *Advances in Quantum Chemistry*, 59:59–97, 2010. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327610590038`.

Gustavsson:1998:FDH

[GMP98] Martin G. H. Gustavsson and Ann-Marie Mårtensson-Pendrill. Four decades of hyperfine anomalies. *Advances in Quantum Chemistry*, 30:343–360, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860516X.

Gross:2008:MD

[GNM08] Allan Gross, Ole John Nielsen, and Kurt V. Mikkelsen. From molecules to droplets. *Advances in Quantum Chemistry*, 55:355–385, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002171.

Gonze:1998:IFC

[Gon98] Xavier Gonze. Interatomic force constants in periodic solids from density functional perturbation theory. *Advances in Quantum Chemistry*, 33:225–239, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604384.

Goscinski:2002:APR

[Gos02a] Osvaldo Goscinski. Appendix. preliminary research report 217 (1968). *Advances in Quantum Chemistry*, 41:57–85, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410477.

Goscinski:2002:CEP

[Gos02b] Osvaldo Goscinski. Conjugate eigenvalue problems and generalized Sturmians. *Advances in Quantum Chemistry*, 41:51–56, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410465.

Gadre:1991:BAM

[GP91] Shridhar R. Gadre and Rajeev K. Pathak. Bounds to atomic and molecular energy functionals. *Advances in Quantum Chemistry*, 22:211–300, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603652.

GarciadeAbajo:2004:RCE

[GP04] F. J. García de Abajo and V. H. Ponce. Resonant-coherent excitation of channeled ions. *Advances in Quantum Chemistry*, 46 (part 2):65–89, 2004. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460031.

Galynska:2014:MDW

[GP14] Marta Galyńska and Petter Persson. Material dependence of water interactions with metal oxide nanoparticles: TiO_2, SiO_2, GeO_2, and SnO_2. *Advances in Quantum Chemistry*, 69:303–332, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459000088.

Guo:2021:CFI

[GPEB21] Yangyang Guo, Lukáš F. Pašteka, Ephraim Eliav, and Anastasia Borschevsky. Ionization potentials and electron affinity of oganesson with relativistic coupled cluster method. *Advances in Quantum Chemistry*, 83:107–123, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000095.

Green:1973:AIP

[Gre73] A. E. S. Green. An analytic independent particle model for atoms. I. Initial studies. *Advances in Quantum Chemistry*, 7:221–262, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605638.

Greiner:1998:CV

[Gre98] Walter Greiner. Correlations in the vacuum. *Advances in Quantum Chemistry*, 30:195–208, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605080.

Greiner:2008:SVE

[Gre08] Walter Greiner. Structure of vacuum and elementary matter: From superheavies via hypermatter to antimatter-the vacuum decay in supercritical fields. *Advances in Quantum Chemistry*, 53:99–150, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760753008X.

Goodson:2004:SSM

[GS04a] David Z. Goodson and Alexey V. Sergeev. Singularity structure of Møller-plesset perturbation theory. *Advances in Quantum Chemistry*, 47:193–208, 2004. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470117.

Grande:2004:IEL

[GS04b] P. L. Grande and G. Schiwietz. Ionization and energy loss beyond perturbation theory. *Advances in Quantum Chemistry*, 45 (part 1):7–46, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450023.

Gonis:1998:PPC

[GSTvE98] A. Gonis, T. C. Schulthess, P. E. A. Turchi, and J. van Ek. The n-particle picture and the calculation of the electronic structure of atoms, molecules, and solids. *Advances in Quantum Chemistry*, 33:85–104, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604311.

Goussev:2010:QTR

[GSWW10] Arseni Goussev, Roman Schubert, Holger Waalkens, and Stephen Wiggins. Quantum theory of reactive scattering in phase space. *Advances in Quantum Chemistry*, 60:269–332, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600056.

Gemeri:2023:ESO

[GTB23] D. Gemeri, J. C. Tremblay, and H. Bahmann. Electronic structure in organic dye-sensitized solar cells: Insight from density functional theory and electron dynamics. *Advances in Quantum Chemistry*, 88:329–350, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S006532762300031X.

Gutsev:1997:NPW

[Gut97] Gennady L. Gutsev. Numerical pseudopotentials within DV–Xα framework. *Advances in Quantum Chemistry*, 29:137–157, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602671.

Gutman:2006:CGT

[Gut06] Ivan Gutman. Chemical graph theory-the mathematical connection. *Advances in Quantum Chemistry*, 51:125–138, 2006.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510032.

Garza:2009:CSB

[GV09] Jorge Garza and Rubicelia Vargas. Comparative study between the Hartree–Fock and Kohn–Sham models for the lowest singlet and triplet states of the confined helium atom. *Advances in Quantum Chemistry*, 57:241–254, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760900611X.

Gallup:1982:PVB

[GVCN82] G. A. Gallup, R. L. Vance, J. R. Collins, and J. M. Norbeck. Practical valence-bond calculations. *Advances in Quantum Chemistry*, 16:229–272, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603548.

Guerra:2009:MPE

[GVFG09] Doris Guerra, Rubicelia Vargas, Patricio Fuentealba, and Jorge Garza. Modeling pressure effects on the electronic properties of Ca, Sr, and Ba by the confined atoms model. *Advances in Quantum Chemistry*, 58:1–12, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007059.

Gianinetti:1998:ESM

[GVFR98] E. Gianinetti, I. Vandoni, A. Famulari, and M. Raimondi. Extension of the SCF–MI method to the case of K fragments, one of which is an open-shell system. *Advances in Quantum Chemistry*, 31:251–266, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601914.

Glushkov:2001:DGB

[GW01] V. N. Glushkov and S. Wilson. Distributed Gaussian basis sets: Variationally optimized s-type sets. *Advances in Quantum Chemistry*, 39:123–143, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390083.

Gebremedhin:2017:ASP

[GW17] Daniel H. Gebremedhin and Charles A. Weatherford. Application of the space-pseudo-time method to density functional theory. *Advances in Quantum Chemistry*, 73:231–247, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000313.

Gebremedhin:2018:OPE

[GW18] Daniel Gebremedhin and Charles Weatherford. One-particle effective potential for helium atom. *Advances in Quantum Chemistry*, 76:211–222, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300576.

Gebremedhin:2023:HFC

[GW23] Daniel Gebremedhin and Charles Weatherford. Hartree–Fock calculations on atoms with Coulomb Sturmian basis sets. *Advances in Quantum Chemistry*, 88:119–132, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000278.

Gordon:2003:OOC

[GWM+03] I. Gordon, P. Wagner, V. V. Moshchalkov, Y. Bruynseraede, L. Pinsard, and A. Revcolevschi. Orbital ordering and the cooperative Jahn–Teller effect in single crystals of the magnetic perovskite $La_{7/8}Sr_{1/8}MnO_3$. *Advances in Quantum Chemistry*, 44:563–578, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440379.

Gebremedhin:2019:NCW

[GWW19] Daniel Gebremedhin, Charles Weatherford, and Brian Wilson. Normalizing cluster wavefunctions in the interstitial region within the muffin-tin approximation. *Advances in Quantum Chemistry*, 79:97–112, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300218.

Harris:2013:FCW

[HA13] F. E. Harris and V. V. Albert. Fully correlated wavefunctions for three- and four-body systems. *Advances in Quantum Chemistry*, 67:3–18, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000017.

Hall:1964:ACA

[Hal64] G. G. Hall. Accuracy of calculated atomic and molecular properties. *Advances in Quantum Chemistry*, 1:241–254, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603809.

Hall:1991:LJP

[Hal91] George G. Hall. The Lennard-Jones paper of 1929 and the foundations of molecular orbital theory. *Advances in Quantum Chemistry*, 22:1–6, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603615.

Harris:1967:MOT

[Har67] Frank E. Harris. Molecular orbital theory. *Advances in Quantum Chemistry*, 3:61–127, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600878.

Harriman:1990:DDM

[Har90] John E. Harriman. Density and density matrices in density functional theory. *Advances in Quantum Chemistry*, 21:27–46, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605900.

Harris:2004:CMC

[Har04] Frank E. Harris. Current methods for Coulomb few-body problems. *Advances in Quantum Chemistry*, 47:129–155, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470087.

Harris:2005:ASH

[Har05] Frank E. Harris. Angular symmetry and Hylleraas coordinates in four-body problems. *Advances in Quantum Chemistry*, 50:61–75, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500042.

Harris:2017:ECW

[Har17] Frank E. Harris. Exponentially correlated wave functions for four-body systems. *Advances in Quantum Chemistry*, 73:81–102, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000568`.

Harris:2018:AES

[Har18] Frank E. Harris. Atomic electronic structure computations with Hylleraas-CI wave functions. *Advances in Quantum Chemistry*, 76:187–210, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327617300345`.

Hattig:2005:SOE

[Hät05] Christof Hättig. Structure optimizations for excited states with correlated second-order methods: CC2 and ADC(2). *Advances in Quantum Chemistry*, 50:37–60, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605500030`.

Hoggan:2014:RAQ

[HB14] P. E. Hoggan and A. Bouferguene. Relative advantages of quantum Monte Carlo simulation for changing electron correlation: CO reactions on copper and platinum catalysts. *Advances in Quantum Chemistry*, 68:89–103, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128005361000058`.

Hirschfelder:1964:RDP

[HBE64] Joseph O. Hirschfelder, W. Byers Brown, and Saul T. Epstein. Recent developments in perturbation theory. *Advances in Quantum Chemistry*, 1:255–374, 1964. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603810`.

Hoffges:1998:RFS

[HBE+98] J. T. Höffges, H. W. Baldauf, T. Eichler, S. R. Helmfrid, and H. Walther. Resonance fluorescence of a single ion. *Advances in Quantum Chemistry*, 30:65–75, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605031`.

Holroyd:2019:TBT

[HBGvM19] Leo F. Holroyd, Michael Bühl, Marie-Pierre Gaigeot, and Tanja van Mourik. Thermodynamics of 5-bromouracil tautomerization from first-principles molecular dynamics simulations. *Advances in Quantum Chemistry*, 78:109–128, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300200.

Hizhnyakov:2003:JTE

[HBKS03] V. Hizhnyakov, V. Boltrushko, H. Kaasik, and I. Sildos. Jahn–Teller effect in the excited state: Anomalous temperature dependence of the zero-phonon line. *Advances in Quantum Chemistry*, 44:135–149, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440094.

Hirata:2000:RDF

[HBT+00] Masaru Hirata, Turgut Bastug, Shoichi Tachimori, Rika Sekine, Jun Onoe, and Hirohide Nakamatsu. Relativistic density functional calculations for potential energy curves of uranyl nitrate hydrate. *Advances in Quantum Chemistry*, 37:325–333, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760037023X.

Hands:2003:VIS

[HDB03] I. D. Hands, J. L. Dunn, and C. A. Bates. Vibronic-induced shifts in the optical spectra of doped fullerenes. *Advances in Quantum Chemistry*, 44:335–353, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440227.

Hoggan:2024:CSQ

[HDFT24] Philip E. Hoggan, Noëlie Duchamp, Chloé Feschet, and Maria M. Tarragó. Chapter seven — quantum Monte Carlo method modeling hydrogen production using methane at Ni(111): the adsorbed formyl to CO step. *Advances in Quantum Chemistry*, 89:359–371, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000680.

Hehenberger:2018:POL

[Heh18] Michael Hehenberger. Per-Olov Löwdin's impact on a "Lost Son". *Advances in Quantum Chemistry*, 77:1–18, 2018. CO-

DEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300680.

Hess:2022:PTI

[Hes22] B. Andes Hess. The propensity of terpenes to invoke concerted reactions in their biosynthesis. *Advances in Quantum Chemistry*, 85:??, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000120.

Hirshberg:2017:MFM

[HG17] Barak Hirshberg and R. Benny Gerber. Mean-field methods for time-dependent quantum dynamics of many-atom systems. *Advances in Quantum Chemistry*, 75:1–26, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300023.

Hanstorp:1998:TED

[HHK+98] D. Hanstorp, G. Haeffler, A. E. Klinkmüller, U. Ljungblad, U. Berzinsh, I. Yu. Kiyan, and D. J. Pegg. Two electron dynamics in photodetachment. *Advances in Quantum Chemistry*, 30:311–334, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605146.

Haque:2021:COE

[HHU+21] Mohammad M. Haque, Abul K. F. Haque, Mohammad Alfaz Uddin, Malik Maaza, Mohammad Atiqur R. Patoary, Arun K. Basak, and Bidhan C. Saha. Elastic scattering of $e^{\pm}$ by Cd, Hg, and Pb atoms at 1 eV $\leq E_i \leq$ 1 GeV. *Advances in Quantum Chemistry*, 84:1–72, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300046.

Helgaker:1988:ACG

[HJ88] Trygve Helgaker and Poul Jørgensen. Analytical calculation of geometrical derivatives in molecular electronic structure theory. *Advances in Quantum Chemistry*, 19:183–245, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606164.

Hattig:1999:DCS

[HJ99] Christof Hättig and Poul Jørgensen. Dispersion coefficients for second hyperpolarizabilities using coupled-cluster cubic response theory. *Advances in Quantum Chemistry*, 35:111–148, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860458X.

Hizhnyakov:2003:CDM

[HK03] V. Hizhnyakov and H. Kaasik. Critical dependence of multiphonon transitions on interaction strength and temperature. *Advances in Quantum Chemistry*, 44:151–168, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440100.

Hohenberg:1990:BST

[HKS90] P. C. Hohenberg, Walter Kohn, and L. J. Sham. The beginnings and some thoughts on the future. *Advances in Quantum Chemistry*, 21:7–26, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605894.

Hybertsen:1990:SEA

[HL90] Mark S. Hybertsen and Steven G. Louie. Self-energy approach to quasiparticle energies using a density functional treatment of dielectric screening. *Advances in Quantum Chemistry*, 21:155–174, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605961.

Hartmann:1997:SWD

[HL97] Eberhard Hartmann and Christa Lauterbach. Scattered-wave description of inner-shell processes in small molecules and clusters. *Advances in Quantum Chemistry*, 29:373–387, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602798.

Hayes:2019:CTH

[HM19] Wayne W. Hayes and Joseph R. Manson. Classical theory of hyperthermal gas scattering from surfaces. *Advances in Quantum Chemistry*, 80:319–359, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300395.

Hoggan:2021:NEC

[HM21] Philip E. Hoggan and Monika Musiał, editors. *New Electron Correlation Methods and Their Applications, and Use of Atomic Orbitals with Exponential Asymptotes*, volume 83 of *Advances in quantum chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2021. ISBN 0-12-823546-2 (hardcover). ISSN 0065-3276. xvii + 334 pp. LCCN QD453 .A28 83; QD462 .N49 2021.

Huzinaga:1973:POH

[HMC73] Sigeru Huzinaga, Denis McWilliams, and Antonio A. Cantu. Projection operators in Hartree–Fock theory. *Advances in Quantum Chemistry*, 7:187–220, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605626`.

Haque:2018:EII

[HMH+18] Abul K. F. Haque, Malik Maaza, Md. M. Haque, Md. Atiqur R. Patoary, Md. Alfaz Uddin, Md. Ismail Hossain, Md. Selim Mahbub, Arun K. Basak, and Bidhan C. Saha. Electron-impact ionization cross sections for inner L- and M-subshells of atomic targets at relativistic energies. *Advances in Quantum Chemistry*, 77:121–165, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327617300230`.

Hubac:2001:MBW

[HMW01] I. Hubač, P. Mach, and S. Wilson. Multireference Brillouin–Wigner methods for many-body systems. *Advances in Quantum Chemistry*, 39:225–240, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605390149`.

Hoggan:2016:ECM

[HO16] Philip E. Hoggan and Telhat Ozdogan, editors. *Electron correlation in molecules — ab initio beyond Gaussian quantum chemistry*, volume 73. Elsevier, Amsterdam, The Netherlands, 2016. CODEN AQCHA9. ISBN 0-12-803060-7, 0-12-803061-5. ISSN 0065-3276. xvi + 423 pp. LCCN QD462 .E43 2016. URL `https://www.sciencedirect.com/science/bookseries/00653276/73`.

Hoggan:2017:P

[HO17] Philip E. Hoggan and Telhat Ozdogan. Preface. *Advances in Quantum Chemistry*, 73:xi–xii, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300247.

Hoggan:2013:AQCa

[Hog13a] Philip E. Hoggan. Advances in quantum chemistry. *Advances in Quantum Chemistry*, 67:i, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000285.

Hoggan:2013:AQCb

[Hog13b] Philip E. Hoggan. Advances in quantum chemistry. *Advances in Quantum Chemistry*, 67:iii, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000303.

Hoggan:2013:Cb

[Hog13c] Philip E. Hoggan. Contributors. *Advances in Quantum Chemistry*, 67:xi–xiii, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000340.

Hoggan:2013:Ca

[Hog13d] Philip E. Hoggan. Copyright. *Advances in Quantum Chemistry*, 67:iv, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000315.

Hoggan:2013:EB

[Hog13e] Philip E. Hoggan. Editorial board. *Advances in Quantum Chemistry*, 67:ii, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000297.

Hoggan:2013:P

[Hog13f] Philip E. Hoggan. Preface. *Advances in Quantum Chemistry*, 67:ix–x, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000339.

Hoggan:2013:PME

[Hog13g] Philip E. Hoggan. *Proceedings of MEST 2012: Exponential Type Orbitals for Molecular Electronic Structure Theory*, volume 67 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. xiii + 290 pp. LCCN QC451 .U57 2013 .v67.

Hoggan:2014:PME

[Hog14] Philip E. Hoggan. *Proceedings of MEST 2012: Electronic structure methods with applications to experimental chemistry*, volume 68 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. xvi + 320 pp. LCCN QC451 .U57 2014 .v68.

Hoggan:2018:P

[Hog18a] Philip Hoggan. Preface. *Advances in Quantum Chemistry*, 76:xv–xvi, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300837.

Hoggan:2018:AQC

[Hog18b] Philip E. Hoggan, editor. *Advances in Quantum Chemistry*, volume 76 of *Advances in quantum chemistry*. Elsevier, Amsterdam, The Netherlands, 2018. CODEN AQCHA9. ISBN 0-12-813002-4, 0-12-813003-2 (e-book). ISSN 0065-3276. xvi + 357 pp. LCCN QC176.8.E4. URL https://www.sciencedirect.com/science/bookseries/00653276/76.

Hoggan:2018:Cb

[Hog18c] Philip E. Hoggan. Contributors. *Advances in Quantum Chemistry*, 76:xi–xiv, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300825.

Hoggan:2018:Ca

[Hog18d] Philip E. Hoggan. Copyright. *Advances in Quantum Chemistry*, 76:iv, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300801.

Hoggan:2018:QMC

[Hog18e] Philip E. Hoggan. Quantum Monte Carlo calculations for industrial catalysts: Accurately evaluating the H_2 dissociation reaction barrier on Pt(111). *Advances in Quantum Chemistry*, 76:271–278, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300679.

Hoggan:2018:SP

[Hog18f] Philip E. Hoggan. Series page. *Advances in Quantum Chemistry*, 76:ii–??, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300795.

Hoggan:2021:CEQ

[Hog21] Philip E. Hoggan. Quantum Monte Carlo with ground-state input to investigate platinum-doped aluminum catalyst: H_2 production from adsorbed CO. *Advances in Quantum Chemistry*, 83:155–170, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000137.

Hoggan:2023:AQC

[Hog23a] Philip E. Hoggan, editor. *Advances in Quantum Chemistry*, volume 88 of *Advances in quantum chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2023. ISBN 0-443-18663-4 (hardback), 0-443-18664-2 (ePub). ISSN 0065-3276. 312 pp. LCCN QD462.

Hoggan:2023:P

[Hog23b] Philip E. Hoggan. Preface. *Advances in Quantum Chemistry*, 88: xv–xvii, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000631.

Hoggan:2023:QMC

[Hog23c] Philip E. Hoggan. Quantum Monte Carlo method describing supported metal catalysis: Ni(111)/alumina decomposing methane as a route to hydrogen. *Advances in Quantum Chemistry*, 88:291–304, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000011.

Higashiguchi:2008:AES

[HOI+08] Yoshitsune Higashiguchi, Hiroaki Ochiai, Kazuyuki Igei, Kengo Ohmori, and Yoshinori Hayafuji. Atomic and electronic structures of boron clusters in crystalline silicon: The case of X@B_6 and X@B_{12}, X = H–Br. *Advances in Quantum Chemistry*, 54:89–102, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000081.

Hanstorp:1998:P

[HP98] Dag Hanstorp and Hans Persson. Preface. *Advances in Quantum Chemistry*, 30:xiii, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604980.

Hoggan:2017:AGT

[HPB17] Philip E. Hoggan, Jorge E. Pérez, and Ahmed Bouferguene. An application of the Gaussian transform for approximating some Bessel functions and multicenter integrals involving 1s Slater-type orbitals. *Advances in Quantum Chemistry*, 73:139–144, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000349.

Hanstorp:1998:AQC

[HPL98] Dag Hanstorp, Hans Persson, and Ingvar Lindgren, editors. *Advances in Quantum Chemistry: Modern trends in atomic physics*, volume 30 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1998. CODEN AQCHA9. ISBN 0-12-034830-6 (hardcover). ISSN 0065-3276. xiii + 506 pp. LCCN QD453 .A28 v.30. US$125.00. URL http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348306&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/article/pii/S0065327608604955; https://www.sciencedirect.com/science/book/9780120348305. The symposium Modern Trends in Atomic Physics was held on May 24–25, 1995, at the Hjortviken Conference Centre just outside Göteborg in Sweden. It was organized in honor of professor Ingvar Lindgren on the occasion of his 65th birthday.

Hofer:2010:IQM

[HPRR10] Thomas S. Hofer, Andreas B. Pribil, Bernhard R. Randolf, and Bernd M. Rode. Ab initio quantum mechanical charge field molecular dynamics: a nonparametrized first-principle approach to liquids and solutions. *Advances in Quantum Chemistry*, 59:213–246, 2010. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590075.

Haque:2017:EIA

[HPU+17] A. K. Fazlul Haque, M. Atiqur R. Patoary, M. Alfaz Uddin, Arun K. Basak, and Bidhan C. Saha. Electron impact atomic and ionic ionization: Analytical, semiempirical, and semiclassical methods. *Advances in Quantum Chemistry*, 73:363–414, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000398.

Hoffmann:1986:FCC

[HS86] Mark R. Hoffmann and Henry F. Schaefer III. A full coupled-cluster singles, doubles, and triples model for the description of electron correlation. *Advances in Quantum Chemistry*, 18:207–279, 1986. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600507.

Harris:2005:HCW

[HS05] Frank E. Harris and Vedene H. Smith, Jr. Highly compact wavefunctions for two-electron systems. *Advances in Quantum Chemistry*, 48:407–419, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480211.

Harada:2019:PCS

[HS19] Ryuhei Harada and Yasuteru Shigeta. Parallel cascade selection molecular dynamics simulations for transition pathway sampling of biomolecules. *Advances in Quantum Chemistry*, 78:129–147, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300212.

Hoffmann:1998:GPC

[HSR98] Marcin Hoffmann, Agnieszka Szarecka, and Jacek Rychlewski. Gas-phase conformational analysis of (R,R)-tartaric acid, its diamide, N,N,N',N'-tetramethyldiamide, and model compounds. *Advances in Quantum Chemistry*, 32:109–125, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604098.

Henningsson:2004:PIP

[HSS+04] A. Henningsson, A. Stashans, A. Sandell, H. Rensmo, S. Södergren, H. Lindström, L. Vayssieres, A. Hagfeldt, S. Lunell, and H. Siegbahn. Proton insertion in polycrystalline WO_3 studied with electron spectroscopy and semi-empirical calculations. *Advances in Quantum Chemistry*, 47:23–36, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470026.

Hirata:2000:ESC

[HTS+00] Masaru Hirata, Shoichi Tachimori, Rika Sekine, Jun Onoe, and Hirohide Nakamatsu. Electronic structures and chemical bonding of actinyl nitrates dihydrates. *Advances in Quantum Chemistry*, 37:335–351, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370241.

Hughes:1998:HPS

[Hug98] Vernon W. Hughes. High precision spectroscopy of positronium and muonium. *Advances in Quantum Chemistry*, 30:99–123, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605055.

Hurley:1973:THF

[Hur73] A. C. Hurley. Thermochemistry in the Hartree–Fock approximation. *Advances in Quantum Chemistry*, 7:315–334, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605675.

Haque:2011:EII

[HUS+11] A. K. Fazlul Haque, M. Alfaz Uddin, M. Shahjahan, M. Rashid Talukder, Arun K. Basak, and Bidhan C. Saha. Electron impact inner-shell ionization of atoms. *Advances in Quantum Chemistry*, 61:317–380, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000061.

Hubac:2001:GBW

[HW01] I. Hubac and S. Wilson. On the generalized Brillouin–Wigner perturbation theory and the many-body problem. *Advances in Quantum Chemistry*, 39:209–223, 2001. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390137.

Hylleraas:1964:STE

[Hyl64] Egil A. Hylleraas. The Schrödinger two-electron atomic problem. *Advances in Quantum Chemistry*, 1:1–33, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603731.

Head:1989:NBO

[HZ89] John D. Head and Michael C. Zerner. Newton based optimization methods for obtaining molecular conformation. *Advances in Quantum Chemistry*, 20:239–290, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606280.

Ignatenko:2019:NCD

[IBB+19] Anna V. Ignatenko, Anna A. Buyadzhi, Vasily V. Buyadzhi, Anna A. Kuznetsova, Alexander A. Mashkantsev, and Eugeny V. Ternovsky. Nonlinear chaotic dynamics of quantum systems: Molecules in an electromagnetic field. *Advances in Quantum Chemistry*, 78:149–170, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300303.

Ishii:2008:NTP

[IFAY08] Tomohiko Ishii, Yukikazu Fuke, Naoko Aizawa, and Masahiro Yamashita. Novel theoretical prediction method of the Haldane gap among the azido-bridged compounds by DV–Xα molecular orbital calculation. *Advances in Quantum Chemistry*, 54:35–46, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000044.

IHaya:1964:RDG

[I'H64] Y. I'Haya. Recent developments in the generalized Hückel method. *Advances in Quantum Chemistry*, 1:203–240, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603792.

Ishizumi:2008:PSS

[IKN+08] Keisuke Ishizumi, Hironori Kawanishi, Ryo Nakao, Isao Takahashi, Hikaru Terauchi, and Yoshinori Hayafuji. Particle size and surface effects on critical thickness for ferroelectricity of $BaTiO_3$ by ab initio calculations. *Advances in Quantum Chemistry*, 54:103–113, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000093.

Ivanov:1998:SOR

[IL98] Stanislav Ivanov and Mel Levy. Second-order relations involving correlation energy and its functional derivative. *Advances in Quantum Chemistry*, 33:11–29, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860427X.

Iyengar:2008:SDA

[ILS08] Srinivasan S. Iyengar, Xiaohu Li, and Isaiah Sumner. The study of dynamically averaged vibrational spectroscopy of atmospherically relevant clusters using ab initio molecular dynamics in conjunction with quantum wavepackets. *Advances in Quantum Chemistry*, 55:333–353, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760700216X.

IHaya:1980:VAO

[IM80] Y. J. I'Haya and Tetsuo Morikawa. Variational approach to orthogonality and normality of basis ket-vectors. *Advances in Quantum Chemistry*, 12:43–63, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603135.

Ishii:2003:MEC

[IOA03] Takugo Ishii, Kazuyoshi Ogasawara, and Hirohiko Adachi. Many-electron calculation for the analysis of optical absorption spectra in Cr^{4+}-doped solid-state laser crystals. *Advances in Quantum Chemistry*, 42:67–76, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420418.

Ishii:2000:FPC

[IOI+00] Takugo Ishii, Kazuyoshi Ogasawara, Yukiko Ito, Isao Tanaka, and Hirohiko Adachi. First-principles calculation for multiplet structure of emerald. *Advances in Quantum Chemistry*, 37:85–96, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760037006X.

Ivanov:2001:FDC

[IS01] Mikhail V. Ivanov and Peter Schmelcher. Finite-difference calculations for atoms and diatomic molecules in strong magnetic and static electric fields. *Advances in Quantum Chemistry*, 40:361–379, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400256`.

Ito:2000:EIT

[ITI+00] Yukiko Ito, Isao Tanaka, Takugo Ishii, Kazuyoshi Ogasawara, and Hirohiko Adachi. The effect of intrinsic trigonal distortion on the multiplet structures of ruby and emerald. *Advances in Quantum Chemistry*, 37:97–110, 2000. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327600370071`.

Itoh:2003:ESD

[Ito03] Shinichi Itoh. Electronic structure of Er doped GaAs. *Advances in Quantum Chemistry*, 42:209–214, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603420509`.

Jalbout:2007:EAD

[JA07] Abraham F. Jalbout and Ludwik Adamowicz. Electron attachment to DNA base complexes. *Advances in Quantum Chemistry*, 52:231–251, 2007. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327606520106`.

Jansen:1965:QCC

[Jan65] Laurens Jansen. Quantum chemistry and crystal physics: Stability of crystals of rare gas atoms and alkali halides in terms of three-atom and three-ion exchange interactions. *Advances in Quantum Chemistry*, 2:119–194, 1965. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860074X`.

Janoschek:1997:SSM

[Jan97] Rudolf Janoschek. SiN_2 and SiN_4 molecules: An ab initio study of molecular and electronic structure, stability, and IR activity. *Advances in Quantum Chemistry*, 28:235–245, 1997.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860218X.

Joudieh:2018:IML

[JcH18] Nabil Joudieh, Ali Ba c, and Philip E. Hoggan. Ab initio molecular local nuclear magnetic shielding tensors. *Advances in Quantum Chemistry*, 76:167–183, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300254.

Jehle:1965:CFI

[Jeh65] Herbert Jehle. Charge fluctuation interactions in molecular biophysics. *Advances in Quantum Chemistry*, 2:195–212, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600751.

Johnson:2008:ATM

[JG08] Matthew S. Johnson and Michael E. Goodsite. Applications of theoretical methods to atmospheric science. *Advances in Quantum Chemistry*, 55:1–4, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002018.

Jaramillo-Gonzalez:2016:AES

[JGCRC16] Caterine Jaramillo-González, Rodrigo Morales Cueto, and William Rodríguez-Córdoba. Absorption and emission spectra of anthracene-9-carboxylic acid in solution within the polarizable continuum model: a long-range corrected time dependent density functional study. *Advances in Quantum Chemistry*, 72:61–94, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000234.

Jorgensen:2008:IEP

[JGNJ08] Solvejg Jørgensen, Mette M.-L. Grage, Gunnar Nyman, and Matthew S. Johnson. Isotope effects in photodissociation: Chemical reaction dynamics and implications for atmospheres. *Advances in Quantum Chemistry*, 55:101–135, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002079.

Jensen:1999:MMS

[JH99] Morten Østergaard Jensen and Aage E. Hansen. The molecular magnetic shielding field: Response graph illustrations of the benzene field. *Advances in Quantum Chemistry*, 35:193–215, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860461X.

Jacak:2020:IPC

[JJ20] Witold A. Jacak and Janusz E. Jacak. Ion plasmon collective oscillations underlying saltatory conduction in myelinated axons and topological-homotopy concept of memory. *Advances in Quantum Chemistry*, 82:113–157, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300095.

Jalkanen:2005:LRP

[JJD05] K. J. Jalkanen, V. Würtz Jürgensen, and I. M. Degtyarenko. Linear response properties required to simulate vibrational spectra of biomolecules in various media: (R)-phenyloxirane (a comparative theoretical and spectroscopic vibrational study). *Advances in Quantum Chemistry*, 50:91–124, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500066.

Jenkins:2019:AQC

[JKMB19a] Samantha Jenkins, Steven R. Kirk, Jean Maruani, and Erkki J. Brändas, editors. *Advances in Quantum Chemistry*, volume 78 of *Advances in quantum chemistry*. Elsevier, Amsterdam, The Netherlands, 2019. CODEN AQCHA9. ISBN 0-12-816084-5. ISSN 0065-3276. xix + 465 pp. LCCN QC176.8.E4. URL https://www.sciencedirect.com/science/journal/00653276/78. Quantum systems in physics, chemistry and biology — theory, interpretation, and results.

Jenkins:2019:P

[JKMB19b] Samantha Jenkins, Steven R. Kirk, Jean Maruani, and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 78:xiii–xv, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300097.

Judd:2003:IQ

[JL03] B. R. Judd and Edwin Lo. Icosahedral quarks. *Advances in Quantum Chemistry*, 44:13–19, 2003. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440021.

Jerosimic:2019:DBS

[JMWG19] Stanka V. Jerosimić, Milan Z. Milovanović, Roland Wester, and Franco A. Gianturco. Dipole-bound states contribution to the formation of anionic carbonitriles in the ISM: Calculations using multireference methods for C_3N^-. *Advances in Quantum Chemistry*, 80:47–86, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300346.

Johnson:1973:SWT

[Joh73] Keith H. Johnson. Scattered-wave theory of the chemical bond. *Advances in Quantum Chemistry*, 7:143–185, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605614.

Jorgensen:1974:PSS

[Jør74] Christian Klixbüll Jørgensen. Photoelectron spectra showing relaxation effects in the continuum and electrostatic and chemical influences of the surrounding atoms. *Advances in Quantum Chemistry*, 8:137–182, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600611.

Jorgensen:1978:KIS

[Jør78] Christian Klixbüll Jørgensen. Kossel isoelectronic series and photoelectron spectra. *Advances in Quantum Chemistry*, 11:51–91, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602348.

Jost:2008:NML

[Jos08] R. Jost. A new model of low resolution absorption cross section. *Advances in Quantum Chemistry*, 55:75–100, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002067.

Joseph:2021:CTC

[JS21] Dwayne C. Joseph and Bidhan C. Saha. Charge exchange in slow collisions of Si^{3+} with hydrogen atom: Molecular-orbital close-coupling approaches in the adiabatic representation. *Advances in Quantum Chemistry*, 84:73–94, 2021. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300058.

Jankowski:2008:ABM

[JSF08] Karol Jankowski, Romuald Slupski, and Jesus R. Flores. Asymptotic behavior of MP2 correlation energies for closed-shell atoms. *Advances in Quantum Chemistry*, 53:151–175, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530091.

Joseph:2014:SQM

[JSG+14] D. C. Joseph, B. C. Saha, J-P. Gu, H. P. Liebermann, P. Funke, and R. J. Buenker. The $(SiH)^{3+}$ quasi-molecule in the adiabatic representation. *Advances in Quantum Chemistry*, 68:191–202, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000101.

Kaijser:2015:FHM

[Kai15] Per Kaijser. Frank Harris, a master of mountains. *Advances in Quantum Chemistry*, 71:1–9, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000039.

Kaplan:1998:REC

[Kap98] I. G. Kaplan. Role of electron correlation in nonadditive forces and *ab initio* model potentials for small metal clusters. *Advances in Quantum Chemistry*, 31:137–156, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601860.

Karelson:1997:QCT

[Kar97] Mati Karelson. Quantum chemical treatment of molecules in condensed disordered media. *Advances in Quantum Chemistry*, 28:141–157, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602129.

Karlsson:2002:SEI

[Kar02] Göran Karlsson. The scientific, educational and internationalization influence of Per-Olov Löwdin. *Advances in Quantum Chemistry*, 41:1–8, 2002. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760241043X.

Karshenboim:2008:CPP

[Kar08] Savely G. Karshenboim. Conceptual problems in phenomenological interpretation in searches for variation of constants and violation of various invariances. *Advances in Quantum Chemistry*, 53:237–252, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530121.

Karlsson:2024:COS

[Kar24] Erik B. Karlsson. Chapter one — specific quantum effects in low energy neutron scattering from protons. *Advances in Quantum Chemistry*, 89:1–59, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000710.

Kato:2003:CSD

[Kat03] Tatsuhisa Kato. Cage structure distortion of fullerenes. *Advances in Quantum Chemistry*, 44:313–317, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440203.

Kawai:1997:DXC

[Kaw97] Jun Kawai. DV–Xα calculation of X-ray emission spectra. *Advances in Quantum Chemistry*, 29:329–355, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602774.

Kucharski:1986:FOM

[KB86] Stanislaw A. Kucharski and Rodney J. Bartlett. Fifth-order many-body perturbation theory and its relationship to various coupled-cluster approaches. *Advances in Quantum Chemistry*, 18:281–344, 1986. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600519.

Kleinman:1998:UEK

[KB98] Leonard Kleinman and D. M. Bylander. Using the exact Kohn–Sham exchange energy density functional and potential to study errors introduced by approximate correlation functionals. *Advances in Quantum Chemistry*, 33:151–165, 1998.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604347.

Kiraz:2023:QMC

[KBH23] Aslı Öztürk Kiraz, Ali Bağcı, and Philip E. Hoggan. Quantum Monte Carlo method for metal-film catalysis: Water addition to CO adsorbed on Pt/Al(111), efficient hydrogen production. *Advances in Quantum Chemistry*, 88:273–289, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000187.

Koppel:2003:CJT

[KBS03] H. Köppel, I. Bâldea, and P. G. Szalay. Combined Jahn–Teller and pseudo-Jahn–Teller effects in the benzene radical cation. *Advances in Quantum Chemistry*, 44:199–217, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440136.

Koroteev:2019:ECS

[KC19] Yury M. Koroteev and Evgenii V. Chulkov. Electronic and crystal structure of the Pt(111)-(2×2)-K and Cu(111)-(2×2)-K systems. *Advances in Quantum Chemistry*, 80:175–197, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300371.

Klein:1970:SAS

[KCM70] D. J. Klein, C. H. Carlisle, and F. A. Matsen. Symmetry adaptation to sequences of finite groups. *Advances in Quantum Chemistry*, 5:219–260, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860341X.

Kolesov:2011:QCE

[KD11] Grigory Kolesov and Yuri Dahnovsky. Quantum correlation effects in electron dynamics in molecular wires and solar cells: The nonequilibrium Green's function approach. *Advances in Quantum Chemistry*, 61:261–315, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012386013200005X.

Klobukowski:1997:EAS

[KDG97] M. Klobukowski, G. H. F. Diercksen, and J. M. García de la Vega. Electron affinity of SF_6. *Advances in Quantum*

Chemistry, 28:189–203, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602154.

Kowada:1997:AEC

[KE97] Y. Kowada and D. E. Ellis. Application of the embedded cluster method to the electronic state of silicate glasses. *Advances in Quantum Chemistry*, 29:233–251, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602725.

Kaldor:1998:HAC

[KE98] Uzi Kaldor and Ephraim Eliav. High-accuracy calculations for heavy and super-heavy elements. *Advances in Quantum Chemistry*, 31:313–336, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860194X.

Kowada:2000:ECM

[KE00] Yoshiyuki Kowada and D. E. Ellis. Embedded cluster models for electronic states of silicate glasses. *Advances in Quantum Chemistry*, 37:271–290, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370198.

Kertesz:1982:ESP

[Ker82] Miklós Kertész. Electronic structure of polymers. *Advances in Quantum Chemistry*, 15:161–214, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601239.

Klaiman:2012:RFG

[KG12] Shachar Klaiman and Ido Gilary. On resonance: a first glance into the behavior of unstable states. *Advances in Quantum Chemistry*, 63:1–31, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000011.

Kuznetsova:2019:SMA

[KGI+19] Anna A. Kuznetsova, Alexander V. Glushkov, Anna V. Ignatenko, Andrey A. Svinarenko, and Valentin B. Ternovsky. Spectroscopy of multielectron atomic systems in a DC electric field. *Advances in Quantum Chemistry*, 78:287–306, 2019.

CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327618300297`.

Keith:1998:SSE

[KGW98] G. J. A. Keith, P. J. Grout, and S. Wilson. Systematic sequences of even-tempered Gaussian primitives for diatomic molecules in solution: a preliminary study using continuum solvation models. *Advances in Quantum Chemistry*, 32:285–313, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604189`.

Kato:2003:VIJ

[KH03] Takashi Kato and Kazuyuki Hirao. Vibronic interactions and Jahn–Teller effects in charged hydrocarbons. *Advances in Quantum Chemistry*, 44:257–271, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440161`.

Khetselius:2019:ORM

[Khe19] Olga Yu Khetselius. Optimized relativistic many-body perturbation theory calculation of wavelengths and oscillator strengths for Li-like multicharged ions. *Advances in Quantum Chemistry*, 78:223–251, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532761830025X`.

Khodyrev:2004:TEL

[Kho04] V. A. Khodyrev. The treatment of energy loss in terms of induced current density. *Advances in Quantum Chemistry*, 45 (part 1):125–158, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604450060`.

Korona:2023:RHM

[KHPP23] Tatiana Korona, Michał Hapka, Katarzyna Pernal, and Konrad Patkowski. Review — how to make symmetry-adapted perturbation theory more accurate? *Advances in Quantum Chemistry*, 87:37–72, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327623000382`.

Kimura:1997:ESS

[KIHA97] Hitoshi Kimura, Syunji Imanaga, Yoshinori Hayafuji, and Hirohiko Adachi. The electronic structure of silicon clusters. *Advances in Quantum Chemistry*, 29:193–206, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602701.

Kawanishi:2008:ESA

[KIT+08] Hironori Kawanishi, Keisuke Ishizumi, Isao Takahashi, Hikaru Terauchi, and Yoshinori Hayafuji. Electronic structures of $ATiO_3$ perovskite oxides (A = Ba, Sr, and Pb): Comparative first-principles study. *Advances in Quantum Chemistry*, 54:133–143, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000111.

Kryachko:1985:MAD

[KK85] Eugene S. Kryachko and Toshikatsu Koga. Modern aspects of diatomic interaction theory. *Advances in Quantum Chemistry*, 17:97–223, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603020.

Kovacs:1997:CTA

[KKA97] Zs. Kovács, L. Kövér, and H. Adachi. Charge transfer in Al–Ni alloys: a spin-selective study. *Advances in Quantum Chemistry*, 29:421–431, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602816.

Kreibich:1998:APO

[KKGG98] T. Kreibich, S. Kurth, T. Grabo, and E. K. U. Gross. Asymptotic properties of the optimized effective potential. *Advances in Quantum Chemistry*, 33:31–48, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604281.

Kochanski:1997:DTW

[KKK+97] E. Kochanski, R. Kelterbaum, S. Klein, M. M. Rohmer, and A. Rahmouni. Decades of theoretical work on protonated hydrates. *Advances in Quantum Chemistry*, 28:273–291, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860221X.

Klahn:1981:RLI

[Kla81] Bruno Klahn. Review of the linear independence properties of infinite sets of functions used in quantum chemistry. *Advances in Quantum Chemistry*, 13:155–209, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602932.

Kleinpoppen:1977:AEA

[Kle77] Hans Kleinpoppen. Analysis of electron–atom collisions. *Advances in Quantum Chemistry*, 10:77–141, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605791.

Kleppner:2008:P

[Kle08] Daniel Kleppner. Preface. *Advances in Quantum Chemistry*, 53: xvi–xix, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530157.

Kjaergaard:2008:APS

[KLG+08] Henrik G. Kjaergaard, Joseph R. Lane, Anna L. Garden, Daniel P. Schofield, Timothy W. Robinson, and Michael J. Mills. Atmospheric photolysis of sulfuric acid. *Advances in Quantum Chemistry*, 55:137–158, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002080.

Kalemos:1998:ESS

[KM98] Apostolos Kalemos and Aristides Mavridis. On the electronic structure of ScB^+: Ground and low-lying excited states. *Advances in Quantum Chemistry*, 32:69–91, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604074.

Kirchner:2013:ICW

[KMHL13] Tom Kirchner, Mitsuko Murakami, Marko Horbatsch, and Hans Jürgen Lüdde. Ion collisions with water molecules: a time-dependent density functional theory approach. *Advances in Quantum Chemistry*, 65:315–337, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012396455700011X.

Korona:1997:CSA

[KMJ97] Tatiana Korona, Robert Moszynski, and Bogumił Jeziorski. Convergence of symmetry-adapted perturbation theory for the interaction between helium atoms and between a hydrogen molecule and a helium atom. *Advances in Quantum Chemistry*, 28:171–188, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602142`.

Kuleff:2001:RMC

[KMR01] A. I. Kuleff, J. Maruani, and P. P. Raychev. Reproduction of metal-cluster magic numbers using a q-deformed, 3-dimensional, harmonic oscillator model. *Advances in Quantum Chemistry*, 40:279–304, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400219`.

Kryachko:2001:TST

[KN01] Eugene S. Kryachko and Minh Tho Nguyen. Thiouracils: Structures, tautomerism, interaction with water, and functioning in RNA and modified DNA base pairs. *Advances in Quantum Chemistry*, 40:79–102, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400104`.

Kinoshita:2008:ICE

[KNI+08] Yusuke Kinoshita, Takayuki Noguchi, Takeshi Inoue, Takumi Tomita, and Yoshinori Hayafuji. Ab initio calculation of the electronic structure of ZnO with an impurity from Li to Bi. *Advances in Quantum Chemistry*, 54:325–339, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760700024X`.

Kurisaki:2008:ELU

[KNM+08] Tsutomu Kurisaki, Yuichi Nakazono, Shuji Matsuo, Rupert C. C. Perera, James H. Underwood, and Hisanobu Wakita. Evaluation of laboratory ultra-soft X-ray absorption spectrometer by Li-K XANES measurements and their DV–Xα calculations. *Advances in Quantum Chemistry*, 54:315–323, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327607000238`.

Kurokawa:2017:GCC

[KNN17] Yusaku I. Kurokawa, Hiroyuki Nakashima, and Hiroshi Nakatsuji. General coalescence conditions for the exact wave functions: Higher-order relations for Coulombic and non-Coulombic systems. *Advances in Quantum Chemistry*, 73:59–79, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000520`.

Kereselidze:2018:HAP

[KO18] Tamaz Kereselidze and John F. Ogilvie. The hydrogen-atom problem and Coulomb Sturmian functions in spheroidal coordinates. *Advances in Quantum Chemistry*, 77:391–421, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327618300030`.

Kuros:2019:EPB

[KO19] Arkadiusz Kuroś and Anna Okopińska. Entanglement properties of bound and resonant few-body states. *Advances in Quantum Chemistry*, 78:31–55, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327618300339`.

Kobe:1968:FTA

[Kob68] Donald H. Kobe. Field theoretic approach to atomic helium. *Advances in Quantum Chemistry*, 4:109–140, 1968. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603913`.

Kobus:1997:DME

[Kob97] Jacek Kobus. Diatomic molecules: Exact solutions of HF equations. *Advances in Quantum Chemistry*, 28:1–14, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602038`.

Kolos:1970:AAA

[Koł70] Włodzimierz Kołos. Adiabatic approximation and its accuracy. *Advances in Quantum Chemistry*, 5:99–133, 1970. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608603378`.

Komasa:2005:SNP

[Kom05] Jacek Komasa. In search for the negative polarizability states — the E F $^1\Sigma_g^+$ state of hydrogen molecule. *Advances in Quan-*

tum Chemistry, 48:151–159, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480119.

Kara:2023:ART

[KÖO23] Mehmet Kara, Telhat Özdoğan, and Metin Orbay. Analysis of research trends on the investigation of molecular integrals over Slater type orbitals. *Advances in Quantum Chemistry*, 88:59–74, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000205.

Kurtz:1999:P

[KOS99] H. A. Kurtz, J. V. Ortiz, and J. R. Sabin. Preface. *Advances in Quantum Chemistry*, 35:ix–x, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604517.

Kotani:1968:PPE

[Kot68] Masao Kotani. Paramagnetic properties and electronic structure of iron in heme proteins. *Advances in Quantum Chemistry*, 4:227–266, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603950.

Kawasaki:2000:ESG

[KOT$^+$00] Shinji Kawasaki, Fujio Okino, Hidekazu Touhara, Ning Liu, and Toyohisa Nakajima. The electronic structures of graphite and fullerene, and their compounds. *Advances in Quantum Chemistry*, 37:301–309, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370216.

Koures:2015:SIM

[Kou15] Vasilios G. Koures. Statistical inference with minimum relative entropy: a robust numerical algorithm employing sinc quadrature. *Advances in Quantum Chemistry*, 71:247–263, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761500012X.

Kover:1997:F

[Köv97] L. Kövér. Foreword. *Advances in Quantum Chemistry*, 29:xv–xvi, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602610`.

Kover:2003:IAS

[Köv03] László Kövér. Interpreting Auger spectra in cluster approximation. *Advances in Quantum Chemistry*, 42:331–352, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603420595`.

Kover:2008:LES

[Köv08] L. Kövér. Local electronic structures from analyzing and modeling high-energy Auger and photoelectron spectra of solids. *Advances in Quantum Chemistry*, 54:175–191, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327607000147`.

Katriel:1977:TIH

[KP77] Jacob Katriel and Ruben Pauncz. Theoretical interpretation of Hund's rule. *Advances in Quantum Chemistry*, 10:143–185, 1977. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605808`.

Krause:1999:QCS

[Kra99] Jeffrey L. Krause. Quantum control in semiconductor heterostructures. *Advances in Quantum Chemistry*, 35:249–260, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604633`.

Kristoffel:2003:VRS

[Kri03] N. Kristoffel. Vibronic renormalization of superconductivity gaps in a two-band model of cuprates. *Advances in Quantum Chemistry*, 44:555–561, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440367`.

Kaplan:2001:BCC

[KRL01] I. G. Kaplan, Szczepan Roszak, and Jerzy Leszczynskin. Binding in clusters with closed-subshell atoms (alkaline-earth elements). *Advances in Quantum Chemistry*, 40:257–278, 2001.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400207.

Krstic:2016:RDH

[Krs16] Predrag Krstic. Response of a DNA hydrogen bond to a force in liquid. *Advances in Quantum Chemistry*, 72:13–28, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615300010.

Kryachko:1981:SPR

[Kry81] Eugene S. Kryachko. Symmetry properties of reduced density matrices. *Advances in Quantum Chemistry*, 14:1–61, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603251.

Kryachko:2003:NCG

[Kry03] Eugene S. Kryachko. Nonadiabatic coupling: General features and relation to molecular properties. *Advances in Quantum Chemistry*, 44:119–133, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440082.

Kaijser:1977:EMD

[KS77] Per Kaijser and Vedene H. Smith, Jr. Evaluation of momentum distributions and Compton profiles for atomic and molecular systems. *Advances in Quantum Chemistry*, 10:37–76, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860578X.

Kaplan:1988:DIR

[KS88] I. G. Kaplan and V. N. Smutny. β-decay-induced rearrangement of the molecular electron shell and the problem of determining the neutrino rest mass. *Advances in Quantum Chemistry*, 19:289–348, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606188.

Kleinman:1990:DGE

[KS90] Leonard Kleinman and Viraht Sahni. Density-gradient expansions. *Advances in Quantum Chemistry*, 21:201–234, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605985.

Karwowski:1997:P

[KS97a] Jacek Karwowski and John R. Sabin. Preface. *Advances in Quantum Chemistry*, 28:xv–xvi, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602002.

Kilpatrick:1997:ADT

[KS97b] P. L. Kilpatrick and N. S. Scott. Abstract data types in the construction of knowledge-based quantum chemistry software. *Advances in Quantum Chemistry*, 28:345–359, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602269.

Kathmann:2008:IMI

[KSG08] Shawn M. Kathmann, Gregory K. Schenter, and Bruce C. Garrett. The impact of molecular interactions on atmospheric aerosol radiative forcing. *Advances in Quantum Chemistry*, 55:429–447, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002201.

Kim:2008:XRA

[KsKsN08] Sung Kwan Kim, Yang soo Kim, and Kwang soo No. X-ray absorption near-edge structure and optical properties of hafnium oxynitride thin films. *Advances in Quantum Chemistry*, 54:81–88, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760700007X.

Kishino:2008:FPC

[KSY08] S. Kishino, K. Sueoka, and H. Yoshida. First-principles calculation of energy band structure of gallium arsenide crystals using Madelung potential. *Advances in Quantum Chemistry*, 54:13–21, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000020.

Kozmutza:1998:SWI

[KT98] Cornelia Kozmutza and Ernő Tfirst. A study of weakly interacting systems in localized representation, including the many-body effect. *Advances in Quantum Chemistry*, 31:231–250, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601902.

Karasiev:2015:FDS

[KT15] Valentin V. Karasiev and Samuel B. Trickey. Frank discussion of the status of ground-state orbital-free DFT. *Advances in Quantum Chemistry*, 71:221–245, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000052.

Koyama:2003:ESE

[KTA03] Yukinori Koyama, Isao Tanaka, and Hirohiko Adachi. Electronic structures and electrode potentials of layered lithium insertion electrodes by the first principles calculation. *Advances in Quantum Chemistry*, 42:145–161, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420455.

Kozmutza:2001:IPT

[KTC01] C. Kozmutza, E. Tfirst, and I. G. Csizmadia. Ab initio program for treatment of related systems: Transferable quantities of localized molecular orbitals. *Advances in Quantum Chemistry*, 40:49–77, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400098.

Kowada:2008:CBM

[KTMA08] Y. Kowada, M. Tatsumisago, T. Minami, and H. Adachi. Chemical bonding of mobile cations in superionic conductors. *Advances in Quantum Chemistry*, 54:255–270, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000202.

Kuklja:2014:QCM

[Kuk14] Maija M. Kuklja. Quantum-chemical modeling of energetic materials: Chemical reactions triggered by defects, deformations, and electronic excitations. *Advances in Quantum Chemistry*, 69:71–145, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459000039.

Kurten:2008:IAS

[KV08] Theo Kurtén and Hanna Vehkamäki. Investigating atmospheric sulfuric acid-water-ammonia particle formation using quantum chemistry. *Advances in Quantum Chemistry*, 55:407–427, 2008.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002195.

Kutzelnigg:1999:ECD

[KvH99] Werner Kutzelnigg and Pasquale von Herigonte. Electron correlation at the dawn of the 21st century. *Advances in Quantum Chemistry*, 36:185–229, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604840.

Kwiatkowski:1986:QMP

[KZR86] Jozef S. Kwiatkowski, Theresa Julia Zielinski, and Robert Rein. Quantum-mechanical prediction of tautomeric equilibria. *Advances in Quantum Chemistry*, 18:85–130, 1986. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600489.

Lindroth:2012:ARS

[LA12] Eva Lindroth and Luca Argenti. Atomic resonance states and their role in charge-changing processes. *Advances in Quantum Chemistry*, 63:247–308, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000059.

Ladik:1973:QTD

[Lad73] János J. Ladik. Quantum theory of DNA: Summary of results and study program. *Advances in Quantum Chemistry*, 7:397–445, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605699.

Luo:1995:RTC

[LÅJM95] Yi Luo, Hans Ågren, Poul Jørgensen, and Kurt V. Mikkelsen. Response theory and calculations of molecular hyperpolarizabilities. *Advances in Quantum Chemistry*, 26:165–237, 1995. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601136. See editorial apology [The96].

Larsson:2002:PTE

[Lar02] Sven Larsson. Partitioning technique in electron transfer and excitation energy transfer. *Advances in Quantum Chemistry*, 41:9–33, 2002. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410441.

Larsson:2017:QCS

[Lar17] Sven Larsson. Quantum chemistry and superconductors. *Advances in Quantum Chemistry*, 74:209–226, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300405.

Ludena:2018:KEP

[LASV18] Eduardo V. Ludeña, Darío Arroyo, Edison X. Salazar, and Jorge Vallejo. The kinetic energy Pauli enhancement factor and its role in determining the shell structure of atoms and molecules. *Advances in Quantum Chemistry*, 76:59–78, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300369.

Laughlin:2009:PTH

[Lau09] Cecil Laughlin. Perturbation theory for a hydrogen-like atom confined within an impenetrable spherical cavity. *Advances in Quantum Chemistry*, 57:203–239, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006108.

Lazzeretti:2004:EFG

[Laz04] Paolo Lazzeretti. Electric field gradient effects on magnetic susceptibility. *Advances in Quantum Chemistry*, 47:177–191, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470105.

Louck:1992:CNM

[LB92] J. D. Louck and L. C. Biedenharn. Canonical and noncanonical methods in applications of group theory to physical problems. *Advances in Quantum Chemistry*, 23:127–204, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600301.

Lami:1999:P

[LB99] Alessandro Lami and Vincenzo Barone. Preface. *Advances in Quantum Chemistry*, 36:xv–xvii, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604748.

Landau:2017:ICP

[LBH+17] Arie Landau, Debarati Bhattacharya, Idan Haritan, Anael Ben-Asher, and Nimrod Moiseyev. Ab initio complex potential energy surfaces from standard quantum chemistry packages. *Advances in Quantum Chemistry*, 74:321–346, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300442`.

Ladik:2001:CCH

[LBV01] Janos Ladik, Ferenc Bogar, and Vick Van Doren. Correlation corrected Hartree–Fock and density functional computations on periodic polymers. *Advances in Quantum Chemistry*, 39:19–34, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605390022`.

Lijnen:2003:EKG

[LC03] Erwin Lijnen and Arnout Ceulemans. Embedding of the K_{10} graph on a surface with seven cross-caps and the icosahedral $H \otimes 2h$ Jahn–Teller surface. *Advances in Quantum Chemistry*, 44:183–198, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440124`.

Lacerda:2022:CFN

[LCC22] Evanildo G. Lacerda, Sylvio Canuto, and Kaline Coutinho. New insights on nonlinear solvatochromism in binary mixture of solvents. *Advances in Quantum Chemistry*, 85:57–79, 2022. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327622000089`.

Lazzeretti:1995:RVS

[LDB95] P. Lazzeretti, M. Defranceschi, and G. Berthier. Rototranslational and virial sum rules for geometrical derivatives of second-order properties and nuclear electric hypershieldings. *Advances in Quantum Chemistry*, 26:1–34, 1995. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601100`.

Liu:1999:EED

[LDNP99] Shubin Liu, Frank De Proft, Ágnes Nagy, and Robert G. Parr. Exchange-energy density functionals as linear combinations of homogeneous functionals of density. *Advances in Quantum Chemistry*, 36:77–91, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604797.

Lill:2004:DCC

[LDP+04] Sten O. Nilsson Lill, Peter Dinér, Daniel Pettersen, Mohamed Amedjkouh, and Per Ahlberg. Development of chiral catalysts for stereoselective synthesis by deprotonations — experimentation in interplay with computational chemistry. *Advances in Quantum Chemistry*, 47:1–22, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470014.

Landau:2001:IHF

[LEK01] Arie Landau, Ephraim Eliav, and Uzi Kaldor. Intermediate Hamiltonian Fock-space coupled-cluster method. *Advances in Quantum Chemistry*, 39:171–188, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390113.

Lengyel:1968:FAQ

[Len68] Bela A. Lengyel. Functional analysis for quantum theorists. *Advances in Quantum Chemistry*, 4:1–82, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603895.

Leroy:1985:TAS

[Ler85] Georges Leroy. The theoretical approach to some chemical problems. *Advances in Quantum Chemistry*, 17:1–95, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603019.

Lester:1975:CCS

[Les75] William A. Lester, Jr. Coupled-channel studies of rotational and vibrational energy transfer by collision. *Advances in Quantum Chemistry*, 9:199–214, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600416.

Levy:1990:CSF

[Lev90] Mel Levy. Constrained-search formulation and recent coordinate scaling in density-functional theory. *Advances in Quan-*

tum Chemistry, 21:69–95, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605924.

Levin:2014:BPE

[Lev14] D. Levin. Behavior preserving extension of univariate and bivariate functions. *Advances in Quantum Chemistry*, 68:19–42, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000022.

Liu:2009:MSO

[LF09] Ya-Jun Liu and Wei-Hai Fang. Multireference and spin-orbit calculations on photodissociations of hydrocarbon halides. *Advances in Quantum Chemistry*, 56:1–29, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004012.

Lowdin:1989:CSA

[LFM89] Per-Olov Löwdin, Piotr Froelich, and Manoj Míshra. On the change of spectra associated with unbounded similarity transformations of a many-particle Hamiltonian and the occurrence of resonance states in the method of complex scaling. Part II. Applications to the Hartree–Fock scheme based on the bi-variational principle. *Advances in Quantum Chemistry*, 20:185–237, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606279.

Li:1999:ACC

[LGJP99] Xiangzhu Li, Ireneusz Grabowski, Karol Jankowski, and Josef Paldus. Approximate coupled cluster methods: Combined reduced multireference and almost-linear coupled cluster methods with singles and doubles. *Advances in Quantum Chemistry*, 36:231–251, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604852.

Lunell:1999:TES

[LGK+99] S. Lunell, J. W. Gauld, R. M. Kadam, Y. Itagaki, and A. Lund. Theoretical and experimental studies of the benzene radical cation: Effects of selective deuteration. *Advances in Quantum Chemistry*, 35:339–355, 1999. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604670.

Li:2020:DIM

[LH20] Run R. Li and Mark R. Hoffmann. On the development and implementation of multi-CPU parallel versions of accurate, general purpose, methods of multireference perturbation theories. *Advances in Quantum Chemistry*, 81:105–141, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300083.

Lestrange:2018:TDC

[LHL18] Patrick J. Lestrange, Mark R. Hoffmann, and Xiaosong Li. Time-dependent configuration interaction using the graphical unitary group approach: Nonlinear electric properties. *Advances in Quantum Chemistry*, 76:295–313, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300618.

Linderberg:1998:BTS

[Lin98] Jan Linderberg. Beyond the transition state treatment. *Advances in Quantum Chemistry*, 32:315–330, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604190.

Linderberg:1999:YOS

[Lin99] Jan Linderberg. Yngve Öhrn, scientist, leader, and friend. *Advances in Quantum Chemistry*, 35:1–19, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604529.

Linderberg:2002:APR

[Lin02] Jan Linderberg. Approximate propagator for the radial Dirac problem. *Advances in Quantum Chemistry*, 41:87–106, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410489.

Linderberg:2005:BPA

[Lin05] Jan Linderberg. Bonding in the perchlorate anion and radical. *Advances in Quantum Chemistry*, 48:1–8, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480016.

Linderberg:2017:FNS

[Lin17a] Jan Linderberg. Features of nearly spherical electronic systems. *Advances in Quantum Chemistry*, 75:243–266, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300242.

Linderberg:2017:NOA

[Lin17b] Jan Linderberg. From numerical orbitals to analytical ones and back. *Advances in Quantum Chemistry*, 74:9–32, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300326.

Lindgren:2017:TDP

[Lin17c] Ingvar Lindgren. Time-dependent perturbation theory with application to atomic systems. *Advances in Quantum Chemistry*, 74:83–105, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300375.

Last:2017:EII

[LJ17] Isidore Last and Joshua Jortner. Electron-ion impact energy transfer in nanoplasmas of Coulomb exploding clusters. *Advances in Quantum Chemistry*, 75:27–52, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300035.

Bigot:2008:ECH

[LJK+08] Eric-Olivier Le Bigot, Ulrich D. Jentschura, Svetlana Kotochigova, Peter J. Mohr, and Barry N. Taylor. Extensive calculations of high-precision energy levels in hydrogen and deuterium through a least-squares adjustment. *Advances in Quantum Chemistry*, 53:253–271, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530133.

List:2013:UFP

[LJKH13] Nanna H. List, Hans Jørgen Aa. Jensen, Jacob Kongsted, and Erik D. Hedegård. A unified framework for the polarizable embedding and continuum methods within multiconfigurational self-consistent field theory. *Advances in Quantum Chemistry*, 66:195–238, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124080997000040.

Ludena:1990:DMF

[LK90] Eduardo V. Ludeña and Jaime Keller. Density matrix foundations of density functional theory: The importance of pure-state N-representability in the derivation of extended Kohn–Sham equations. *Advances in Quantum Chemistry*, 21:47–67, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605912.

Ley-Koo:2009:HAC

[LK09] Eugenio Ley-Koo. The hydrogen atom confined in semi-infinite spaces limited by conoidal boundaries. *Advances in Quantum Chemistry*, 57:79–122, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006078.

Lazur:2013:DWT

[LK13] Volodymyr Yu. Lazur and Mykhaylo V. Khoma. Distorted wave theories for one- and two-electron capture in fast atomic collisions. *Advances in Quantum Chemistry*, 65:363–405, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000133.

Lafifi:2014:TII

[LK14] I. Lafifi and D. Khatmi. Theoretical investigation of the intramolecular H-bonding on tautomerism. *Advances in Quantum Chemistry*, 68:257–268, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000137.

Lo:2005:LLE

[LKD05] John M. H. Lo, Mariusz Klobukowski, and Geerd H. F. Diercksen. Low-lying excited states of the hydrogen molecule in cylindrical harmonic confinement. *Advances in Quantum Chemistry*, 48:59–89, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480065.

Luo:2020:QPF

[LL20] Liaofu Luo and Jun Lv. Quantum protein folding. *Advances in Quantum Chemistry*, 82:181–211, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300010.

Ludena:1998:RDL

[LLBK+98] E. V. Ludeña, R. López-Boada, V. Karasiev, R. Pino, E. Valderrama, J. Maldonado, R. Colle, and J. Hinze. Recent developments in the local-scaling transformation version of density functional theory. *Advances in Quantum Chemistry*, 33:49–70, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604293.

Lowdin:1992:SSG

[LM92] Per-Olov Löwdin and István Mayer. Some studies of the general Hartree–Fock method. *Advances in Quantum Chemistry*, 24:79–114, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860101X.

Lavin:1997:ORR

[LM97] C. Lavín and I. Martin. The oxonium Rydberg radical: Electronic transitions. *Advances in Quantum Chemistry*, 28:205–218, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602166.

Luders:2003:JTD

[LM03] Martin Lüders and Nicola Manini. Jahn–Teller distortions and excitation energies in ${C_{60}}^{n+}$. *Advances in Quantum Chemistry*, 44:289–304, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440185.

Lison:2019:PEC

[LMK19] Artur Lisoń, Monika Musiał, and Stanisław A. Kucharski. Potential energy curves of the NaH molecule and its cation with the Fock space coupled cluster method. *Advances in Quantum Chemistry*, 79:221–237, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300140.

Leon:2001:FSO

[LMSP01] V. M. León, M. Martín, L. Sandoval, and A. Palma. Floquet states and operator algebra. *Advances in Quantum Chemistry*, 39:357–366, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390204.

Linderberg:2017:POL

[LÖBS17] Jan Linderberg, Yngve Öhrn, Erkki J. Brändas, and John R. Sabin. Per-Olov Löwdin. *Advances in Quantum Chemistry*, 74: 1–7, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300302`.

Longo:1999:SDP

[Lon99] Ricardo L. Longo. Spin density properties from the electron propagator: Hyperfine and nuclear spin-spin couplings. *Advances in Quantum Chemistry*, 35:53–76, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604554`.

Linderberg:2002:AQC

[LÖS02] Jan Linderberg, Yngve Öhrn, and John R. Sabin. Advancing quantum chemistry: Per-Olov Löwdin 1916–2000. *Advances in Quantum Chemistry*, 41:x–xv, 2002. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327602410428`.

Lowdin:1964:AQC

[Löw64a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 1 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1964. CODEN AQCHA9. ISSN 0065-3276. xi + 385 pp. LCCN QD453 .A28 v.1. URL `https://www.sciencedirect.com/science/article/pii/S006532760860369X`.

Lowdin:1964:P

[Löw64b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 1: vii–viii, 1964. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860372X`.

Lowdin:1965:AQC

[Löw65a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 2 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1965. CODEN AQCHA9. ISSN 0065-3276. xi + 372 pp. LCCN QD453 .A28 v.2. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600660`.

Lowdin:1965:P

[Löw65b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 2: vii–viii, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600696.

Lowdin:1965:QGA

[Löw65c] Per-Olov Löwdin. Quantum genetics and the aperiodic solid. Some aspects of the biological problems of heredity, mutations, aging and tumors in view of the quantum theory of the DNA molecule. *Advances in Quantum Chemistry*, 2:213–360, 1965. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600763.

Lowdin:1967:AQC

[Löw67a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 3 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1967. CODEN AQCHA9. ISSN 0065-3276. xiv + 392 pp. LCCN QD453 .A28 v.3. URL https://www.sciencedirect.com/science/article/pii/S0065327608600805.

Lowdin:1967:P

[Löw67b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 3: vii–viii, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600830.

Lowdin:1967:QTT

[Löw67c] Per-Olov Löwdin. Quantum theory of time-dependent phenomena treated by the evolution operator technique. *Advances in Quantum Chemistry*, 3:323–381, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600921.

Lowdin:1968:AQC

[Löw68a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 4 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1968. CODEN AQCHA9. ISSN 0065-3276. xiv + 334 pp. LCCN QD453 .A28 v.4. URL https://www.sciencedirect.com/science/article/pii/S0065327608603858.

Lowdin:1968:P

[Löw68b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 4: vii–viii, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603883.

Lowdin:1970:AQC

[Löw70a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 5 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1970. CODEN AQCHA9. ISBN 0-12-034805-5 (hardcover). ISSN 0065-3276. xv + 303 pp. LCCN QD453 .A28 v.5. URL https://www.sciencedirect.com/science/article/pii/S0065327608603317; https://www.sciencedirect.com/science/book/9780120348053.

Lowdin:1970:NP

[Löw70b] Per-Olov Löwdin. On the nonorthogonality problem. *Advances in Quantum Chemistry*, 5:185–199, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603391. Contribution to Professor Ivar Waller's 70-Year Anniversary Volume.

Lowdin:1970:P

[Löw70c] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 5: xi–xii, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603342.

Lowdin:1972:AQC

[Löw72a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 6 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1972. CODEN AQCHA9. ISBN 0-12-034806-3 (hardcover). ISSN 0065-3276. xvi + 413 pp. LCCN QD453 .A28 v.6. URL https://www.sciencedirect.com/science/article/pii/S0065327608605377; https://www.sciencedirect.com/science/book/9780120348060.

Lowdin:1972:P

[Löw72b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 6: xi–xii, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605407.

Lowdin:1973:AQC

[Löw73a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 7 of *Advances in Quantum Chemistry*. Academic Press

Inc., New York, USA, 1973. CODEN AQCHA9. ISBN 0-12-034807-1 (hardcover). ISSN 0065-3276. xvi + 457 pp. LCCN QD453 .A28 v.7. URL https://www.sciencedirect.com/science/article/pii/S0065327608605547; https://www.sciencedirect.com/science/book/9780120348077.

Lowdin:1973:P

[Löw73b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 7: xi–xii, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605572.

Lowdin:1974:AQC

[Löw74a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 8 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1974. CODEN AQCHA9. ISBN 0-12-034808-X (hardcover). ISSN 0065-3276. xvii + 291 pp. LCCN QD453 .A28 v.8. URL https://www.sciencedirect.com/science/article/pii/S0065327608600532; https://www.sciencedirect.com/science/book/9780120348084.

Lowdin:1974:P

[Löw74b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 8: xi–xii, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600568.

Lowdin:1975:AQC

[Löw75a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 9 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1975. CODEN AQCHA9. ISBN 0-12-034809-8 (hardcover). ISSN 0065-3276. x + 304 pp. LCCN QD453 .A28 v.9. URL https://www.sciencedirect.com/science/article/pii/S0065327608600349; https://www.sciencedirect.com/science/book/9780120348091.

Lowdin:1975:P

[Löw75b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 9: ix–x, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600374.

Lowdin:1977:AQC

[Löw77a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 10 of *Advances in Quantum Chemistry*. Academic Press

Inc., New York, USA, 1977. CODEN AQCHA9. ISBN 0-12-034810-1 (hardcover). ISSN 0065-3276. xii + 338 pp. LCCN QD453 .A28 v.10. URL https://www.sciencedirect.com/science/article/pii/S0065327608605730; https://www.sciencedirect.com/science/book/9780120348107.

Lowdin:1977:P

[Löw77b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 10: xi–xii, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605766.

Lowdin:1978:AQC

[Löw78a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 11 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1978. CODEN AQCHA9. ISBN 0-12-034811-X (hardcover). ISSN 0065-3276. xii + 487 pp. LCCN QD453 .A28 v.11. URL https://www.sciencedirect.com/science/article/pii/S0065327608602282; https://www.sciencedirect.com/science/book/9780120348114.

Lowdin:1978:P

[Löw78b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 11: xi–xii, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602312.

Lowdin:1980:AQC

[Löw80a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 12 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1980. CODEN AQCHA9. ISBN 0-12-034812-8 (hardcover). ISSN 0065-3276. x + 325 pp. LCCN QD453 .A28 v.12. URL https://www.sciencedirect.com/science/article/pii/S0065327608603081; https://www.sciencedirect.com/science/book/9780120348121.

Lowdin:1980:MSC

[Löw80b] Per-Olov Löwdin. Molecular structure calculations. *Advances in Quantum Chemistry*, 12:263–316, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603184.

Lowdin:1980:P

[Löw80c] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 12: ix–x, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603111.

Lowdin:1981:AQCa

[Löw81a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 13 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1981. CODEN AQCHA9. ISBN 0-12-034813-6 (hardcover). ISSN 0065-3276. x + 251 pp. LCCN QD453 .A28 v.13. URL https://www.sciencedirect.com/science/article/pii/S0065327608602877; https://www.sciencedirect.com/science/book/9780120348138.

Lowdin:1981:AQCb

[Löw81b] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 14 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1981. CODEN AQCHA9. ISBN 0-12-034814-4 (hardcover). ISSN 0065-3276. x + 248 pp. LCCN QD453 .A28 v.14. URL https://www.sciencedirect.com/science/article/pii/S0065327608603214; https://www.sciencedirect.com/science/book/9780120348145.

Lowdin:1981:Pa

[Löw81c] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 13: ix–x, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602907.

Lowdin:1981:Pb

[Löw81d] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 14: ix–x, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860324X.

Lowdin:1982:AQCa

[Löw82a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 15 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1982. CODEN AQCHA9. ISBN 0-12-034815-2 (hardcover). ISSN 0065-3276. x + 277 pp. LCCN QD453 .A28 v.15. URL https://www.sciencedirect.com/science/article/pii/S0065327608601173; https://www.sciencedirect.com/science/book/9780120348152.

Lowdin:1982:AQCb

[Löw82b] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 16 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1982. CODEN AQCHA9. ISBN 0-12-034816-0 (hardcover). ISSN 0065-3276. x + 285 pp. LCCN

QD453 .A28 v.16. URL https://www.sciencedirect.com/science/article/pii/S0065327608603469; https://www.sciencedirect.com/science/book/9780120348169.

Lowdin:1982:Pa

[Löw82c] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 15: ix–x, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601203.

Lowdin:1982:Pb

[Löw82d] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 16: ix–x, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603494.

Lowdin:1985:AQC

[Löw85a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 17 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1985. CODEN AQCHA9. ISBN 0-12-034817-9 (hardcover). ISSN 0065-3276. x + 344 pp. LCCN QD453 .A28 v.17. URL https://www.sciencedirect.com/science/article/pii/S006532760860297X; https://www.sciencedirect.com/science/book/9780120348176.

Lowdin:1985:P

[Löw85b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 17: ix–x, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603007.

Lowdin:1985:SAH

[Löw85c] Per-Olov Löwdin. Some aspects on the Hamiltonian and Liouvillian formalism, the special propagator methods, and the equation of motion approach. *Advances in Quantum Chemistry*, 17:285–334, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603056.

Lowdin:1986:AQC

[Löw86a] Per-Olov Löwdin, editor. *Advances in Quantum Chemistry*, volume 18 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1986. CODEN AQCHA9. ISBN 0-12-034818-7 (hardcover). ISSN 0065-3276. viii + 350 pp. LCCN

QD453 .A28 v.18. URL https://www.sciencedirect.com/science/article/pii/S0065327608600441; https://www.sciencedirect.com/science/book/9780120348183.

Lowdin:1986:P

[Löw86b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 18: vii–viii, 1986. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600465.

Lowdin:1988:ANF

[Löw88a] Per-Olov Löwdin. Announcement of new format. *Advances in Quantum Chemistry*, 19:xiii, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606127.

Lowdin:1988:CSA

[Löw88b] Per-Olov Löwdin. On the change of spectra associated with unbounded similarity transformations of a many-particle Hamiltonian and the occurrence of resonance states in the method of complex scaling. Part I. General theory. *Advances in Quantum Chemistry*, 19:87–138, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606140.

Lowdin:1988:P

[Löw88c] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 19: xi–xii, 1988. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606115.

Lowdin:1989:P

[Löw89] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 20: xi–xii, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606243.

Lowdin:1991:P

[Löw91] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 22: ix–x, 1991. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603603.

Lowdin:1992:LAL

[Löw92a] Per-Olov Löwdin. On linear algebra, the least square method, and the search for linear relations by regression analysis in quantum chemistry and other sciences. *Advances in Quantum Chemistry*, 23:83–126, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600295.

Lowdin:1992:Pa

[Löw92b] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 23: ix–x, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600271.

Lowdin:1992:Pb

[Löw92c] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 24: ix–x, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600994.

Lowdin:1994:P

[Löw94] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 25: ix–x, 1994. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600167.

Lowdin:1995:P

[Löw95] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 26: ix–x, 1995. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601094.

Lowdin:1996:P

[Löw96a] Per-Olov Löwdin. Preface. *Advances in Quantum Chemistry*, 27: xi–xii, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860249X.

Lowdin:1996:SPL

[Löw96b] Per-Olov Löwdin. Some properties of linear functionals and adjoint operators. *Advances in Quantum Chemistry*, 27:371–397, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602555.

Lowdin:1998:SAB

[Löw98] Per-Olov Löwdin. Some aspects on the Bloch–Lindgren equation and a comparison with the partitioning technique. *Advances in Quantum Chemistry*, 30:415–432, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605201.

Li:1997:PTL

[LP97] Xiangzhu Li and Josef Paldus. Perturbation theory for low-spin open-shell states. *Advances in Quantum Chemistry*, 28:15–32, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860204X`.

Lanzardo:2024:CER

[LPC24] Carmina J. Alturria Lanzardo, Jorge E. Pérez, and Juan C. Cesco. Chapter eight — revisiting the Coulomb potential corresponding to the product of two 1s STOs by using the Laguerre functions. *Advances in Quantum Chemistry*, 89:373–381, 2024. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000692`.

Li:2003:TPG

[LPDB03] Huanming Li, Victor Z. Polinger, Janette L. Dunn, and Colin A. Bates. Tunneling path and ground state crossover in linear $T \otimes (e \oplus t_2)$ and quadratic $G \otimes (g \oplus h)$ Jahn–Teller systems. *Advances in Quantum Chemistry*, 44:89–102, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440069`.

Linder:1972:UTV

[LR72] Bruno Linder and David A. Rabenold. Unified treatment of van der Waals forces between two molecules of arbitrary sizes and electron delocalizations. *Advances in Quantum Chemistry*, 6:203–233, 1972. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605468`.

Lembarki:1998:GCE

[LRCR98] A. Lembarki, H. Razafinjanahary, H. Chermette, and F. Rogemond. Gradient-corrected exchange potential functional with the correct asymptotic behaviour. *Advances in Quantum Chemistry*, 33:105–130, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604323`.

Lindgren:2003:DDF

[LS03] Ingvar Lindgren and Sten Salomonson. Differentiability in density-functional theory. *Advances in Quantum Chemistry*, 43: 95–117, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603430037`.

Li:2007:DTR

[LS07] Xifeng Li and Michael D. Sevilla. DFT treatment of radiation produced radicals in DNA model systems. *Advances in Quantum Chemistry*, 52:59–87, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520040.

Loos:2019:SCE

[LSC19] Pierre-François Loos, Anthony Scemama, and Michel Caffarel. Self-consistent electron-nucleus cusp correction for molecular orbitals. *Advances in Quantum Chemistry*, 79:113–132, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300164.

Lowdin:1988:AQC

[LSZ88] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 19 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1988. CODEN AQCHA9. ISBN 0-12-034819-5 (hardcover). ISSN 0065-3276. xii + 365 pp. LCCN QD453 .A28 v.19. URL https://www.sciencedirect.com/science/article/pii/S0065327608606085; https://www.sciencedirect.com/science/book/9780120348190.

Lowdin:1989:AQC

[LSZ89] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 20 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1989. CODEN AQCHA9. ISBN 0-12-034820-9 (hardcover). ISSN 0065-3276. xiii + 453 pp. LCCN QD453 .A28 v.20. URL https://www.sciencedirect.com/science/article/pii/S0065327608606218; https://www.sciencedirect.com/science/book/9780120348206.

Lowdin:1991:AQC

[LSZ91] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 22 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1991. CODEN AQCHA9. ISBN 0-12-034822-5 (hardcover). ISSN 0065-3276. x + 385 pp. LCCN QD453 .A28 v.22. URL https://www.sciencedirect.com/science/article/pii/S0065327608603573; https://www.sciencedirect.com/science/book/9780120348220.

Lowdin:1992:AQCa

[LSZ92a] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 23 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1992. CODEN AQCHA9. ISBN 0-12-034823-3 (hardcover). ISSN 0065-3276. x + 363 pp. LCCN QD453 .A28 v.23. URL https://www.sciencedirect.com/science/article/pii/S0065327608600246; https://www.sciencedirect.com/science/book/9780120348237.

Lowdin:1992:AQCb

[LSZ92b] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 24 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1992. CODEN AQCHA9. ISBN 0-12-034824-1 (hardcover). ISSN 0065-3276. x + 298 pp. LCCN QD453 .A28 v.24. URL https://www.sciencedirect.com/science/article/pii/S0065327608600969; https://www.sciencedirect.com/science/book/9780120348244.

Lowdin:1994:AQC

[LSZ94] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 25 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1994. CODEN AQCHA9. ISBN 0-12-034825-X (hardcover). ISSN 0065-3276. x + 320 pp. LCCN QD453 .A28 v.25. URL https://www.sciencedirect.com/science/article/pii/S0065327608600131; https://www.sciencedirect.com/science/book/9780120348251.

Lowdin:1995:AQC

[LSZ95] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 26 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1995. CODEN AQCHA9. ISBN 0-12-034826-8 (hardcover). ISSN 0065-3276. x + 367 pp. LCCN QD453 .A28 v.26. URL https://www.sciencedirect.com/science/article/pii/S0065327608601069; https://www.sciencedirect.com/science/book/9780120348268.

Lowdin:1996:AQC

[LSZ96] Per-Olov Löwdin, John R. Sabin, and Michael C. Zerner, editors. *Advances in Quantum Chemistry*, volume 27 of *Ad-*

vances in Quantum Chemistry. Academic Press Inc., New York, USA, 1996. CODEN AQCHA9. ISBN 0-12-034827-6 (hardcover). ISSN 0065-3276. xii + 407 pp. LCCN QD453 .A28 v.27. US$126.00. URL http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348276&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/article/pii/S0065327608602452; https://www.sciencedirect.com/science/book/9780120348275.

Lowdin:1997:AQCb

[LSZ+97a] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki Brändas, Laszlo Kövér, Jun Kawai, and Hirohiko Adachi, editors. *Advances in Quantum Chemistry: Electronic structure of clusters*, volume 29 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1997. CODEN AQCHA9. ISBN 0-12-034829-2 (hardcover). ISSN 0065-3276. xvi + 471 pp. LCCN QD453 .A28 v.29. US$110.00. URL http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348292&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/book/9780120348299. This volume includes the papers presented at the first International Workshop on DV-X Methods. DVA-X '96 took place in the ATOMKI, Debrecen, Hungary, on 2–3 September 1996.

Lowdin:1997:AQCa

[LSZ+97b] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Jacek Karwowski, and Mati Karelson, editors. *Advances in Quantum Chemistry: Recent advances in computational chemistry*, volume 28 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1997. CODEN AQCHA9. ISBN 0-12-034828-4 (hardcover). ISSN 0065-3276. xix + 370 pp. LCCN QD453 .A28 v.28. US$139.95. URL http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348284&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/article/pii/S0065327608601975; https://www.sciencedirect.com/science/book/9780120348282. Papers written to honor Geerd H. F. Diercksen on his 60th birthday. Most of the papers were presented at the symposium Recent Advances in Computational Chemistry (Munich, 20–30 March 1996).

Lowdin:1998:AQCd

[LSZ+98a] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki

Brändas, and Jorge M. Seminario, editors. *Advances in Quantum Chemistry: Density functional theory*, volume 33 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1998. CODEN AQCHA9. ISBN 0-12-034832-2 (hardcover). ISSN 0065-3276. xviii + 398 pp. LCCN QD453 .A28 v.33. US$120.00. URL http://www.academicpress.com/pecs/chem/serials.html; http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348322&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/book/9780120348329.

Lowdin:1998:AQCb

[LSZ+98b] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki Brändas, S. Wilson, J. Maruani, Y. G. Smeyers, P. J. Grout, and R. McWeeny, editors. *Advances in Quantum Chemistry: Quantum systems in chemistry and physics, part I*, volume 31 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1998. CODEN AQCHA9. ISBN 0-12-034831-4 (hardcover). ISSN 0065-3276. xix + 345 pp. LCCN QD453 .A28 v.31. US$99.95. URL http://www.academicpress.com/pecs/chem/serials.html; http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348314&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/article/pii/S0065327608601744; https://www.sciencedirect.com/science/article/pii/S0065327608601756; https://www.sciencedirect.com/science/book/9780120348312. Copyright year 1999.

Lowdin:1998:AQCc

[LSZ+98c] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki Brändas, S. Wilson, J. Maruani, Y. G. Smeyers, P. J. Grout, and R. McWeeny, editors. *Advances in Quantum Chemistry: Quantum systems in chemistry and physics, part II*, volume 32 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1998. CODEN AQCHA9. ISBN 0-12-034833-0 (hardcover). ISSN 0065-3276. xix + 338 pp. LCCN QD453 .A28 v.32. US$99.95. URL http://www.academicpress.com/pecs/chem/serials.html; http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348330&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/article/pii/S0065327608604001; https://www.sciencedirect.com/science/article/pii/S0065327608604220; https://www.sciencedirect.com/science/book/9780120348336.

Lowdin:1999:AQCc

[LSZ+99a] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki Brändas, Alessandro Lami, and Vincenzo Barone, editors. *Advances in Quantum Chemistry: From electronic structure to time-dependent processes: a volume in honor of Giuseppe Del Re*, volume 36 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1999. CODEN AQCHA9. ISBN 0-12-034836-5 (hardcover). ISSN 0065-3276. xxii + 394 pp. LCCN QD453 .A28 v.36. US$145.00. URL `http://www.academicpress.com/pecs/chem/serials.html`; `http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348365&LOCATION=US&FORM=FORM2`; `http://www.hbuk.co.uk/ap/`; `https://www.sciencedirect.com/science/article/pii/S0065327608604712`; `https://www.sciencedirect.com/science/book/9780120348367`.

Lowdin:1999:AQCb

[LSZ+99b] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki Brändas, J. V. Ortiz, and Henry Kurtz, editors. *Advances in Quantum Chemistry: Propagating insight: a tribute to Yngve Öhrn*, volume 35 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1999. CODEN AQCHA9. ISBN 0-12-034835-7 (hardcover). ISSN 0065-3276. x + 380 pp. LCCN QD453 .A28 v.35. US$145.00. URL `http://www.academicpress.com/pecs/chem/serials.html`; `http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348357&LOCATION=US&FORM=FORM2`; `http://www.hbuk.co.uk/ap/`; `https://www.sciencedirect.com/science/article/pii/S0065327608604487`; `https://www.sciencedirect.com/science/book/9780120348350`.

Lowdin:2000:AQCa

[LSZ+00] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, Erkki Brändas, Hirohiko Adachi, Masayuki Uda, and Rika Sekine, editors. *Advances in Quantum Chemistry: DV-Xα for atomic spectroscopy and materials science*, volume 37 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 2000. CODEN AQCHA9. ISBN 0-12-034837-3 (hardcover). ISSN 0065-3276. xvi + 393 pp. LCCN QD453 .A28 v.37. US$145.00. URL `http://www.academicpress.com/pecs/chem/serials.html`; `http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348373&LOCATION=US&FORM=FORM2`; `http://www.hbuk.co.uk/ap/`; `https://www.sciencedirect.com/science/book/9780120348374`. Copyright year 2001.

Lowdin:1999:AQCa

[LSZB99] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 34 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1999. CODEN AQCHA9. ISBN 0-12-034834-9 (hardcover). ISSN 0065-3276. x + 388 pp. LCCN QD453 .A28 v.34. US$125.00. URL http://www.academicpress.com/pecs/chem/serials.html; http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348349&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/article/pii/S0065327608605262; https://www.sciencedirect.com/science/book/9780120348343.

Lowdin:2000:AQCb

[LSZB00] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, and Erkki Brändas, editors. *Advances in Quantum Chemistry: From electronic structure to time-dependent processes*, volume 38 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 2000. CODEN AQCHA9. ISBN 0-12-034838-1 (hardcover). ISSN 0065-3276. ix + 287 pp. LCCN QD453 .A28 v.38. US$145.00. URL http://www.academicpress.com/pecs/chem/serials.html; http://www.apcatalog.com/cgi-bin/AP?ISBN=0120348381&LOCATION=US&FORM=FORM2; http://www.hbuk.co.uk/ap/; https://www.sciencedirect.com/science/book/9780120348381.

Lowdin:1990:AQC

[LSZT90] Per-Olov Löwdin, John R. Sabin, Michael C. Zerner, and Samuel B. Trickey, editors. *Advances in Quantum Chemistry: Density functional theory of many-fermion systems*, volume 21 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 1990. CODEN AQCHA9. ISBN 0-12-034821-7 (hardcover). ISSN 0065-3276. xii + 405 pp. LCCN QD453 .A28 v.21. URL https://www.sciencedirect.com/science/article/pii/S0065327608605857; https://www.sciencedirect.com/science/book/9780120348213.

Labzowsky:1998:RSC

[LT98] L. N. Labzowsky and M. A. Tokman. The reference state Coulomb-Breit QED corrections for the few-electron highly charged ions. *Advances in Quantum Chemistry*, 30:393–413, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605195.

Ludena:2021:COI

[LT21] Eduardo V. Ludeña and Orlando Tapia. On interpretations of quantum mechanics and a novel nonrepresentational framework. *Advances in Quantum Chemistry*, 83:1–29, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000150.

Langreth:1990:RFN

[LV90] David C. Langreth and S. H. Vosko. Response functions and nonlocal approximations. *Advances in Quantum Chemistry*, 21:175–199, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605973.

Liu:2001:SCP

[LvWH+01] Wenjian Liu, Christoph van Wüllen, Young Kyu Han, Yoon Jeong Choi, and Yoon Sup Lee. Spectroscopic constants of Pb and eka-lead compounds: Comparison of different approaches. *Advances in Quantum Chemistry*, 39:325–355, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390198.

Lykos:1964:PEA

[Lyk64] Peter G. Lykos. The pi-electron approximation. *Advances in Quantum Chemistry*, 1:171–201, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603780.

Liu:2003:ECB

[LYM03] Yi Liu, Hiroshi Yukawa, and Masahiko Morinaga. Energetics and chemical bonding of lithium absorbed carbon nanotubes. *Advances in Quantum Chemistry*, 42:315–330, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420583.

Lyons:2008:PLL

[Lyo08] James R. Lyons. Photolysis of long-lived predissociative molecules as a source of mass-independent isotope fractionation: The example of SO_2. *Advances in Quantum Chemistry*, 55:57–74, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002055.

Minaev:2001:SUC

[MÅ01] Boris F. Minaev and Hans Ågren. Spin uncoupling in chemical reactions. *Advances in Quantum Chemistry*, 40:191–211, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400165.

Muino:2004:NSE

[MA04] R. Díez Muiño and A. Arnau. Nonlinear screening and electron capture processes of ions in metals. *Advances in Quantum Chemistry*, 45 (part 1):201–221, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450096.

Mammino:2019:CHB

[Mam19] Liliana Mammino. Complexes of hyperguinones A and B with a Cu^{2+} ion: A DFT study. *Advances in Quantum Chemistry*, 78:83–108, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300340.

Marcus:2008:MIO

[Mar08a] R. A. Marcus. Mass-independent oxygen isotope fractionation in selected systems. mechanistic considerations. *Advances in Quantum Chemistry*, 55:5–19, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760700202X.

Marshall:2008:CST

[Mar08b] Paul Marshall. Computational studies of the thermochemistry of the atmospheric iodine reservoirs HOI and $IONO_2$. *Advances in Quantum Chemistry*, 55:159–175, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002092.

Mizuno:2003:TCP

[MAS03] Masataka Mizuno, Hideki Araki, and Yasuharu Shirai. Theoretical calculation of positron lifetimes for defects in solids. *Advances in Quantum Chemistry*, 42:109–126, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420431.

Matsen:1964:SFQ

[Mat64] F. A. Matsen. Spin-free quantum chemistry. *Advances in Quantum Chemistry*, 1:59–114, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603755.

Matsen:1978:UGM

[Mat78] F. A. Matsen. The unitary group and the many-body problem. *Advances in Quantum Chemistry*, 11:223–250, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602385.

Matsen:1996:FDN

[Mat96] F. A. Matsen. Freeon dynamics: a novel theory of atoms and molecules. *Advances in Quantum Chemistry*, 27:1–70, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602506.

Mayer:1980:SPE

[May80] István Mayer. The spin-projected extended Hartree–Fock method. *Advances in Quantum Chemistry*, 12:189–262, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603172.

Morcillo:2019:SAC

[MBAPS19] Milagros F. Morcillo, Enrique F. Borja, José M. Alcaraz-Pelegrina, and Antonio Sarsa. Stability after confinement of the H atom. *Advances in Quantum Chemistry*, 79:323–336, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300152.

Morpurgo:1999:SMP

[MBM99] Simone Morpurgo, Mario Bossa, and Giorgio O. Morpurgo. Solvent-mediated proton transfer reactions in cytosine: An ab initio study. *Advances in Quantum Chemistry*, 36:169–183, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604839.

Munoz:2007:EDM

[MBO+07] A. Muñoz, F. Blanco, J. C. Oller, J. M. Pérez, and G. García. Energy deposition models at the molecular level in biological systems. *Advances in Quantum Chemistry*, 52:21–57, 2007.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520039.

Mata:2010:QMA

[MC10] Ricardo A. Mata and B. J. Costa Cabral. QM/MM approaches to the electronic spectra of hydrogen-bonding systems with connection to many-body decomposition schemes. *Advances in Quantum Chemistry*, 59:99–144, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761059004X.

Mussard:2018:TDL

[MCA⁺18] Bastien Mussard, Emanuele Coccia, Roland Assaraf, Matthew Otten, Cyrus J. Umrigar, and Julien Toulouse. Time-dependent linear-response variational Monte Carlo. *Advances in Quantum Chemistry*, 76:255–270, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300424.

Mironov:2003:FOP

[MCC03] V. S. Mironov, L. F. Chibotaru, and A. Ceulemans. First-order phase transition in UO_2: The interplay of the $5f^2$–$5f^2$ superexchange interaction and Jahn–Teller effect. *Advances in Quantum Chemistry*, 44:599–616, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440409.

McGuire:2004:UGF

[McG04] E. J. McGuire. The use of Green's functions in the calculation of proton stopping power. *Advances in Quantum Chemistry*, 45 (part 1):159–174, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450072.

Maciel:2008:EPA

[MCG⁺08] Glauciete S. Maciel, David Cappelletti, Gaia Grossi, Fernando Pirani, and Vincenzo Aquilanti. Elementary processes in atmospheric chemistry: Quantum studies of intermolecular dimer formation and intramolecular dynamics. *Advances in Quantum Chemistry*, 55:311–332, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002158.

Musial:2014:PEC

[MCM14] M. Musiał, J. Cembrzyńska, and L. Meissner. Potential energy curves via double ionization potential calculations: Example of HF molecule. *Advances in Quantum Chemistry*, 68: 153–172, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000083.

Malinovskaya:2012:UMR

[MCP12] Svetlana A. Malinovskaya, Tom Collins, and Vishesha Patel. Ultrafast manipulation of Raman transitions and prevention of decoherence using chirped pulses and optical frequency combs. *Advances in Quantum Chemistry*, 64:211–258, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000077.

McWeeny:1998:SQS

[McW98] Roy McWeeny. Separability of quantum systems: a density matrix approach. *Advances in Quantum Chemistry*, 31:15–35, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601811.

McWeeny:1999:EPR

[McW99] Roy McWeeny. On the Einstein–Podolsky–Rosen paradox. *Advances in Quantum Chemistry*, 36:365–384, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860492X.

McWeeny:2001:SS

[McW01] Roy McWeeny. Symbols in science. *Advances in Quantum Chemistry*, 40:1–16, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400062.

Mahapatra:1998:SSM

[MDBM98] Uttam Sinha Mahapatra, Barnali Datta, Barun Bandyopadhyay, and Debashis Mukherjee. State-specific multi-reference coupled cluster formulations: Two paradigms. *Advances in Quantum Chemistry*, 30:163–193, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605079.

Masiello:2005:CFE

[MDÖ05] David Masiello, Erik Deumens, and Yngve Öhrn. On the canonical formulation of electrodynamics and wave mechanics. *Advances in Quantum Chemistry*, 49:249–297, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490061.

Mezey:1996:FGQ

[Mez96] Paul G. Mezey. Functional groups in quantum chemistry. *Advances in Quantum Chemistry*, 27:163–222, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860252X.

Monreal:2004:CEP

[MF04] R. C. Monreal and F. Flores. Charge exchange processes in low energy ion-metal collisions. *Advances in Quantum Chemistry*, 45 (part 1):175–199, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450084.

Manaa:2014:REM

[MF14] M. Riad Manaa and Laurence E. Fried. The reactivity of energetic materials under high pressure and temperature. *Advances in Quantum Chemistry*, 69:221–252, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459000064.

Mitnik:2021:CEG

[MFA21] Dario Mitnik, Ana Laura Frapiccini, and Lorenzo Ugo Ancarani. Generalized Sturmian functions in prolate spheroidal coordinates: Continuum states. *Advances in Quantum Chemistry*, 83:239–253, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000046.

Mendez-Fragoso:2015:HSN

[MFCT15] Ricardo Méndez-Fragoso and Remigio Cabrera-Trujillo. On a hyperbolic solution to the nonlinear Schrödinger equation for a square well potential coupled to a contact impurity at the delocalization threshold. *Advances in Quantum Chemistry*, 71:341–352, 2015. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000143.

Mendez-Fragoso:2011:RAM

[MFLK11] Ricardo Méndez-Fragoso and Eugenio Ley-Koo. Rotations of asymmetric molecules and the hydrogen atom in free and confined configurations. *Advances in Quantum Chemistry*, 62:137–213, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000048.

Mendez-Fragoso:2015:AMT

[MFLK15] Ricardo Méndez-Fragoso and Eugenio Ley-Koo. Angular momentum theory in bases of Lamé spheroconal harmonics. *Advances in Quantum Chemistry*, 71:115–152, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000040.

Moule:2001:CSR

[MFMCN01] D. C. Moule, W. Fraessdorf, C. Muñoz-Caro, and A. Niño. A computer simulation of the ring puckering and oxygen wagging dynamics in the S_0 state of cyclobutanone. *Advances in Quantum Chemistry*, 40:345–359, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400244.

Marx:2020:QCN

[MG20] Gerard Marx and Chaim Gilon. Quantum considerations of neural memory. *Advances in Quantum Chemistry*, 82:13–23, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300071.

Macetti:2021:CTQ

[MG21] Giovanni Macetti and Alessandro Genoni. Quantum mechanics/extremely localized molecular orbital embedding technique: Theoretical foundations and further validation. *Advances in Quantum Chemistry*, 83:269–285, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532762100006X.

Miraglia:2022:AIC

[MG22] Jorge E. Miraglia and Maria Silvia Gravielle. Atomic ionization, capture, and stopping cross sections by ion impact examined with the Benford law. *Advances in Quantum Chemistry*, 85:??, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000107.

Musial:2023:PQC

[MG23a] Monika Musiał and Ireneusz Grabowski, editors. *Polish Quantum Chemistry from Kołos to Now*, volume 87 of *Advances in quantum chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2023. ISBN 0-443-18594-8, 0-443-18595-6 (e-book). ISSN 0065-3276. xv + 420 pp. LCCN QD462. URL https://www.sciencedirect.com/bookseries/advances-in-quantum-chemistry/vol/87/suppl/C.

Musial:2023:P

[MG23b] Monika Musiał and Ireneusz Grabowski. Preface. *Advances in Quantum Chemistry*, 87:xv, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000473.

Mercero:2023:NOF

[MGAUP23] Jose M. Mercero, Rafael Grande-Aztatzi, Jesus M. Ugalde, and Mario Piris. Natural orbital functional theory studies of all-metal aromaticity: the Al_3^- anion. *Advances in Quantum Chemistry*, 88:229–248, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000217.

Masik:1998:MBW

[MH98] J. Mášik and I. Hubač. Multireference Brillouin–Wigner coupled-cluster theory: Single-root approach. *Advances in Quantum Chemistry*, 31:75–104, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601847.

Musial:2021:P

[MH21] Monika Musiał and Philip E. Hoggan. Preface. *Advances in Quantum Chemistry*, 83:xv–xvii, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000289.

Moszynski:1997:TMS

[MHWvdA97] Robert Moszynski, Tino G. A. Heijmen, Paul E. S. Wormer, and Ad van der Avoird. Theoretical modeling of spectra and collisional processes of weakly interacting complexes. *Advances in Quantum Chemistry*, 28:119–140, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602117.

Micha:1974:EHM

[Mic74] David A. Micha. Effective Hamiltonian methods for molecular collisions. *Advances in Quantum Chemistry*, 8:231–287, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600635.

Micha:1999:DMT

[Mic99] David A. Micha. Density matrix treatment of electronic rearrangement. *Advances in Quantum Chemistry*, 35:317–337, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604669.

Micha:2002:FAM

[Mic02] David A. Micha. From few-atom to many-atom quantum dynamics. *Advances in Quantum Chemistry*, 41:139–159, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410519.

Micha:2015:GRT

[Mic15] David A. Micha. Generalized response theory for a photoexcited many-atom system. *Advances in Quantum Chemistry*, 71:195–220, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000118.

Micha:2017:QPM

[Mic17] David A. Micha. Quantum partitioning methods for few-atom and many-atom dynamics. *Advances in Quantum Chemistry*, 74:107–128, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300363.

Micha:2022:EDM

[Mic22] David A. Micha. Energy deposition in a many-atom system with dissipative dynamics. *Advances in Quantum Chemistry*, 85:??,

2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000016.

Mintmire:2022:CND

[Min22] J. W. Mintmire. Density-functional methods for extended helical systems. *Advances in Quantum Chemistry*, 85:177–196, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000065.

Miyazaki:2003:CER

[Miy03] T. Miyazaki. Comment from experimental results on "Was H_2^- Observed in Solid H_2? A Theoretical Answer"(H. U. Suter, B. Engels and S. Lunell, Adv. Quantum Chem. **40** (2001) 133). *Advances in Quantum Chemistry*, 43:217–218, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430074. See [SEL01].

Morrison:2018:NHF

[MK18] John C. Morrison and Jacek Kobus. Numerical Hartree Fock and many-body calculations for diatomic molecules. *Advances in Quantum Chemistry*, 76:103–116, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300588.

Musial:2023:RAM

[MK23] Monika Musiał and Stanisław A. Kucharski. Review — advanced models of coupled-cluster theory for the ground, excited, and ionized states. *Advances in Quantum Chemistry*, 87:73–113, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000254.

Musial:2004:AIO

[MKB04] Monika Musiał, Stanislaw A. Kucharski, and Rodney J. Bartlett. Approximate inclusion of the T_3 and R_3 operators in the equation-of-motion coupled-cluster method. *Advances in Quantum Chemistry*, 47:209–222, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470129.

Morishita:1997:ESO

[MKH+97] Masao Morishita, Koichiro Koyama, Akinori Hatamoto, Masahiko Morinaga, and Hirohiko Adachi. Electronic states of oxygen ions of molten slags used for iron and steel making. *Advances in Quantum Chemistry*, 29:285–296, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602750.

Morishita:2000:MIC

[MKK+00] Masao Morishita, Koichiro Koyama, Tadayoshi Kikko, Masahiko Morinaga, and Hirohiko Adachi. A method of incorporating the composition into the calculation of the OKa X-ray emission spectrum of the glassy state SiO_2–Na_2O binary slag with the DV-Xα molecular orbital calculation. *Advances in Quantum Chemistry*, 37:163–177, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370125.

Maruani:2001:MCT

[MKK+01] J. Maruani, A. Khoudir, A. Kuleff, M. Tronc, G. Giorgi, and C. Bonnelle. A method of combined treatment for the evaluation of core excitation energies in molecules involving heavy atoms: application to CrF_6, MoF_6, and WF_6. *Advances in Quantum Chemistry*, 39:307–324, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390186.

Mercouris:2010:SSE

[MKN10] Theodoros Mercouris, Yannis Komninos, and Cleanthes A. Nicolaides. The state-specific expansion approach to the solution of the polyelectronic time-dependent schrödinger equation for atoms and molecules in unstable states. *Advances in Quantum Chemistry*, 60:333–405, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600068.

Malinovskaya:2018:APC

[ML18] Svetlana A. Malinovskaya and Gengyuan Liu. Adiabatic passage control methods for ultracold alkali atoms and molecules via chirped laser pulses and optical frequency combs. *Advances in Quantum Chemistry*, 77:241–294, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300029.

Martin:1998:VET

[MLPD+98] I. Martin, C. Lavín, Y. Pérez-Delgado, J. Karwowski, and G. H. F. Diercksen. Vertical electron transitions in Rydberg radicals. *Advances in Quantum Chemistry*, 32:181–196, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860413X.

Molina:1998:PMP

[MLR+98] L. M. Molina, M. J. López, A. Rubio, L. C. Balbás, and J. A. Alonso. Pure and mixed Pb clusters of interest for liquid ionic alloys. *Advances in Quantum Chemistry*, 33:329–348, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604438.

Mishra:1996:CSA

[MM96] Manoj K. Mishra and Milan N. Medikeri. Characterization of shape and Auger resonances using the dilated one electron propagator method. *Advances in Quantum Chemistry*, 27:223–295, 1996. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602531.

Mishra:1999:SPC

[MM99] Vandana K. Mishra and Manoj K. Mishra. Selective photodynamic control of chemical reactions: a Rayleigh–Ritz variational approach. *Advances in Quantum Chemistry*, 35:261–281, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604645.

Montanari:2013:DFI

[MM13] Claudia C. Montanari and Jorge E. Miraglia. The dielectric formalism for inelastic processes in high-energy ion-matter collisions. *Advances in Quantum Chemistry*, 65:165–201, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000078.

Mendez:2018:LEH

[MMM18] Alejandra M. P. Mendez, Dario M. Mitnik, and Jorge E. Miraglia. Local effective Hartree Fock potentials obtained by the depurated inversion method. *Advances in Quantum Chemistry*, 76:117–132, 2018. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300709.

Mendez:2019:CPU

[MMM19] Alejandra M. P. Mendez, Darío M. Mitnik, and Jorge E. Miraglia. Collision processes using effective potentials. *Advances in Quantum Chemistry*, 79:179–200, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300267.

Mendez:2022:CEE

[MMM22] Alejandra M. P. Mendez, Darío M. Mitnik, and Claudia C. Montanari. The electronic stopping power of heavy targets. *Advances in Quantum Chemistry*, 85:157–175, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000090.

Musial:2016:PEC

[MMSK16] Monika Musiał, Anna Motyl, Patrycja Skupin, and Stanisław A. Kucharski. Potential energy curves for the low-lying electronic states of KLi with Fock space coupled cluster method. *Advances in Quantum Chemistry*, 72:201–216, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000209.

Mineva:1998:DFO

[MNR+98] T. Mineva, N. Neshev, N. Russo, E. Sicilia, and M. Toscano. Density functional orbital reactivity indices: Fundamentals and applications. *Advances in Quantum Chemistry*, 33:273–292, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604402.

Mozos:2003:DFT

[MOB+03] JoséLuis Mozos, Pablo Ordejón, Mads Brandbyge, Jeremy Taylor, and Kurt Stokbro. Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. *Advances in Quantum Chemistry*, 42:299–314, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420571.

Mohr:1998:QEF

[Moh98] Peter Mohr. Quantum electrodynamics and the fundamental constants. *Advances in Quantum Chemistry*, 30:77–97, 1998.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605043.

Mohr:2008:QSP

[Moh08] Peter J. Mohr. The quantum SI: a possible new international system of units. *Advances in Quantum Chemistry*, 53:27–36, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530030.

Monkhorst:2005:GME

[Mon05] Hendrik J. Monkhorst. GW method for extended, periodic systems with a mixed Slater-orbital/plane-wave basis and Fourier transform techniques. *Advances in Quantum Chemistry*, 48:35–45, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480041.

Mukherjee:1989:UCE

[MP89] Debashis Mukherjee and Sourav Pal. Use of cluster expansion methods in the open-shell correlation problem. *Advances in Quantum Chemistry*, 20:291–373, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606292.

Muller-Plathe:1997:CQC

[MP97] Florian Müller-Plathe. Combining quantum chemistry and molecular simulation. *Advances in Quantum Chemistry*, 28:81–87, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602087.

Matras:2022:CTA

[MP22] Morten Matras and John W. Perram. Artificial intelligence and E-learning. *Advances in Quantum Chemistry*, 85:31–38, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000028.

Mitxelena:2019:AAN

[MPU19] Ion Mitxelena, Mario Piris, and Jesus M. Ugalde. Advances in approximate natural orbital functional theory. *Advances in Quantum Chemistry*, 79:155–177, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300176.

Mejia-Rodriguez:2015:HFV

[MRHdCK15] Daniel Mejía-Rodríguez, Xiaomin Huang, Jorge M. del Campo, and Andreas M. Köster. Hybrid functionals with variationally fitted exact exchange. *Advances in Quantum Chemistry*, 71:41–67, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000167`.

Marino:1999:DFC

[MRS+99] T. Marino, N. Russo, E. Sicilia, M. Toscano, and T. Mineva. Density functional computations and mass spectrometric measurements. can this coupling enlarge the knowledge of gas-phase chemistry? *Advances in Quantum Chemistry*, 36:93–120, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604803`.

McWeeny:1965:TPC

[MS65] R. McWeeny and E. Steiner. The theory of pair-correlated wave functions. *Advances in Quantum Chemistry*, 2:93–117, 1965. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600738`.

Margenau:1967:NIF

[MS67] H. Margenau and J. Stamper. Nonadditivity of intermolecular forces. *Advances in Quantum Chemistry*, 3:129–160, 1967. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760860088X`.

Majernikova:2003:GSQ

[MS03] Eva Majerníková and S. Shpyrko. Ground state of quantum Jahn–Teller model: Selftrapping vs. correlated phonon-assisted tunneling. *Advances in Quantum Chemistry*, 44:631–648, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603440422`.

Musial:2017:PEC

[MSM17] Monika Musiał, Patrycja Skupin, and Anna Motyl. Potential energy curves of NaK molecule from all-electron multireference-coupled cluster calculations. *Advances in Quantum Chemistry*, 73:249–262, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000192`.

Matsuo:2003:TAX

[MST+03] Shuji Matsuo, Kaori Shirozu, Yuichi Tateishi, Hisanobu Wakita, and Takushi Yokoyama. Theoretical analysis of XANES for aqueous aluminum salt solutions. *Advances in Quantum Chemistry*, 42:407–417, 2003. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327603420649`.

Micha:2004:QCD

[MT04] David A. Micha and Brian Thorndyke. The quantum-classical density operator for electronically excited molecular systems. *Advances in Quantum Chemistry*, 47:293–314, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604470178`.

Mukoyama:1997:XRE

[MTA97] Takeshi Mukoyama, Kazuo Taniguchi, and Hirohiko Adachi. X-ray emission in molecules. *Advances in Quantum Chemistry*, 29:297–328, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602762`.

Mukoyama:2000:KSK

[MTA00] Takeshi Mukoyama, Kazuo Taniguchi, and Hirohiko Adachi. Kβ /Kα X-ray intensity ratios in 3d elements by photoionization and electron-capture decay. *Advances in Quantum Chemistry*, 37:139–151, 2000. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327600370101`.

Mathar:2004:ESM

[MTS04] Richard J. Mathar, S. B. Trickey, and John R. Sabin. Electronic stopping and momentum density of diamond from first-principles treatment of the microscopic dielectric function. *Advances in Quantum Chemistry*, 45 (part 1):277–288, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604450126`.

Mukoyama:2003:NAE

[MU03] Takeshi Mukoyama and Masayuki Uda. A new approach to electron transition during inner-shell ionization. *Advances in Quantum Chemistry*, 42:283–297, 2003. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760342056X.

Muramatsu:2003:TPS

[Mur03] Yasuji Muramatsu. Theoretically predicted soft X-ray emission and absorption spectra of graphitic-structured BC_2N. *Advances in Quantum Chemistry*, 42:353–361, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420601.

Muramatsu:2008:SXR

[Mur08] Yasuji Muramatsu. Soft X-ray absorption spectral analysis of amorphous carbon and carbon black using the DV–Xα method. *Advances in Quantum Chemistry*, 54:209–218, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000160.

Martin:2001:SRS

[MVL01] I. Martín, A. M. Velasco, and C. Lavín. Similarities in the Rydberg spectra of the isovalent radicals CH_3 and SiH_3. *Advances in Quantum Chemistry*, 39:145–162, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390095.

Moncrieff:1998:DGB

[MW98] D. Moncrieff and S. Wilson. Distributed Gaussian basis sets in correlation energy studies: The second order correlation energy for the ground state of the hydrogen molecule. *Advances in Quantum Chemistry*, 31:157–172, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601872.

Matsuo:2008:XRA

[MW08] Shuji Matsuo and Hisanobu Wakita. X-ray absorption spectroscopic study on polymerization of aqueous aluminate by DV–Xα molecular-orbital method. *Advances in Quantum Chemistry*, 54:193–207, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000159.

Mohn:2005:RTB

[MWL+05] Chris E. Mohn, David J. D. Wilson, Ola B. Lutnæs, Trygve Helgaker, and Kenneth Ruud. The rotational g tensor as a benchmark for *Ab Initio* molecular property calculations. *Advances in Quantum Chemistry*, 50:77–90, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500054.

Morishita:2008:TSM

[MYM08] Masao Morishita, Hiroaki Yamamoto, and Yasutomo Matsumoto. Thermal spectroscopy of magnesium-zinc binary compounds near absolute zero Kelvin: Coefficient of the electronic contribution to heat capacity and density of states in the vicinity of the Fermi level. *Advances in Quantum Chemistry*, 54:1–12, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000019.

Matsuo:2000:SSB

[MYW00] Shuji Matsuo, Toshio Yamaguchi, and Hisanobu Wakita. A structural study of dibromo(1,4,8,11-tetraazacyclotetradecane) copper(II) and diaqua(1,4,8,11-tetraazacyclotetradecane) copper(II) difluoride four hydrate complexes in crystal and in aqueous solution by X-ray absorption near edge structure measurements and DV-Xα calculations. *Advances in Quantum Chemistry*, 37:153–162, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370113.

Nagy:2004:SPE

[NA04] István Nagy and Barnabás Apagyi. Stopping power of an electron gas for heavy unit charges: Models in the kinetic approximation. *Advances in Quantum Chemistry*, 46 (part 2):267–291, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460109.

Nagy:2019:CMA

[NA19] Istvan Nagy and Inigo Aldazabal. Correlated model atom in a time-dependent external field: Sign effect in the energy shift. *Advances in Quantum Chemistry*, 80:23–45, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300358.

Nagy:1997:DFT

[Nag97] Ágnes Nagy. Density functional theory for excited states. *Advances in Quantum Chemistry*, 29:159–178, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602683.

Nagy:2001:EPS

[Nag01] Á. Nagy. Effective potential of a single excited state along the adiabatic path. *Advances in Quantum Chemistry*, 39:35–46, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390034.

Nagy:2003:TES

[Nag03] Á. Nagy. Theories for excited states. *Advances in Quantum Chemistry*, 42:363–381, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420613.

Nakagawa:2000:BIE

[Nak00] Katsumi Nakagawa. Bond index and energy partition method for DV-Xα. *Advances in Quantum Chemistry*, 37:365–374, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370265.

Nalewajski:2000:CCI

[Nal00] Roman F. Nalewajski. Coupling constant integration analysis of density functionals for subsystems. *Advances in Quantum Chemistry*, 38:217–277, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600380054.

Nalewajski:2003:ESC

[Nal03] Roman F. Nalewajski. Electronic structure and chemical reactivity: Density functional and information-theoretic perspectives. *Advances in Quantum Chemistry*, 43:119–184, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430049.

Nalewajski:2006:PIB

[Nal06] Roman F. Nalewajski. Probing the interplay between electronic and geometric degrees-of-freedom in molecules and reactive systems. *Advances in Quantum Chemistry*, 51:235–305,

2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510068.

Nalewajski:2009:MLD

[Nal09] Roman F. Nalewajski. Multiple, localized, and delocalized/conjugated bonds in the orbital communication theory of molecular systems. *Advances in Quantum Chemistry*, 56:217–250, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760800405X.

Nalewajski:2023:ECR

[Nal23] Roman F. Nalewajski. Electronic convection in resultant information-theoretic description of molecular states and communications. *Advances in Quantum Chemistry*, 87:115–139, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000102.

Nadykto:2008:CQC

[NAY+08] Alexey B. Nadykto, Anas Al Natsheh, Fangqun Yu, Kurt V. Mikkelsen, and Jason Herb. Computational quantum chemistry: a new approach to atmospheric nucleation. *Advances in Quantum Chemistry*, 55:449–478, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002213.

Nicolaides:2010:P

[NB10] Cleanthes A. Nicolaides and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 60:ix–x, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600135.

Nasiri:2020:TMN

[NBA20] Saeed Nasiri, Sergiy Bubin, and Ludwik Adamowicz. Treating the motion of nuclei and electrons in atomic and molecular quantum mechanical calculations on an equal footing: Non-Born–Oppenheimer quantum chemistry. *Advances in Quantum Chemistry*, 81:143–166, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300149.

Nicolaides:2010:AQC

[NBS10] Cleanthes A. Nicolaides, Erkki Brändas, and John R. Sabin, editors. *Advances in Quantum Chemistry: Unstable states in the* *continuous Spectra, part 1*, volume 60 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2010. CODEN AQCHA9. ISBN 0-12-380900-2 (hardcover). ISSN 0065-3276. xiii + 549 pp. LCCN QD453 .A28 v.60. URL https://www.sciencedirect.com/science/book/9780123809001. Founding editor Per-Olov Löwdin (1916–2000).

Nicolaides:2012:USC

[NBS12] Cleanthes A. Nicolaides, Erkki Brändas, and John R. Sabin, editors. *Unstable states in the continuous spectra. Part II, Interpretation, theory, and applications*, volume 63 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2012. CODEN AQCHA9. ISBN 0-12-397009-1 (e-book). ISSN 0065-3276. ix + 348 pp. LCCN QC451 .U57 2012 .v63. URL https://www.sciencedirect.com/science/book/9780123970091. Founding editor Per-Olov Löwdin (1916–2000).

Nakano:2003:DJT

[NeMM03] Motohiro Nakano, Gen etsu Matsubayashi, and Takasuke Matsuo. Dynamic Jahn–Teller character of manganese(III) spin-crossover complex [Mn(taa)] (H_3 taa = tris(1-(2-azolyl)-2-azabuten-4-yl)amine). *Advances in Quantum Chemistry*, 44:617–630, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440410.

Nesbet:1967:AHF

[Nes67] R. K. Nesbet. Approximate Hartree–Fock calculations on small molecules. *Advances in Quantum Chemistry*, 3:1–24, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600854.

Nesbet:1975:TLE

[Nes75] R. K. Nesbet. Theory of low energy electron scattering by complex atoms. *Advances in Quantum Chemistry*, 9:215–297, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600428.

Nesbet:1998:SCP

[Nes98] R. K. Nesbet. In search of the correlation potential. *Advances in Quantum Chemistry*, 33:71–83, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860430X.

Nesbet:2003:LNP

[Nes03] Robert K. Nesbet. Local and nonlocal potential functions in density functional theory. *Advances in Quantum Chemistry*, 43:1–23, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430013.

Nekovee:1998:QMC

[NFW+98] Maziar Nekovee, W. M. C. Foulkes, A. J. Williamson, G. Rajagopal, and R. J. Needs. A quantum Monte Carlo approach to the adiabatic connection method. *Advances in Quantum Chemistry*, 33:189–207, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604360.

Nanba:2003:CBS

[NHM03] Tokuro Nanba, Tatsuya Hagiwara, and Yoshinari Miura. Chemical bonding state of sodium silicates. *Advances in Quantum Chemistry*, 42:187–198, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420480.

Nakajima:2003:NES

[NHYU03] Y. Nakajima, M. Hoshino, D. Yamashita, and M. Uda. Near edge structures of Mg-, Co-, Cu- and Zn-tetraphenylporphyrins measured by PESA and calculated with DV–Xα. *Advances in Quantum Chemistry*, 42:399–405, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420637.

Nicolaides:2010:TSS

[Nic10] Cleanthes A. Nicolaides. Theory and state-specific methods for the analysis and computation of field-free and field-induced unstable states in atoms and molecules. *Advances in Quantum Chemistry*, 60:163–267, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600044.

Nicolaides:2011:SPS

[Nic11] Cleanthes A. Nicolaides. State- and property-specific quantum chemistry. *Advances in Quantum Chemistry*, 62:35–103, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000085.

Nicolaides:2017:RCF

[Nic17] Cleanthes A. Nicolaides. Resonances in the continuum, field-induced nonstationary states, and the state- and property-specific treatment of the many-electron problem. *Advances in Quantum Chemistry*, 74:149–181, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300296.

Nikitin:1970:TNT

[Nik70] E. E. Nikitin. The theory of nonadiabatic transitions: Recent development with exponential models. *Advances in Quantum Chemistry*, 5:135–184, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860338X.

Nakatsugawa:2003:ESS

[NIO03] H. Nakatsugawa, E. Iguchi, and Y. Oohara. Electronic structures of $Sr_{1-x}La_xRuO_3$. *Advances in Quantum Chemistry*, 42:215–222, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420510.

Nakamatsu:2000:ACX

[NM00] Hirohide Nakamatsu and Takeshi Mukoyama. Assignment of Ce XANES spectra for CeO_2 and $CeO_{1.75}$ and effect of oxygen vacancy. *Advances in Quantum Chemistry*, 37:111–125, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370083.

Nikolaev:2003:MEH

[NM03] A. V. Nikolaev and K. H. Michel. Many electron- and hole terms of molecular ions ${C_{60}}^{n\pm}$. *Advances in Quantum Chemistry*, 44:305–312, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440197.

Nooijen:2009:RFD

[Noo09] Marcel Nooijen. Reflections on formal density functional theory. *Advances in Quantum Chemistry*, 56:181–216, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004048.

Nordling:1998:FDA

[Nor98] Carl Nordling. Four decades of atomic physics: a review of Ingvar Lindgren's career until now. *Advances in Quantum Chemistry*, 30:1–4, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604992.

Nikiforov:2003:CDE

[NP03] A. E. Nikiforov and S. E. Popov. Cooperative dynamical effect in rhombohedral $LaMnO_3$. *Advances in Quantum Chemistry*, 44:587–598, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440392.

Nalewajski:2011:BDO

[NSM11] Roman F. Nalewajski, Dariusz Szczepanik, and Janusz Mrozek. Bond differentiation and orbital decoupling in the orbital-communication theory of the chemical bond. *Advances in Quantum Chemistry*, 61:1–48, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000012.

Nishiyama:2020:NQB

[NTT20] Akihiro Nishiyama, Shigenori Tanaka, and Jack A. Tuszynski. Nonequilibrium quantum brain dynamics. *Advances in Quantum Chemistry*, 82:159–180, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300186.

Ohrn:1981:MEP

[ÖB81] Y. Öhrn and G. Born. Molecular electron propagator theory and calculations. *Advances in Quantum Chemistry*, 13:1–88, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602919.

Oddershede:2022:JSS

[OB22a] Jens Oddershede and Erkki J. Brändas. *Jack Sabin, Scientist and Friend*, volume 85 of *Advances in quantum chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2022. ISBN 0-323-99188-2. ISSN 0065-3276. xvii + 387 pp. LCCN QD462.

Oddershede:2022:P

[OB22b] Jens Oddershede and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 85:xv–xvii, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000284.

Oprea:2023:CMP

[OB23] Diana-Gabriela Oprea and Hugh G. A. Burton. Convergence of Møller–Plesset perturbation theory for excited reference states. *Advances in Quantum Chemistry*, 88:249–271, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000126.

Olsen:2017:MPS

[OBHM17] Stine T. Olsen, Asbjørn Bols, Thorsten Hansen, and Kurt V. Mikkelsen. Molecular properties of sandwiched molecules between electrodes and nanoparticles. *Advances in Quantum Chemistry*, 75:53–102, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300266.

Oddershede:1978:PPC

[Odd78] Jens Oddershede. Polarization propagator calculations. *Advances in Quantum Chemistry*, 11:275–352, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602403.

Oddershede:2005:PJH

[Odd05] Jens Oddershede. Poul Jørgensen and his science. *Advances in Quantum Chemistry*, 50:xxi–xxix, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500194.

OLeary:1975:UTM

[ODE75] Brian O'Leary, Brian J. Duke, and James E. Eilers. Utilization of transferability in molecular orbital theory. *Advances in Quantum Chemistry*, 9:1–67, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600386.

Ozdogan:2017:ACM

[OE17] Telhat Ozdogan and Melek Eraslan. Analytic calculation of momentum distribution and Compton profiles of atoms using Hartree–Fock–Roothaan method: Applications to atoms $2 \leq Z \leq 10$. *Advances in Quantum Chemistry*, 73:173–182, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000532.

Ozdogan:2023:HFR

[ÖEO23] Telhat Özdoğan, Melek Eraslan, and Metin Orbay. Hartree–Fock–Roothaan theory of molecular Compton profiles via the position space method. *Advances in Quantum Chemistry*, 88:151–158, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000266.

Ohno:1967:MOC

[Ohn67] Kimio Ohno. Molecular orbital calculations of π electron systems. *Advances in Quantum Chemistry*, 3:239–322, 1967. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860091X.

Ohrn:2002:DDM

[Öhr02] Yngve Öhrn. Density, density matrix, or propagator. *Advances in Quantum Chemistry*, 41:35–49, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410453.

Ohrn:2005:JLS

[Öhr05] Yngve Öhrn. Jan Linderberg, scientist, teacher, friend. *Advances in Quantum Chemistry*, 50:xiii–xix, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500182.

Ohrn:2015:TDT

[Öhr15] Yngve Öhrn. Time-dependent treatment of molecular processes. *Advances in Quantum Chemistry*, 70:69–109, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327614000033.

Ohrn:2016:DEG

[Öhr16] Yngve Öhrn. The Dirac equation as guide to nonrelativistic Hamiltonian terms. *Advances in Quantum Chemistry*, 72:217–227, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000337.

Ohrn:2017:TDV

[Öhr17] Yngve Öhrn. The time-dependent variational principal in quantum mechanics and its application. *Advances in Quantum Chemistry*, 74:33–51, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300314.

Olsen:2005:P

[OJ05] Jeppe Olsen and Hans Jørgen Aagaard Jensen. Preface. *Advances in Quantum Chemistry*, 50:xi, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500170.

Olsen:2011:MPT

[OK11] Jógvan Magnus Haugaard Olsen and Jacob Kongsted. Molecular properties through polarizable embedding. *Advances in Quantum Chemistry*, 61:107–143, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123860132000036.

Oliveira:1990:DFT

[Oli90] L. N. Oliveira. Density functional treatment of excited states. *Advances in Quantum Chemistry*, 21:135–154, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860595X.

Oliva:2012:ELB

[Oli12] Josep M. Oliva. Energy landscapes in boron chemistry: Bottom-top approach toward design of novel molecular architectures. *Advances in Quantum Chemistry*, 64:105–119, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000041.

Ogurtsov:2003:JTO

[OM03] I. Ya. Ogurtsov and V. Mirzac. On the Jahn–Teller origin of the phosphorus molecule P_4 activation by one- and two-electron reduction. *Advances in Quantum Chemistry*, 44:401–412, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440264.

Onishi:2012:QCF

[Oni12] Taku Onishi. Quantum chemistry in functional inorganic materials. *Advances in Quantum Chemistry*, 64:31–81, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000028.

Onishi:2015:QCP

[Oni15] Taku Onishi. Quantum chemistry in proton-conductors: Mechanism elucidation and materials design. *Advances in Quantum Chemistry*, 70:31–67, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327614000070.

Onoe:2000:AND

[Ono00] Jun Onoe. Atomic-number dependence of relativistic effects on chemical bonding. *Advances in Quantum Chemistry*, 37:311–323, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370228.

Ovchinnikov:1982:PNR

[OO82] A. A. Ovchinnikov and M. Ya. Ovchinnikova. Problems of nonlinear radiationless processes in chemistry. *Advances in Quantum Chemistry*, 16:161–227, 1982. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603536.

Ogilvie:2005:DFA

[OO05] J. F. Ogilvie and J. Oddershede. Dunham's formalism applied in reduction of spectral data of diatomic molecules and the development of computational spectrometry. *Advances in Quantum Chemistry*, 48:253–317, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480168.

Ozay:2013:RRR

[ÖÖ13] S. Özay and E. Öztekin. Recurrence relations for radial parts of STOs and evaluation of overlap integrals via the Fourier transform methods. *Advances in Quantum Chemistry*, 67:245–265, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000108.

Oddershede:2017:CCD

[OOSS17] Jens Oddershede, John F. Ogilvie, Stephan P. A. Sauer, and John R. Sabin. Continuum contributions to dipole oscillator-strength sum rules for hydrogen in finite basis sets. *Advances in Quantum Chemistry*, 75:229–241, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300229.

Oliferenko:2006:ACE

[OPPZ06] Alexander A. Oliferenko, Sergei A. Pisarev, Vladimir A. Palyulin, and Nikolai S. Zefirov. Atomic charges via electronegativity equalization: Generalizations and perspectives. *Advances in Quantum Chemistry*, 51:139–156, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510044.

Orlando:2023:ENE

[ORL23] Roberto Orlando, Pina Romaniello, and Pierre-François Loos. Exploring new exchange-correlation kernels in the Bethe–Salpeter equation: a study of the asymmetric Hubbard dimer. *Advances in Quantum Chemistry*, 88:183–211, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000229.

Ortiz:1999:TEO

[Ort99] J. V. Ortiz. Toward an exact one-electron picture of chemical bonding. *Advances in Quantum Chemistry*, 35:33–52, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604542.

Ortiz:2022:CSR

[Ort22] J. V. Ortiz. Recent progress in electron-propagator, extended-Koopmans-theorem and self-consistent-field approaches to the interpretation and prediction of electron binding energies. *Advances in Quantum Chemistry*, 85:109–155, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000041.

Oddershede:2005:JOA

[OS05] Lene B. Oddershede and John R. Sabin. Jens Oddershede — adventurer in quantum chemistry. *Advances in Quantum Chemistry*, 48:xvii–xix, 2005. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480272.

Ogasawara:1997:ACH

[OTA97] Kazuyoshi Ogasawara, Isao Tanaka, and Hirohiko Adachi. Analysis of core-hole effect in cation $L_{2,3}$-edge of MgO, α-Al_2O_3 and SiO_2 based on DV–Xα cluster calculations. *Advances in Quantum Chemistry*, 29:441–466, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860283X.

Oba:2003:ESA

[OTA03] Fumiyasu Oba, Isao Tanaka, and Hirohiko Adachi. Electronic states associated with bond disorder at ZnO grain boundaries. *Advances in Quantum Chemistry*, 42:175–186, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420479.

Ogasawara:2008:CSF

[OW08] Kazuyoshi Ogasawara and Shinta Watanabe. Current situation and future development of discrete variational multielectron method. *Advances in Quantum Chemistry*, 54:297–314, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000226.

Ogasawara:2000:SEC

[OYI+00] Kazuyoshi Ogasawara, Masateru Yamamoto, Takugo Ishii, Hidenori Ida, Hirohiko Adachi, and Isao Tanaka. Separation of the effects of charge transfer, covalency, and electron correlations on the multiplet structure of ruby based on first-principles cluster calculations. *Advances in Quantum Chemistry*, 37:69–83, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370058.

Palma:2004:OAF

[Pal04] Alejandro Palma. Operator algebra: From Franck–Condon to Floquet theory. *Advances in Quantum Chemistry*, 47:223–238, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470130.

Paul:2013:ASP

[Pau13] Helmut Paul. On the accuracy of stopping power codes and ion ranges used for hadron therapy. *Advances in Quantum Chemistry*, 65:39–61, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780123964557000029`.

Peyerimhoff:1975:SES

[PB75] Sigrid D. Peyerimhoff and Robert J. Buenker. A series of electronic spectral calculations using nonempirical CI techniques. *Advances in Quantum Chemistry*, 9:69–104, 1975. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608600398`.

Piecuch:1999:ENC

[PB99] Piotr Piecuch and Rodney J. Bartlett. EOMXCC: a new coupled-cluster method for electronic excited states. *Advances in Quantum Chemistry*, 34:295–380, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605341`.

Perera:2005:RRT

[PB05] S. Ajith Perera and Rodney J. Bartlett. A reinvestigation of Ramsey's theory of NMR coupling. *Advances in Quantum Chemistry*, 48:434–467, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605480235`.

Perera:2014:GMM

[PB14] Ajith Perera and Rodney J. Bartlett. Geometric metastability in molecules as a way to enhance energy storage. *Advances in Quantum Chemistry*, 69:147–170, 2014. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128003459000040`.

Poznanski:2020:PMP

[PB20a] Roman R. Poznański and Erkki J. Brändas. Panexperiential materialism: a physical exploration of qualitativeness in the brain. *Advances in Quantum Chemistry*, 82:301–367, 2020. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327620300198`.

Poznanski:2020:P

[PB20b] Roman R. Poznański and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 82:xi–xvii, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300411.

Poznanski:2020:QBL

[PB20c] Roman R. Poznański and Erkki J. Brändas, editors. *Quantum Boundaries of Life*, volume 82 of *Advances in quantum chemistry*. Academic Press Inc., New York, USA, 2020. CODEN AQCHA9. ISBN 0-12-822616-1 (e-book), 0-12-822639-0 (hardcover). ISSN 0065-3276. xvii + 378 pp. LCCN QD453 .A28 82.

Pichl:2004:CCS

[PBK04] Lukás Pichl, Robert J. Buenker, and Mineo Kimura. Calculation of cross-sections for proton and antiproton stopping in molecules. *Advances in Quantum Chemistry*, 46 (part 2):165–193, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460079.

Persson:2002:QCS

[PBOL02] P. Persson, R. Bergström, L. Ojamäe, and S. Lunell. Quantum-chemical studies of metal oxides for photoelectrochemical applications. *Advances in Quantum Chemistry*, 41:203–263, 2002. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327602410544.

Paldus:1975:TID

[PČ75] J. Paldus and J. Čížek. Time-independent diagrammatic approach to perturbation theory of Fermion systems. *Advances in Quantum Chemistry*, 9:105–197, 1975. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600404.

Paidarova:2010:USQ

[PD10] Ivana Paidarová and Philippe Durand. Unstable states: From quantum mechanics to statistical physics. *Advances in Quantum Chemistry*, 60:1–49, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600019.

Ponra:2023:BES

[PEMC23] Abraham Ponra, Anne Justine Etindele, Ousmanou Motapon, and Mark E. Casida. Binding energies for successive addition reactions of $^{\bullet}$OH to C_{60}: a laboratory for testing frontier molecular orbital theory. *Advances in Quantum Chemistry*, 88:351–372, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000199.

Perdew:1990:SCS

[Per90] John P. Perdew. Size-consistency, self-interaction correction, and derivative discontinuity in density functional theory. *Advances in Quantum Chemistry*, 21:113–134, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605948.

Percus:1998:AFR

[Per98a] J. K. Percus. Auxiliary field representation of fermion kinetic energy density functional. *Advances in Quantum Chemistry*, 33:131–150, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604335.

Persson:1998:CLS

[Per98b] J. R. Persson. Collinear laser spectroscopy on radioactive isotopes. *Advances in Quantum Chemistry*, 30:335–342, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605158.

Perram:2017:CVD

[Per17] John W. Perram. Criterion for the validity of D'Alembert's equations of motion. *Advances in Quantum Chemistry*, 75:103–116, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300333.

Pereira:2020:CQI

[Per20] Alfredo Pereira. Classical-quantum interfaces in living neural tissue supporting conscious functions. *Advances in Quantum Chemistry*, 82:213–252, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300174.

Petrongolo:1998:RTD

[Pet98] Carlo Petrongolo. Recent theoretical developments in conical-intersection effects in triatomic spectra. *Advances in Quantum Chemistry*, 32:127–144, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604104.

Perdew:1998:WDG

[PEZB98] John P. Perdew, Matthias Ernzerhof, Ales Zupan, and Kieron Burke. Why density-gradient corrections improve atomization energies and barrier heights. *Advances in Quantum Chemistry*, 33:1–9, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604268.

Paul:2007:ISP

[PGJ07] Helmut Paul, Oksana Geithner, and Oliver Jäkel. The influence of stopping powers upon dosimetry for radiation therapy with energetic ions. *Advances in Quantum Chemistry*, 52:289–306, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520131.

Pitarke:2004:NBS

[PGN04] J. M. Pitarke, I. G. Gurtubay, and V. U. Nazarov. Nonlinear, band-structure, and surface effects in the interaction of charged particles with solids. *Advances in Quantum Chemistry*, 45 (part 1):247–275, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604450114.

Pernal:2017:EEM

[PGP17] Katarzyna Pernal, Nikitas I. Gidopoulos, and Ewa Pastorczak. Excitation energies of molecules from ensemble density functional theory: Multiconfiguration approaches. *Advances in Quantum Chemistry*, 73:199–229, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000283.

Paragi:1997:CEB

[PGV97] G. Paragi, I. K. Gyémánt, and Zs. Varga. Core-electron binding energy shifts in aluminium. *Advances in Quantum Chemistry*, 29:433–439, 1997. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602828.

Phillips:1998:AOL

[Phi98] William D. Phillips. Atoms in optical lattices: Cooling, trapping and squeezing atoms with light. *Advances in Quantum Chemistry*, 30:19–39, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605018.

Pawlowski:2005:CMA

[PJH05] Filip Pawlowski, Poul Jørgensen, and Christof Hättig. Cauchy moments of Ne, Ar, and Kr atoms calculated using the approximate Coupled Cluster Triples model CC3. *Advances in Quantum Chemistry*, 48:9–21, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480028.

Pavlov:2001:RDM

[PKYM01] R. L. Pavlov, A. I. Kuleff, P. Tz. Yotov, and J. Maruani. Reduced density-matrix treatment of spin-spin interaction terms in many-electron systems. *Advances in Quantum Chemistry*, 39:295–305, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390174.

Politzer:1998:DFC

[PL98] Peter Politzer and Pat Lane. Density functional calculations of reaction energetics: Application to alkyl azide decomposition. *Advances in Quantum Chemistry*, 33:293–302, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604414.

PerezdelValle:2001:LEE

[PLA01] C. Perez del Valle, R. Lefebvre, and O. Atabek. Localization of energy exchanges in field-assisted double-barrier resonant tunneling. *Advances in Quantum Chemistry*, 40:179–190, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400153.

Politzer:2014:DPS

[PM14] Peter Politzer and Jane S. Murray. Detonation performance and sensitivity: a quest for balance. *Advances in Quan-*

tum Chemistry, 69:1–30, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459000015.

Perera:2016:IPL

[PM16] Ajith Perera and Jorge A. Morales. Implementation of a parallel linear-response coupled-cluster-theory module in ACES III: First application to the static polarizabilities of the C_{20} isomers and of the biphospholylidene dioxide and disulfide oligomers. *Advances in Quantum Chemistry*, 72:29–60, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000350.

Puchalski:2023:RKW

[PMK23] Mariusz Puchalski, Robert Moszyński, and Jacek Komasa. Review — from the Kołos–Wolniewicz calculations to the quantum-electrodynamic treatment of the hydrogen molecule: Competition between theory and experiment. *Advances in Quantum Chemistry*, 87:1–36, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000370.

Polinger:2003:TJT

[Pol03] Victor Polinger. Tunneling in Jahn–Teller systems and multidimensional WKB approximation. *Advances in Quantum Chemistry*, 44:59–88, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440057.

Porter:2004:BEC

[Por04] L. E. Porter. The Barkas-effect correction to Bethe–Bloch stopping power. *Advances in Quantum Chemistry*, 46 (part 2):91–119, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460043.

Pullman:1968:AES

[PP68] Alberte Pullman and Bernard Pullman. Aspects of the electronic structure of the purine and pyrimidine bases of the nucleic acids and of their interactions. *Advances in Quantum Chemistry*, 4:267–325, 1968. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603962.

Pendrill:1998:APL

[PR98] L. R. Pendrill and L. Robertsson. Atomic physics and the laser metrology of time and length. *Advances in Quantum Chemistry*, 30:445–468, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605225.

Pecul:2005:ICO

[PR05] Magdalena Pecul and Kenneth Ruud. The ab initio calculation of optical rotation and electronic circular dichroism. *Advances in Quantum Chemistry*, 50:185–212, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500091.

Paidarova:2005:CDQ

[PS05a] Ivana Paidarová and Stephan P. A. Sauer. Calculations of dipole and quadrupole polarizability radial functions for LiH and HF: a comparison of different linear response methods. *Advances in Quantum Chemistry*, 48:185–208, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480132.

Perram:2005:EFW

[PS05b] John W. Perram and Edgar R. Smith. Elliptic functions of the worst kind: Non-linear quantisation of the classical spherical pendulum. *Advances in Quantum Chemistry*, 48:111–125, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480089.

Pluta:2021:CFT

[PS21] Tadeusz Pluta and Grzegorz Skrzyński. Time-dependent DFT calculations of the dipole moment and polarizability for excited states. *Advances in Quantum Chemistry*, 83:305–327, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000071.

Pierdominici-Sottile:2010:AMQ

[PSAP10] Gustavo Pierdominici-Sottile, Sebastián Fernández Alberti, and Juliana Palma. Applications of mixed-quantum/classical trajectories to the study of nuclear quantum effects in chemical reactions and vibrational relaxation processes. *Advances in Quantum Chemistry*, 59:247–282, 2010. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590087.

Persson:1998:RCP

[PSS98] Hans Persson, Sten Salomonson, and Per Sunnergren. Regularization corrections to the partial-wave renormalization procedure. *Advances in Quantum Chemistry*, 30:379–392, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605183.

Perez:2013:TEP

[PTBH13] J. E. Pérez, O. E. Taurian, A. Bouferguene, and P. E. Hoggan. On a transformation for the electrostatic potential, generated by the product of two 1*s* Slater type orbitals, giving an efficient expression. *Advances in Quantum Chemistry*, 67:65–71, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000042.

Perez:2013:BSC

[PTC+13] J. E. Pérez, O. E. Taurian, J. C. Cesco, A. E. Rosso, C. C. Denner, C. J. Alturria Lanzardo, F. S. Ortiz, and A. Bouferguene. A basis sets composed of only 1*s* Slater orbitals and 1*s* Gaussian orbitals to perform molecular calculations, SCF-LCAO approach. *Advances in Quantum Chemistry*, 67:55–64, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000030.

Politzer:2012:PRF

[PTLGOM12] Peter Politzer, Alejandro Toro-Labbé, Soledad Gutiérrez-Oliva, and Jane S. Murray. Perspectives on the reaction force. *Advances in Quantum Chemistry*, 64:189–209, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000065.

Pullman:1977:QMA

[Pul77] Bernard Pullman. Quantum-mechanical approach to the conformational basis of molecular pharmacology. *Advances in Quantum Chemistry*, 10:251–328, 1977. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605821.

Patil:2009:PCH

[PV09] S. H. Patil and Y. P. Varshni. Properties of confined hydrogen and helium atoms. *Advances in Quantum Chemistry*, 57:1–24, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609006054.

Pu:2008:AHL

[PWZ+08] Liang Pu, Qing Wang, Yong Zhang, Qiang Miao, Yang soo Kim, and Zhibing Zhang. Architecture of hydrates and local structure of acetic acid aqueous solution: Ab initio calculations and Car–Parrinello molecular dynamics (CPMD) simulations on hydrogen-bonding rings, network, and intra-hydrate protonation in multi-hydrates of acetic acid monomer. *Advances in Quantum Chemistry*, 54:271–295, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000214.

Pyykko:1978:RQC

[Pyy78] Pekka Pyykkö. Relativistic quantum chemistry. *Advances in Quantum Chemistry*, 11:353–409, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602415.

Quiney:2001:DEA

[QGW01] H. M. Quiney, V. N. Glushkov, and S. Wilson. The Dirac equation in the algebraic approximation. VII. A comparison of molecular finite difference and finite basis set calculations using distributed Gaussian basis sets. *Advances in Quantum Chemistry*, 39:241–259, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390150.

Quiney:1998:IRQ

[QSG98] H. M. Quiney, H. Skaane, and I. P. Grant. Ab initio relativistic quantum chemistry: Four components good, two components bad! *Advances in Quantum Chemistry*, 32:1–49, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604050.

Quack:2020:FAS

[QSW20] Martin Quack, Georg Seyfang, and Gunther Wichmann. Fundamental and approximate symmetries, parity violation and tunneling in chiral and achiral molecules. *Advances in Quantum Chemistry*, 81:51–104, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300150.

Randazzo:2019:TDS

[RA19] Juan Martín Randazzo and Lorenzo Ugo Ancarani. Two-dimensional Sturmian basis set for bound state calculations. *Advances in Quantum Chemistry*, 79:79–95, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300243.

Ramsey:1998:SHC

[Ram98] Norman F. Ramsey. Spectroscopy with highly coherent radiation. *Advances in Quantum Chemistry*, 30:5–18, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605006.

Ramsey:2008:MRC

[Ram08] Norman F. Ramsey. Magnetic resonance contributions to other sciences. *Advances in Quantum Chemistry*, 53:1–6, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530017.

Randic:2018:AR

[Ran18] Milan Randić. Aromaticity revisited. *Advances in Quantum Chemistry*, 77:167–199, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300734.

Ryzhkov:2008:TES

[RAR+08] A. Ryzhkov, P. A. Ariya, F. Raofie, H. Niki, and G. W. Harris. Theoretical and experimental studies of the gas-phase cl-atom initiated reactions of benzene and toluene. *Advances in Quantum Chemistry*, 55:275–295, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002134.

Roman-Ancheyta:2015:ACS

[RAR15] Ricardo Román-Ancheyta and José Récamier. Approximate coherent states for nonlinear systems. *Advances in Quantum Chemistry*, 71:299–322, 2015. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000076.

Raychev:1995:QGA

[Ray95] Peter Raychev. Quantum groups: Application to nuclear and molecular spectroscopy. *Advances in Quantum Chemistry*, 26:239–357, 1995. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601148.

Ruud:2020:P

[RB20] Kenneth Ruud and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 81:xiii–xvii, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300290.

Rizzo:2005:BCB

[RC05] Antonio Rizzo and Sonia Coriani. Birefringences: a challenge for both theory and experiment. *Advances in Quantum Chemistry*, 50:143–184, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760550008X.

Rubinsztein-Dunlop:1998:OTA

[RDNFH98] H. Rubinsztein-Dunlop, T. A. Nieminen, M. E. J. Friese, and N. R. Heckenberg. Optical trapping of absorbing particles. *Advances in Quantum Chemistry*, 30:469–492, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605237.

Rein:1973:PPI

[Rei73] Robert Rein. On physical properties and interactions of polyatomic molecules: With application to molecular recognition in biology. *Advances in Quantum Chemistry*, 7:335–396, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605687.

Ruiz:2013:DA

[RF13] M. B. Ruiz and A. M. Frolov. On the β^--decay in the ^{8}Li and ^{9}Li atoms. *Advances in Quantum Chemistry*, 67:267–289, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012411544600011X.

Raimondi:1998:NIV

[RFG+98] M. Raimondi, A. Famulari, E. Gianinetti, M. Sironi, R. Specchio, and I. Vandoni. New ab initio VB interaction potential for molecular dynamics simulation of liquid water. *Advances in Quantum Chemistry*, 32:263–284, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604177.

Rastelli:1999:RDD

[RGA99] Augusto Rastelli, Remo Gandolfi, and Mirko Sarzi Amadè. Regioselectivity and diastereoselectivity in the 1,3-dipolar cycloadditions of nitrones with acrylonitrile and maleonitrile: The origin of endo/exo selectivity. *Advances in Quantum Chemistry*, 36:151–167, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604827.

Rivarola:2013:CDW

[RGFC13] Roberto D. Rivarola, Mariel E. Galassi, Pablo D. Fainstein, and Christophe Champion. Computation of distorted wave cross sections for high-energy inelastic collisions of heavy ions with water molecules. *Advances in Quantum Chemistry*, 65:231–267, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000091.

Remacle:2004:SGC

[RK04] F. Remacle and E. S. Kryachko. Small gold clusters $Au_{5 \leq n \leq 8}$ and their cationic and anionic cousins. *Advances in Quantum Chemistry*, 47:423–464, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470233.

Ruiz:2017:STB

[RLF17] María Belén Ruiz, Federico Latorre, and Alexei M. Frolov. Singlet and triplet bound state spectra in the four-electron Be-like atomic systems. *Advances in Quantum Chemistry*, 73:119–138, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000210.

Roos:2004:ESO

[RM04] Björn O. Roos and Per-Åke Malmqvist. On the effects of spin-orbit coupling on molecular properties: Dipole moment and polarizability of PbO and spectroscopic constants for the ground and excited states. *Advances in Quantum Chemistry*, 47:37–49, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604470038`.

Roggero:2017:CIM

[RMMP17] Alessandro Roggero, Paolo Mori, Abhishek Mukherjee, and Francesco Pederiva. Configuration interaction Monte Carlo with coupled clusters wave functions. *Advances in Quantum Chemistry*, 73:315–332, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000544`.

Rahim:2014:CIE

[RMN+14] M. Rahim, F. Madi, L. Nouar, S. Haiahem, D. Fateh, and D. Khatmi. β-cyclodextrin interaction with edaravone: Molecular modeling study. *Advances in Quantum Chemistry*, 68:269–278, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128005361000149`.

Raghunath:2014:ICK

[RNL14] Putikam Raghunath, N. T. Nghia, and Ming-Chang Lin. Ab initio chemical kinetics of key processes in the hypergolic ignition of hydrazine and nitrogen tetroxide. *Advances in Quantum Chemistry*, 69:253–301, 2014. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128003459000076`.

Rosen:1997:TTY

[Ros97] Arne Rosén. Twenty to thirty years of DV–Xα calculations: a survey of accuracy and applications. *Advances in Quantum Chemistry*, 29:1–47, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602622`.

Rosen:1998:PTT

[Ros98] Arne Rosén. A periodic table in three dimensions: a sightseeing tour in the nanometer world. *Advances in Quantum Chemistry*, 30:235–272, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605109.

Rourk:2020:FNE

[Rou20] Christopher J. Rourk. Functional neural electron transport. *Advances in Quantum Chemistry*, 82:25–111, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300162.

Ruedenberg:1972:MED

[RP72] Klaus Ruedenberg and Ronald D. Poshusta. Matrix elements and density matrices for many-electron spin eigenstates built from orthonormal orbitals. *Advances in Quantum Chemistry*, 6:267–298, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605481.

Roggero:2018:ECI

[RP18] Alessandro Roggero and Francesco Pederiva. Extension of the configuration interaction Monte Carlo method to atoms and molecules. *Advances in Quantum Chemistry*, 76:241–253, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300631.

Ramasesha:2000:DMR

[RPSB00] S. Ramasesha, Swapan K. Pati, Z. Shuai, and J. L. Brédas. The density matrix renormalization group method: Application to the low-lying electronic states in conjugated polymers. *Advances in Quantum Chemistry*, 38:121–215, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600380042.

Raab:2005:EET

[RR05] Juraj Raab and Björn O. Roos. Excitation energies for transition metal atoms — a comparison between coupled cluster methods and second-order perturbation theory. *Advances in Quantum Chemistry*, 48:421–433, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480223.

Rosado-Reyes:2008:CSR

[RRMAF08] Claudette M. Rosado-Reyes, Mónica Martínez-Avilés, and Joseph S. Francisco. Computational study of the reaction of n-bromopropane with OH radicals and Cl atoms. *Advances in Quantum Chemistry*, 55:215–244, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002110.

Ruiz:2021:CNH

[RSP21] María Belén Ruiz, James S. Sims, and Bholanath Padhy. High-precision Hy-CI and E-Hy-CI studies of atomic and molecular properties. *Advances in Quantum Chemistry*, 83:171–208, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000125.

Ruiz:2018:CIS

[RT18] María Belén Ruiz and Robert Tröger. Configuration interaction study of the 3P ground state of the carbon atom. *Advances in Quantum Chemistry*, 76:223–238, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300667.

Rinkevicius:2005:RDF

[RTV05] Zilvinas Rinkevicius, Lyudmyla Telyatnyk, and Olav Vahtras. Restricted density functional response theory for open-shell systems. *Advances in Quantum Chemistry*, 50:271–288, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500133.

Ruiz:2023:AEH

[Rui23] María Belén Ruiz. Analytical evaluation of Hylleraas-CI Coulomb and hybrid two-center integrals over Slater-type orbitals. *Advances in Quantum Chemistry*, 88:99–118, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000308.

Rychlewski:1998:ECF

[Ryc98] Jacek Rychlewski. Explicitly correlated functions in molecular quantum chemistry. *Advances in Quantum Chemistry*, 31:173–199, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601884.

Rutkowska-Zbik:2023:MAT

[RZTSW23] Dorota Rutkowska-Zbik, Renata Tokarz-Sobieraj, and Małgorzata Witko. Methane activation and transformation to ethylene on Mo-(oxy)carbide as a key step of CH_4 to aromatics. *Advances in Quantum Chemistry*, 87:319–333, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327623000084`.

Silverstone:2023:SCS

[SÁ23a] Harris J. Silverstone and Gabriel Álvarez. Summation of convergent series by educated match. *Advances in Quantum Chemistry*, 88:29–34, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000345`.

Stanke:2023:NNB

[SA23b] Monika Stanke and Ludwik Adamowicz. Nonrelativistic non-Born–Oppenheimer approach for calculating atomic and molecular spectra using all-particle explicitly correlated Gaussian functions. *Advances in Quantum Chemistry*, 87:263–279, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327623000072`.

Saalmann:2001:RDM

[Saa01] Ulf Saalmann. Reaction dynamics of metallic clusters colliding with atoms. *Advances in Quantum Chemistry*, 40:305–322, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400220`.

Sabin:1997:EDS

[Sab97] John R. Sabin. Energy deposition of swift alphas in neon: An electron nuclear dynamics study. *Advances in Quantum Chemistry*, 28:107–118, 1997. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602105`.

Sabin:2000:MCZ

[Sab00] John R. Sabin. Obituary — Michael Charles Zerner. *Advances in Quantum Chemistry*, 38:viii–ix, 2000. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327600380017`.

Sabin:2007:TSI

[Sab07] John R. Sabin. Theoretical studies of the interaction of radiation with biomolecules. *Advances in Quantum Chemistry*, 52:1–3, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520015.

Sabin:2011:AQCa

[Sab11] John R. Sabin, editor. *Advances in Quantum Chemistry*, volume 61 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2011. CODEN AQCHA9. ISBN 0-12-386013-X (hardcover). ISSN 0065-3276. xiv + 386 pp. LCCN QD453 .A28 v.61. URL https://www.sciencedirect.com/science/book/9780123860132. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2014:EMH

[Sab14a] John R. Sabin, editor. *Energetic materials*, volume 69 of *Advances in quantum chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2014. CODEN AQCHA9. ISBN 0-12-800345-6 (hardcover), 0-12-800450-9 (e-book). ISSN 0065-3276. xii + 344 pp. LCCN TP270 .E54 2014. URL https://www.sciencedirect.com/science/book/9780128003459.

Sabin:2014:P

[Sab14b] John R. Sabin. Preface. *Advances in Quantum Chemistry*, 69:ix, 2014. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459100005.

Sabin:2015:AQC

[Sab15] John R. Sabin, editor. *Advances in Quantum Chemistry*, volume 70. Academic Press Inc., New York, USA, 2015. CODEN AQCHA9. ISBN 0-12-801891-7 (hardcover), 0-12-801915-8 (e-book). ISSN 0065-3276. LCCN QD462. URL https://www.sciencedirect.com/science/book/9780128018910.

Sakai:2003:FPA

[Sak03a] Yoshiyuki Sakai. First-principles analysis of tunneling spectra for rutile TiO_2 (110) surface with oxygen vacancies. *Advances in Quantum Chemistry*, 42:429–438, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420662.

Sakuma:2003:GBP

[Sak03b] Taketo Sakuma. Grain boundary plasticity and failure in oxide ceramics at high temperatures. *Advances in Quantum Chemistry*, 42:23–33, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760342039X.

Salmon:1974:GES

[Sal74] William I. Salmon. Genealogical electronic spin eigenfunctions and antisymmetric many-electron wavefunctions generated directly from Young diagrams. *Advances in Quantum Chemistry*, 8:37–94, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600593.

Stobinska:2010:QEO

[SAL10] M. Stobińska, G. Alber, and G. Leuchs. Quantum electrodynamics of one-photon wave packets. *Advances in Quantum Chemistry*, 60:457–483, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600081.

Salam:2011:MQE

[Sal11] A. Salam. Molecular quantum electrodynamics of radiation-induced intermolecular forces. *Advances in Quantum Chemistry*, 62:1–34, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000012.

Sannigrahi:1992:IMO

[San92] A. B. Sannigrahi. *Ab Initio* molecular orbital calculations of bond index and valency. *Advances in Quantum Chemistry*, 23:301–351, 1992. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600325.

Sanders:1998:RDH

[San98] Frank C. Sanders. Recent developments in high-precision computational methods for simple atomic and molecular systems. *Advances in Quantum Chemistry*, 33:369–387, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604451.

Saue:2005:SIN

[Sau05a] Trond Saue. Spin-interactions and the non-relativistic limit of electrodynamics. *Advances in Quantum Chemistry*, 48:383–405, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760548020X.

Sauer:2005:RTH

[Sau05b] Stephan P. A. Sauer. The rotational g tensor of HF, H_2O, NH_3, and CH_4: a comparison of correlated ab initio methods. *Advances in Quantum Chemistry*, 48:469–490, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480247.

Sekino:1999:EPC

[SB99] Hideo Sekino and Rodney J. Bartlett. On the extensivity problem in coupled-cluster property evaluation. *Advances in Quantum Chemistry*, 35:149–173, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604591.

Sabin:2002:AQC

[SB02] John S. Sabin and Erkki J. Brändas, editors. *Advances in Quantum Chemistry: a tribute to the life and work of Per-Olov Löwdin*, volume 41 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 2002. CODEN AQCHA9. ISBN 0-12-034841-1 (hardcover). ISSN 0065-3276. xvi + 270 pp. LCCN QD453 .A28 v.41. URL https://www.sciencedirect.com/science/book/9780120348411. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2003:AQCb

[SB03] John S. Sabin and Erkki J. Brändas, editors. *Advances in Quantum Chemistry*, volume 43 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2003. CODEN AQCHA9. ISBN 0-12-034843-8 (hardcover). ISSN 0065-3276. xii + 224 pp. LCCN QD453 .A28 v.43. URL https://www.sciencedirect.com/science/book/9780120348435. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2005:AQCb

[SB05] John S. Sabin and Erkki J. Brändas, editors. *Advances in Quantum Chemistry*, volume 49 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2005. CODEN

AQCHA9. ISBN 0-12-034847-0 (hardcover). ISSN 0065-3276. xxx + 486 pp. LCCN QD453 .A28 v.49. URL https://www.sciencedirect.com/science/book/9780120348473. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2006:AQC

[SB06] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 51 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2006. CODEN AQCHA9. ISBN 0-12-034851-9 (hardcover). ISSN 0065-3276. x + 322 pp. LCCN QD453 .A28 v.51. URL https://www.sciencedirect.com/science/bookseries/00653276/51. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2007:AQC

[SB07] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry: Theory of the interaction of radiation with biomolecules*, volume 52 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2007. CODEN AQCHA9. ISBN 0-12-034852-7 (hardcover), 0-08-046740-7 (e-book). ISSN 0065-3276. xii + 323 pp. LCCN QD453 .A28 v.52. URL https://www.sciencedirect.com/science/book/9780120348527. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2009:AQCa

[SB09a] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 56 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2009. CODEN AQCHA9. ISBN 0-12-374780-5 (hardcover), 0-08-088785-6 (e-book). ISSN 0065-3276. xi + 333 pp. LCCN QD453 .A28 v.56. URL https://www.math.utah.edu/pub/tex/bib/advquantumchem.bib; https://www.sciencedirect.com/science/book/9780123747808; https://www.sciencedirect.com/science/bookseries/00653276/56. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2009:P

[SB09b] John R. Sabin and Erkki Brändas. Preface. *Advances in Quantum Chemistry*, 56:ix, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608004103.

Sabin:2011:AQCb

[SB11] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 62 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. xiv + 354 pp. LCCN QD453 .A28 v.62. URL `https://www.sciencedirect.com/science/book/9780123864772`. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2012:AQC

[SB12a] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 64 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2012. CODEN AQCHA9. ISBN 0-12-396498-9 (hardcover). ISSN 0065-3276. xii + 266 pp. LCCN QC451 .U57 2012 .v64. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2012:P

[SB12b] John R. Sabin and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 64:ix, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780123964984000144`.

Sabin:2013:AQC

[SB13a] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 66. Elsevier Academic Press, Amsterdam, The Netherlands, 2013. CODEN AQCHA9. ISBN 0-12-408099-5 (hardcover). ISSN 0065-3276. ix + 248 pp. LCCN QC451 .U57 2013 .v66.

Sabin:2013:Cb

[SB13b] John R. Sabin and Erkki J. Brändas. Contributors. *Advances in Quantum Chemistry*, 66:ix, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780124080997099931`.

Sabin:2013:Ca

[SB13c] John R. Sabin and Erkki J. Brändas. Copyright. *Advances in Quantum Chemistry*, 66:iv, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780124080997099955`.

Sabin:2013:P

[SB13d] John R. Sabin and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 66:vii–viii, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124080997100005.

Sabin:2013:SP

[SB13e] John R. Sabin and Erkki J. Brändas. Series page. *Advances in Quantum Chemistry*, 66:ii, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B978012408099709992X.

Sabin:2015:P

[SB15] John R. Sabin and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 70:ix–xi, 2015. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327614000161.

Sabin:2017:AQCa

[SB17a] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry: Löwdin volume*, volume 74. Elsevier, Amsterdam, The Netherlands, 2017. CODEN AQCHA9. ISBN 0-12-809988-7 (hardcover), 0-12-810400-7. ISSN 0065-3276. xiii + 392 pp. LCCN QD453 .A28 v.74 2017. URL https://www.sciencedirect.com/science/bookseries/00653276/74.

Sabin:2017:AQCb

[SB17b] John R. Sabin and Erkki Brändas, editors. *Advances in quantum chemistry. Ratner volume*, volume 75 of *Advances in quantum chemistry*. Academic Press Inc., New York, USA, 2017. CODEN AQCHA9. ISBN 0-12-812888-7. ISSN 0065-3276. xii + 272 pp. LCCN QD453 .A28 75. URL https://www.sciencedirect.com/science/bookseries/00653276/75.

Sabin:2017:Pa

[SB17c] John R. Sabin and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 74:xiii–xiv, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300187.

Sabin:2017:Pb

[SB17d] John R. Sabin and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 75:xi–xii, 2017. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300515.

Sabin:2018:AQC

[SB18a] John R. Sabin and Erkki Brändas, editors. *Advances in Quantum Chemistry*, volume 77 of *Advances in quantum chemistry*. Elsevier, Amsterdam, The Netherlands, 2018. CODEN AQCHA9. ISBN 0-12-813710-X. ISSN 0065-3276. xii + 432 pp. LCCN QC176.8.E4. URL https://www.sciencedirect.com/science/journal/00653276/77.

Sabin:2018:P

[SB18b] John R. Sabin and Erkki J. Brändas. Preface. *Advances in Quantum Chemistry*, 77:xi–xii, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300133.

Sabin:2003:AQCa

[SBA+03] John R. Sabin, Erkki J. Brändas, Hirohiko Adachi, Masayuki Uda, and Rika Sekine, editors. *Advances in Quantum Chemistry: DV–Xα for advanced nano materials and other interesting topics in materials science*, volume 42 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 2003. CODEN AQCHA9. ISBN 0-12-034842-X (hardcover). ISSN 0065-3276. xvii + 477 pp. LCCN QD453 .A28 v.42. URL https://www.sciencedirect.com/science/book/9780120348428. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2003:AQCc

[SBC+03] John S. Sabin, Erkki J. Brändas, Arnout Ceulemans, Liviu Chibotaru, and Eugene Kryachko, editors. *Advances in Quantum Chemistry: Manifestations of vibronic coupling in chemistry and physics*, volume 44 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2003. CODEN AQCHA9. ISBN 0-12-034844-6 (hardcover). ISSN 0065-3276. xxxvi + 673 pp. LCCN QD453 .A28 v.44. URL https://www.sciencedirect.com/science/book/9780120348442. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2009:AQCb

[SBC09a] John R. Sabin, Erkki Brändas, and Salvador A. Cruz, editors. *Advances in Quantum Chemistry: Theory of confined quantum systems: Part One*, volume 57 of *Advances in Quantum*

Chemistry. Elsevier Academic Press, Amsterdam, The Netherlands, 2009. CODEN AQCHA9. ISBN 0-12-374764-3 (hardcover). ISSN 0065-3276. xii + 334 pp. LCCN QD453 .A28 v.57. URL https://www.sciencedirect.com/science/book/9780123747648. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2009:AQC

[SBC09b] John R. Sabin, Erkki Brändas, and Salvador A. Cruz, editors. *Advances in Quantum Chemistry: Theory of confined quantum systems: Part Two*, volume 58 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2009. CODEN AQCHA9. ISBN 0-12-375074-1 (hardcover). ISSN 0065-3276. x + 281 pp. LCCN QD453 .A28 v.58. URL https://www.sciencedirect.com/science/book/9780123750747. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2010:AQC

[SBC10] John R. Sabin, Erkki Brändas, and Sylvio Canuto, editors. *Advances in Quantum Chemistry: Combining quantum mechanics and molecular mechanics: some recent progress in QM–MM methods*, volume 59 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2010. CODEN AQCHA9. ISBN 0-12-380898-7 (hardcover), 0-12-380899-5 (e-book). ISSN 0065-3276. xvi + 416 pp. LCCN QD453 .A28 v.59. UK£136.00. URL https://www.sciencedirect.com/science/book/9780123808981. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2004:AQCa

[SBCT04a] John S. Sabin, Erkki J. Brändas, and Remigio Cabrera-Trujillo, editors. *Advances in Quantum Chemistry: Theory of the Interaction of Swift Ions with Matter, Part 1*, volume 45 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2004. CODEN AQCHA9. ISBN 0-12-034845-4 (hardcover), 0-08-054407-X (e-book). ISSN 0065-3276. xi + 291 pp. LCCN QD453 .A28 v.45. URL https://www.sciencedirect.com/science/book/9780120348459. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2004:AQCb

[SBCT04b] John S. Sabin, Erkki J. Brändas, and Remigio Cabrera-Trujillo, editors. *Advances in Quantum Chemistry: Theory* *of the Interaction of Swift Ions with Matter, Part 2*, volume 46 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2004. CODEN AQCHA9. ISBN 0-12-034846-2 (hardcover), 0-12-391779-4 (e-book). ISSN 0065-3276. xi + 342 pp. LCCN QD453 .A28 v.46. URL https://www.sciencedirect.com/science/bookseries/00653276/46/part/P2. Founding editor Per-Olov Löwdin (1916–2000).

Sookhun:2003:MOT

[SBDD03] S. S. Sookhun, C. A. Bates, J. L. Dunn, and W. Diery. Multiple occupancy of triply degenerate states in icosahedral symmetry. *Advances in Quantum Chemistry*, 44:319–334, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440215.

Schuch:2008:PAM

[SBF+08] R. Schuch, I. Bergström, T. Fritioff, Sz. Nagy, A. Solders, and M. Suhonen. Precise atomic masses for fundamental physics determined at SMILETRAP. *Advances in Quantum Chemistry*, 53:67–81, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530066.

Soff:1998:QES

[SBG+98] Gerhard Soff, T. Beier, M. Greiner, H. Persson, and G. Plunien. Quantum electrodynamics of strong fields: Status and perspectives. *Advances in Quantum Chemistry*, 30:125–161, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605067.

Smiga:2014:DDE

[ŚBG14] S. Śmiga, A. Buksztel, and I. Grabowski. Density-dependent exchange-correlation potentials derived from highly accurate ab initio calculations. *Advances in Quantum Chemistry*, 68:125–151, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128005361000071.

Sabin:2008:AQCc

[SBGJ08] John R. Sabin, Erkki Brändas, Michael E. Goodsite, and Matthew S. Johnson, editors. *Advances in Quantum Chemistry:*

Applications of theoretical methods to atmospheric science, volume 55 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2008. CODEN AQCHA9. ISBN 0-12-374335-4 (hardcover), 0-08-087805-9 (e-book). ISSN 0065-3276. xvi + 484 pp. LCCN QD453 .A28 v.55. URL https://www.sciencedirect.com/science/book/9780123743350. Founding editor Per-Olov Löwdin (1916–2000).

Saalfrank:2020:MAC

[SBH+20] Peter Saalfrank, Florian Bedurke, Chiara Heide, Tillmann Klamroth, Stefan Klinkusch, Pascal Krause, Mathias Nest, and Jean Christophe Tremblay. Molecular attochemistry: Correlated electron dynamics driven by light. *Advances in Quantum Chemistry*, 81:15–50, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300034.

Sabin:2004:AQCc

[SBK04] John S. Sabin, Erkki J. Brändas, and Eugene Kryachko, editors. *Advances In Quantum Chemistry: a Tribute Volume in Honour of Professor Osvaldo Goscinski*, volume 47 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2004. CODEN AQCHA9. ISBN 0-12-391780-8 (hardcover), 0-08-056062-8 (e-book). ISSN 0065-3276. xxx + 486 pp. LCCN QD453 .A28 v.47. URL https://www.sciencedirect.com/science/book/9780120348473; https://www.sciencedirect.com/science/book/9780123917805. Founding editor Per-Olov Löwdin (1916–2000). The mini-symposium and the birthday celebration on 23–24 October 2003, and the Löwdin Lectures 2003.

Sabin:2008:AQCb

[SBK+08] John R. Sabin, Erkki Brändas, Jun Kawai, Yang-Soo Kim, and Hirohiko Adachi, editors. *Advances in Quantum Chemistry: DV-Xα for industrial–academic cooperation*, volume 54 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2008. CODEN AQCHA9. ISBN 0-12-373926-8 (hardcover). ISSN 0065-3276. xxviii + 363 pp. LCCN QD453 .A28 v.54. URL https://www.sciencedirect.com/science/article/pii/S0065327607000329; https://www.sciencedirect.com/science/book/9780123739261. Founding editor Per-Olov Löwdin (1916–2000).

Stenger:2015:CMC

[SBK15] Frank Stenger, Gerd Baumann, and Vasilios G. Koures. Computational methods for chemistry and physics, and Schrödinger in $3 + 1^1$. *Advances in Quantum Chemistry*, 71:265–298, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000064`.

Sabin:2005:AQCc

[SBLJ05] John R. Sabin, Erkki Brändas, Jan Linderberg, and Poul Jørgensen, editors. *Advances in Quantum Chemistry: Response theory and molecular properties: a tribute to Jan Linderberg and Poul Jørgensen*, volume 50 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2005. CODEN AQCHA9. ISBN 0-12-034850-0 (hardcover). ISSN 0065-3276. xxix + 319 pp. LCCN QD453 .A28 v.50. URL `https://www.sciencedirect.com/science/book/9780120348503`. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2001:AQCa

[SBM+01a] John R. Sabin, Erkki Brändas, Jean Maruani, R. McWeeny, Y. G. Smeyers, and S. Wilson, editors. *Advances in Quantum Chemistry: New perspectives in quantum systems in chemistry and physics, part 1*, volume 39 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 2001. CODEN AQCHA9. ISBN 0-12-034839-X (hardcover). ISSN 0065-3276. xxxi + 381 pp. LCCN QD453 .A28 v.39. URL `https://www.sciencedirect.com/science/book/9780120348398`. Founding editor Per-Olov Löwdin (1916–2000). Proceedings of the Fifth European Workshop on Quantum Systems in Chemistry and Physics which was held April 13–18, 2000, in Uppsala, Sweden.

Sabin:2001:AQCb

[SBM+01b] John R. Sabin, Erkki Brändas, Jean Maruani, R. McWeeny, Y. G. Smeyers, and S. Wilson, editors. *Advances in Quantum Chemistry: New perspectives in quantum systems in chemistry and physics, part 1*, volume 40 of *Advances in Quantum Chemistry*. Academic Press Inc., New York, USA, 2001. CODEN AQCHA9. ISBN 0-12-034840-3 (hardcover). ISSN 0065-3276. xxxi + 395 pp. LCCN QD453 .A28 v.40. US$155.00. URL `https://www.sciencedirect.com/science/book/9780120348404`. Founding editor Per-Olov Löwdin (1916–2000). Proceedings of the Fifth European Workshop on Quantum Systems in Chemistry and Physics which was held April 13–18, 2000, in Uppsala, Sweden.

Sabin:2008:AQCa

[SBSL08] John R. Sabin, Erkki Brändas, Sten Salomonson, and Eva Lindroth, editors. *Advances in Quantum Chemistry: Current trends in atomic physics*, volume 53 of *Advances in Quantum Chemistry*. Elsevier, Amsterdam, The Netherlands, 2008. CODEN AQCHA9. ISBN 0-12-373925-X (hardcover). ISSN 0065-3276. xix + 271 pp. LCCN QD453 .A28 v.53. URL https://www.sciencedirect.com/science/book/9780123739254. Founding editor Per-Olov Löwdin (1916–2000). Papers from a symposium celebrating the 75th birthday of Ingvar Lindgren, held at Chalmers University of Technology on June 2nd and 3rd, 2006.

Silkin:2019:CEE

[SCE19] Vyacheslav M. Silkin, Evgenii V. Chulkov, and Pedro M. Echenique. Collective electronic excitations on the MgB_2 (0001) surfaces. *Advances in Quantum Chemistry*, 80:147–174, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761930036X.

Schmidt:1994:MIM

[Sch94] P. P. Schmidt. The mechanics of ionic motion in molecular channels. *Advances in Quantum Chemistry*, 25:47–139, 1994. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600180.

Szalewicz:2023:HCE

[SCJ+23] Krzysztof Szalewicz, Wojciech Cencek, Bogumił Jeziorski, Konrad Patkowski, and Michał Przybytek. How competitive are expansions in orbital products with explicitly correlated expansions for helium dimer? *Advances in Quantum Chemistry*, 87:231–262, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000291.

Sil:2009:SCA

[SCM09] A. N. Sil, S. Canuto, and P. K. Mukherjee. Spectroscopy of confined atomic systems: Effect of plasma. *Advances in Quantum Chemistry*, 58:115–175, 2009. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327609007084.

Suzuki:2003:ECJ

[SCN03] Shugo Suzuki, Tadahiko Chida, and Kenji Nakao. Electron correlation and Jahn–Teller effect in alkali-metal-doped C_{60}. *Advances in Quantum Chemistry*, 44:535–554, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440355.

Sabin:2015:CMP

[SCT15] John R. Sabin and Remigio Cabrera-Trujillo, editors. *Concepts of mathematical physics in chemistry: a tribute to Frank E. Harris*, volume 71. Academic Press Inc., New York, USA, 2015. CODEN AQCHA9. ISBN 0-12-802824-6, 0-12-802868-8 (e-book). ISSN 0065-3276. xv + 382 pp. LCCN QC19.2.

Sabin:2016:CMP

[SCT16] John R. Sabin and Remigio Cabrera-Trujillo, editors. *Concepts of mathematical physics in chemistry: a tribute to Frank E. Harris. Part B*, volume 72 of *Advances in quantum chemistry*. Academic Press Inc., New York, USA, 2016. CODEN AQCHA9. ISBN 0-12-803984-1, 0-12-803985-X (e-book). ISSN 0065-3276. xii + 235 pp. LCCN QC19.2.

Stolterfoht:2007:CEF

[SCTH+07] N. Stolterfoht, R. Cabrera-Trujillo, R. Hellhammer, Z. Pesić, E. Deumens, Y. Öhrn, and J. R. Sabin. Charge exchange and fragmentation in slow collisions of He^{2+} with water molecules. *Advances in Quantum Chemistry*, 52:149–170, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520076.

Springborg:2004:CPE

[SD04] Michael Springborg and Yi Dong. Conjugated polymers in external DC fields. *Advances in Quantum Chemistry*, 47:369–392, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760447021X.

Szarecka:1998:EBS

[SDGW98] A. Szarecka, G. Day, P. J. Grout, and S. Wilson. On the effects of basis set truncation and electron correlation in conformers of 2-hydroxy-acetamide. *Advances in Quantum Chemistry*, 32:93–107, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604086.

Schmid:1998:FPL

[SED+98] R. N. Schmid, E. Engel, R. M. Dreizler, P. Blaha, and K. Schwarz. Full potential linearized-Augmented-Plane-Wave calculations for 5d transition metals using the relativistic generalized gradient approximation. *Advances in Quantum Chemistry*, 33:209–223, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604372.

Suter:2001:WHO

[SEL01] H. U. Suter, B. Engels, and S. Lunell. Was H_2^- observed in solid H_2? A theoretical answer. *Advances in Quantum Chemistry*, 40:133–142, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400128. See comment [Miy03].

Seminario:1998:P

[Sem98] Jorge M. Seminario. Preface. *Advances in Quantum Chemistry*, 33:xv–xviii, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604256.

Serre:1974:SGN

[Ser74] J. Serre. Symmetry groups of nonrigid molecules. *Advances in Quantum Chemistry*, 8:1–36, 1974. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608600581.

Seybold:2012:QCQ

[Sey12] Paul G. Seybold. Quantum chemical-QSPR estimation of the acidities and basicities of organic compounds. *Advances in Quantum Chemistry*, 64:83–104, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000156.

Simonetta:1980:CAT

[SG80] M. Simonetta and A. Gavezzotti. The cluster approach in theoretical study of chemisorption. *Advances in Quantum Chemistry*, 12:103–158, 1980. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603159.

Schneider:2016:TPP

[SGB16] Barry I. Schneider, Xiaoxu Guan, and Klaus Bartschat. Time propagation of partial differential equations using the short iterative Lanczos method and finite-element discrete variable representation. *Advances in Quantum Chemistry*, 72:95–127, 2016. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615300034.

Stohlker:2008:QEO

[SGK+08] Th. Stöhlker, A. Gumberidze, A. Kumar, R. Reuschl, and M. Trassinelli. Quantum electrodynamics in one- and two-electron high- Z ions. *Advances in Quantum Chemistry*, 53:57–65, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530054.

Stopera:2013:SRD

[SGM+13] Christopher Stopera, Thomas V. Grimes, Patrick M. McLaurin, Austin Privett, and Jorge A. Morales. Some recent developments in the simplest-level electron nuclear dynamics method: Theory, code implementation, and applications to chemical dynamics. *Advances in Quantum Chemistry*, 66:113–194, 2013. CODEN AQCHA9. ISBN 0-12-408099-5. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124080997000039.

Shaik:1995:VBM

[SH95] Sason Shaik and Philippe C. Hiberty. Valence bond mixing and curve crossing diagrams in chemical reactivity and bonding. *Advances in Quantum Chemistry*, 26:99–163, 1995. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601124.

Sharma:2019:PEH

[SH19] Rajesh O. Sharma and Philip E. Hoggan. Physisorption energy of H and H_2 on clean Pt(111) as a useful surface energy reference in Quantum Monte Carlo calculation. *Advances in Quantum Chemistry*, 79:311–322, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300231.

Sklyadneva:2019:EPI

[SHBC19] Irina Yu. Sklyadneva, Rolf Heid, Klaus-Peter Bohnen, and Evgenii V. Chulkov. Electron-phonon interaction on the (110) surface of Ag and Cu. *Advances in Quantum Chemistry*, 80:199–223, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327619300401`.

Sheka:2015:SBC

[She15] Elena Sheka. Stretching and breaking of chemical bonds, correlation of electrons, and radical properties of covalent species. *Advances in Quantum Chemistry*, 70:111–161, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327614000069`.

Shimamura:2012:QBS

[Shi12] Isao Shimamura. Quasi-bound states of electronic and positronic few-body systems: Analysis of multichannel scattering information. *Advances in Quantum Chemistry*, 63:165–245, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780123970091000047`.

Sidi:2018:RDA

[Sid18] Avram Sidi. Recent developments in asymptotic expansions from numerical analysis and approximation theory. *Advances in Quantum Chemistry*, 76:35–57, 2018. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532761730059X`.

Sigmund:2005:ICQ

[Sig05] Peter Sigmund. Interplay of classical and quantum mechanics in the theory of charged-particle stopping. *Advances in Quantum Chemistry*, 48:91–110, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605480077`.

Silverstone:2014:CIB

[Sil14] H. J. Silverstone. On the convergence of the interpenetrating bipolar expansion for the Coulomb potential. *Advances in Quantum Chemistry*, 68:3–18, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128005361000010`.

Simons:1999:SCP

[Sim99] Jack Simons. Semi-classical pictures of non-adiabatic induced electron ejection in molecular anions. *Advances in Quan-*

tum Chemistry, 35:283–316, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604657`.

Simons:2005:RMA

[Sim05] Jack Simons. Response of a molecule to adding or removing an electron. *Advances in Quantum Chemistry*, 50:213–233, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605500108`.

Simons:2007:HVL

[Sim07] Jack Simons. How very low-energy (0.1-2 eV) electrons cause DNA strand breaks. *Advances in Quantum Chemistry*, 52:171–188, 2007. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327606520088`.

Shoji:2015:LSQ

[SIY+15] M. Shoji, H. Isobe, S. Yamanaka, Y. Umena, K. Kawakami, N. Kamiya, J.-R. Shen, T. Nakajima, and K. Yamaguchi. Large-scale QM/MM calculations of hydrogen bonding networks for proton transfer and water inlet channels for water oxidation-theoretical system models of the oxygen-evolving complex of photosystem II. *Advances in Quantum Chemistry*, 70:325–413, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327614000082`.

Shoji:2019:TEG

[SIY+19] Mitsuo Shoji, Hiroshi Isobe, Shusuke Yamanaka, Yasufumi Umena, Keisuke Kawakami, and Nobuo Kamiya Kizashi Yamaguchi. Theoretical elucidation of geometrical structures of the $CaMn_4O_5$ cluster in oxygen evolving complex of photosystem II scope and applicability of estimation formulae of structural deformations via the mixed-valence and Jahn–Teller effects. *Advances in Quantum Chemistry*, 78:307–451, 2019. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327618300248`.

Saha:2022:ESE

[SJAB+22] Bidhan C. Saha, D. H. Jakubassa-Amundsen, A. K. Basak, A. K. F. Haque, M. M. Haque, Mahmudul H. Khandker, and M. Alfaz Uddin. Elastic scattering of electrons and positrons from alkali atoms. *Advances in Quantum Chemistry*, 86:1–149, 2022. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000198.

Sjoqvist:2004:ANT

[Sjö04] Erik Sjöqvist. On the alleged nonlocal and topological nature of the molecular Aharonov–Bohm effect. *Advances in Quantum Chemistry*, 47:239–252, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470142.

Sauer:2005:QCC

[SJO05] Stephan P. A. Sauer, Hans Jørgen Aa. Jensen, and John F. Ogilvie. Quantum-chemical calculations of radial functions for rotational and vibrational g factors, electric dipolar moment and adiabatic corrections to the potential energy for analysis of spectra of HeH^+. *Advances in Quantum Chemistry*, 48:319–334, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760548017X.

Singh:2023:PMS

[SKGŚ23] Aditi Singh, Vignesh Balaji Kumar, Ireneusz Grabowski, and Szymon Śmiga. Physically meaningful solutions of optimized effective potential equations in a finite basis set within KS-DFT framework. *Advances in Quantum Chemistry*, 87:297–317, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000035.

Stachowicz-Kusnierz:2023:BST

[SKK23] Anna Stachowicz-Kuśnierz and Jacek Korchowiec. From bulk to surface — transferability of water atomic charges. *Advances in Quantum Chemistry*, 87:397–414, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000060.

Skodje:2012:RBC

[Sko12] Rex T. Skodje. Resonances in bimolecular chemical reactions. *Advances in Quantum Chemistry*, 63:119–163, 2012. CODEN AQCHA9. ISBN 0-12-397009-1. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123970091000035.

Suarez:2019:DEC

[SKS+19] Luis Enrique Aguilar Suarez, R. K. Kathir, Enrico Siagri, Remco W. A. Havenith, and Shirin Faraji. Determination of electronic couplings in the singlet fission process using a nonorthogonal configuration interaction approach. *Advances in Quantum Chemistry*, 79:263–287, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300279.

Sato:2003:JTE

[SKT+03] Tohru Sato, Yasutaka Kuzumoto, Ken Tokunaga, Hideaki Tanaka, and Hiroshi Imahori. Jahn–Teller effect in circulenes. *Advances in Quantum Chemistry*, 44:239–255, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760344015X.

Shinzato:2008:CCB

[SKT+08] Yoshifumi Shinzato, Kenji Komiya, Yoshitaka Takahashi, Hiroshi Yukawa, Masahiko Morinaga, and Shinichi Orimo. Characteristics of chemical bond in perovskite-type hydrides. *Advances in Quantum Chemistry*, 54:245–253, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000196.

Seel:2020:TMT

[SL20] Maximilian Seel and János Ladik. The tragicomedy of modern theoretical biology. *Advances in Quantum Chemistry*, 81:1–13, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532761930067X.

Slater:1964:EBC

[Sla64] J. C. Slater. Energy band calculations by the Augmented Plane Wave method. *Advances in Quantum Chemistry*, 1:35–58, 1964. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603743.

Slater:1972:SEC

[Sla72] John C. Slater. Statistical exchange-correlation in the self-consistent field. *Advances in Quantum Chemistry*, 6:1–92, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605419.

Slanina:1981:CIC

[Sla81] Zdeněk Slanina. Chemical isomerism and its contemporary theoretical description. *Advances in Quantum Chemistry*, 13:89–153, 1981. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602920`.

Sigaud:2022:CEL

[SM22] Lucas Sigaud and Eduardo C. Montenegro. Long-lived molecular dications: a selected probe for double ionization. *Advances in Quantum Chemistry*, 85:219–244, 2022. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327622000119`.

Skrzynski:2023:PEC

[SM23] Grzegorz Skrzyński and Monika Musiał. Potential energy curves of the $LiRb^+$ molecular ion from ab initio calculations with all electrons correlated. *Advances in Quantum Chemistry*, 88:213–227, 2023. CODEN AQCHA9. ISSN 0065-3276. URL `http://www.sciencedirect.com/science/article/pii/S0065327623000114`.

Sugita:2008:ESB

[SMAS08] Kazuki Sugita, Masataka Mizuno, Hideki Araki, and Yasuharu Shirai. Electronic structure and bonding in amorphous $Zr_{67}Ni_{33}$ and $Zr_{67}Cu_{33}$. *Advances in Quantum Chemistry*, 54:161–174, 2008. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327607000135`.

Smeyers:1992:IGT

[Sme92] Yves G. Smeyers. Introduction to group theory for non-rigid molecules. *Advances in Quantum Chemistry*, 24:1–77, 1992. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608601008`.

Smeyers:1999:HPH

[Sme99] Yves G. Smeyers. The half projected Hartree–Fock model for determining singlet excited states. *Advances in Quantum Chemistry*, 36:253–270, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604864`.

Suzuki:2008:STA

[SN08] Chikashi Suzuki and Toshio Nakagiri. Sulfur trioxide adsorption on pt surface. *Advances in Quantum Chemistry*, 54:61–79, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000068.

Sugihara:2008:FMO

[SNIM08] Sunao Sugihara, Koujiroh Nishiyama, Yuka Igarashi, and Kentaroh Morikawa. Functions of metal oxide for thermoelectric materials and electronic structures. *Advances in Quantum Chemistry*, 54:227–243, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000184.

Sekine:1997:ESM

[SNM+97] Rika Sekine, Hirohide Nakamatsu, Takeshi Mukoyama, Jun Onoe, Masaru Hirata, Masayoshi Kurihara, and Hirohiko Adachi. Electronic structures of metal carbides TiC and UC: Similarity and dissimilarity. *Advances in Quantum Chemistry*, 29:123–136, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860266X.

Shigemi:2000:CSC

[SNMI00] Akio Shigemi, Hirohide Nakamatsu, Takeshi Mukoyama, and Shigero Ikeda. CO shakeup calculations with the DV-Xα method. *Advances in Quantum Chemistry*, 37:127–137, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370095.

Sabin:2005:SPW

[SO05a] John R. Sabin and Jens Oddershede. Stopping power — what next? *Advances in Quantum Chemistry*, 49:299–319, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490073.

Sabin:2005:AQCa

[SO05b] John S. Sabin and Lene B. Oddershede, editors. *Advances in Quantum Chemistry: Jens Oddershede: Adventurer in Quantum Chemistry*, volume 48 of *Advances in Quantum Chemistry*. Elsevier Academic Press, Amsterdam, The Netherlands, 2005. CODEN AQCHA9. ISBN 0-12-034848-9 (hardcover). ISSN 0065-3276. xxviii + 499 pp. LCCN QD453 .A28 v.48. URL https://www.sciencedirect.com/science/book/9780120348480. Founding editor Per-Olov Löwdin (1916–2000).

Sabin:2019:P

[SO19a] John R. Sabin and Jens Oddershede. Preface. *Advances in Quantum Chemistry*, 80:xiii, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300760.

Sabin:2019:RRG

[SO19b] John R. Sabin and Jens Oddershede, editors. *Rufus Ritchie, A Gentleman and A Scholar*, volume 80 of *Advances in quantum chemistry*. Elsevier, Amsterdam, The Netherlands, 2019. CODEN AQCHA9. ISBN 0-12-817185-5, 0-12-817186-3 (e-book). ISSN 0065-3276. xiii + 366 pp. LCCN QD462 .R848 2019. URL https://www.sciencedirect.com/science/journal/00653276/78. Quantum systems in physics, chemistry and biology — theory, interpretation, and results.

Staroverov:2019:UCF

[SO19c] Viktor N. Staroverov and Egor Ospadov. Unified construction of Fermi, Pauli and exchange-correlation potentials. *Advances in Quantum Chemistry*, 79:201–219, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300188.

Sauer:2011:MEE

[SOS11] Stephan P. A. Sauer, Jens Oddershede, and John R. Sabin. Mean excitation energies for biomolecules: Glycine to DNA. *Advances in Quantum Chemistry*, 62:215–242, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123864772000115.

Sabin:2013:DME

[SOS13] John R. Sabin, Jens Oddershede, and Stephan P. A. Sauer. On the determination of the mean excitation energy of water. *Advances in Quantum Chemistry*, 65:63–77, 2013. CODEN AQCHA9. ISBN 0-12-396455-5 (hardcover). ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964557000030.

Sauer:2015:MEE

[SOS15] Stephan P. A. Sauer, Jens Oddershede, and John R. Sabin. The mean excitation energy of atomic ions. *Advances in Quantum Chemistry*, 71:29–40, 2015. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000027`.

Santoro:1999:LCS

[SP99] Fabrizio Santoro and Carlo Petrongolo. Lanczos calculation of the $^2A_1$ /$\tilde{A}^2$ B_2 nonadiabatic Franck–Condon absorption spectrum of NO_2. *Advances in Quantum Chemistry*, 36:323–340, 1999. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608604906`.

Sanchez:2005:ULD

[SPAS05] Marina Sanchez, Patricio F. Provasi, Gustavo A. Aucar, and Stephan P. A. Sauer. On the usage of locally dense basis sets in the calculation of NMR indirect nuclear spin-spin coupling constants: Vicinal fluorine-fluorine couplings. *Advances in Quantum Chemistry*, 48:161–183, 2005. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605480120`.

Sako:2009:ELS

[SPD09] Tokuei Sako, Josef Paldus, and Geerd H. F. Diercksen. The energy level structure of low-dimensional multi-electron quantum dots. *Advances in Quantum Chemistry*, 58:177–201, 2009. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327609007096`.

Sperber:1978:FET

[Spe78] Gunnar Sperber. Fundamentals of equilibrium thermodynamics and statistical mechanics. *Advances in Quantum Chemistry*, 11:411–478, 1978. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608602427`.

Sullivan:2022:CFH

[SPG+22] N. S. Sullivan, M. Pilla, E. B. Genio, J. A. Hamida, and K. A. Muttalib. Hierarchical relaxation in frustrated systems. *Advances in Quantum Chemistry*, 85:303–325, 2022. CODEN AQCHA9.

ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327622000168`.

Sidi:2014:AEB

[SPH14] A. Sidi, D. Pinchon, and P. E. Hoggan. Asymptotic expansions of Barnett–Coulson–Löwdin functions of high order. *Advances in Quantum Chemistry*, 68:43–76, 2014. CODEN AQCHA9. ISBN 0-12-800536-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780128005361000034`.

Sen:2009:ERC

[SPM09] K. D. Sen, V. I. Pupyshev, and H. E. Montgomery, Jr. Exact relations for confined one-electron systems. *Advances in Quantum Chemistry*, 57:25–77, 2009. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327609006066`.

Steinborn:1973:RTR

[SR73] E. O. Steinborn and K. Ruedenberg. Rotation and translation of regular and irregular solid spherical harmonics. *Advances in Quantum Chemistry*, 7:1–81, 1973. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605584`.

Srivastava:2001:OVR

[Sri01] Vipin Srivastava. Orthogonalization of vectors and its relation to cognitive phenomena. *Advances in Quantum Chemistry*, 40:249–255, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400190`.

Sarasola:2004:DFT

[SRZE04] A. Sarasola, R. H. Ritchie, E. Zaremba, and P. M. Echenique. Density functional theory-based stopping power for 3D and 2D systems. *Advances in Quantum Chemistry*, 46 (part 2):1–28, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327604460018`.

Schluter:1990:DFT

[SS90] M. Schlüter and L. J. Sham. Density-functional theory of the band gap. *Advances in Quantum Chemistry*, 21:97–112, 1990. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605936`.

Sahni:1998:RDE

[SS98] Viraht Sahni and Alexander Solomatin. Recent developments in the electronic structure of metal surfaces. *Advances in Quantum Chemistry*, 33:241–271, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604396.

Sherrill:1999:CIM

[SS99] C. David Sherrill and Henry F. Schaefer III. The configuration interaction method: Advances in highly correlated approaches. *Advances in Quantum Chemistry*, 34:143–269, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605328.

Savage:2003:APH

[SS03] E. D. Savage and G. E. Stedman. Antilinear particle–hole conjugation operators in Jahn–Teller theory. *Advances in Quantum Chemistry*, 44:21–43, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440033.

Stolterfoht:2004:IEE

[SS04] N. Stolterfoht and B. Sulik. Interferences in electron emission from H_2 induced by fast ion impact. *Advances in Quantum Chemistry*, 46 (part 2):307–327, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604460122.

Srivastava:2017:CLM

[SS17] Vipin Srivastava and Suchitra Sampath. Cognition of learning and memory: What have Löwdin's orthogonalizations got to do with that? *Advances in Quantum Chemistry*, 74:299–319, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327616300430.

Sorensen:2022:CTI

[SS22] Lea Northcote Sørensen and Stephan P. A. Sauer. Implicit and explicit solvent models have opposite effects on radiation damage rate constant for thymine. *Advances in Quantum Chemistry*, 85:245–265, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000332.

Smith:1997:AAI

[SSCL97] F. J. Smith, M. Sullivan, J. Collis, and S. Loughlin. Applying artificial intelligence in physical chemistry. *Advances in Quantum Chemistry*, 28:319–328, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602245.

Sob:2003:TCP

[SSK03] M. Sob, H. Sormann, and J. Kuriplach. Theoretical calculations of positron annihilation characteristics in inorganic solids — recent advances and problems. *Advances in Quantum Chemistry*, 42:77–108, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760342042X.

Sauer:2019:CME

[SSO19] Stephan P. A. Sauer, John R. Sabin, and Jens Oddershede. Calculation of mean excitation energies. *Advances in Quantum Chemistry*, 80:225–245, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300310.

Sobczyk:2005:DLE

[SSS05] Monika Sobczyk, Piotr Skurski, and Jack Simons. Dissociative low-energy electron attachment to the $C — S$ bond of H_3CSCH_3 influenced by Coulomb stabilization. *Advances in Quantum Chemistry*, 48:239–251, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480156.

Smeyers:1998:IDB

[SSV98] Y. G. Smeyers, M. L. Senent, and M. Villa. *Ab initio* determination of band structures of vibrational spectra of non-rigid molecules: Applications to methylamine and dimethylamine. *Advances in Quantum Chemistry*, 32:145–166, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604116.

Scrocco:1978:EMS

[ST78] Eolo Scrocco and Jacopo Tomasi. Electronic molecular structure, reactivity and intermolecular forces: An euristic interpretation by means of electrostatic molecular potentials. *Advances in*

Quantum Chemistry, 11:115–193, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602361.

Sulik:2007:AMS

[ST07] Béla Sulik and Károly Tőkési. Accelerating multiple scattering of electrons by ion impact: Contribution to molecular fragmentation and radiation damages. *Advances in Quantum Chemistry*, 52:253–276, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520118.

Sabio:2017:SAA

[ST17] Michael Sabio and Sid Topiol. Switching activity of allosteric modulators controlled by a cluster of residues forming a pressure point in the mGluR5 GPCR: a computational investigation. *Advances in Quantum Chemistry*, 75:147–174, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300308.

Steinborn:1973:MIB

[Ste73] E. O. Steinborn. Molecular integrals between real and between complex atomic orbitals. *Advances in Quantum Chemistry*, 7:83–112, 1973. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605596.

Sekine:2000:ACB

[STO+00] Rika Sekine, Kumiko Tanaka, Jun Onoe, Kazuo Takeuchi, and Hirohide Nakamatsu. Analysis of chemical bond in metal clusters: I. Alkali metal and alkaline earth metals. *Advances in Quantum Chemistry*, 37:237–254, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370174.

Samanta:2018:EAE

[STZY18] Kousik Samanta, Tsednee Tsogbayar, Song Bin Zhang, and Danny L. Yeager. Electron–atom and electron–molecule resonances: Some theoretical approaches using complex scaled multiconfigurational methods. *Advances in Quantum Chemistry*, 77: 317–390, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300655.

Sucher:1998:WFB

[Suc98] J. Sucher. What is the force between electrons? *Advances in Quantum Chemistry*, 30:433–443, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605213.

Sutcliffe:1997:NMP

[Sut97] B. T. Sutcliffe. The nuclear motion problem in molecular physics. *Advances in Quantum Chemistry*, 28:65–80, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602075.

Sutcliffe:1998:QSC

[Sut98] B. T. Sutcliffe. Quantum systems in chemistry and physics: Some hopes and fears. *Advances in Quantum Chemistry*, 31:1–13, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860180X.

Sutcliffe:2001:SMP

[Sut01] Brian Sutcliffe. Some mathematical problems in the description of dissociating molecules. *Advances in Quantum Chemistry*, 40:17–36, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327601400074.

Svanberg:1998:HPL

[Sva98] S. Svanberg. High-power lasers and their applications. *Advances in Quantum Chemistry*, 30:209–233, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605092.

Shoemaker:1981:FRC

[SW81] Curtis L. Shoemaker and Robert E. Wyatt. Feshbach resonances in chemical reactions. *Advances in Quantum Chemistry*, 14:169–240, 1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603287.

Shalabi:1998:CMB

[SW98] A. S. Shalabi and S. Wilson. On the convergence of the many-body perturbation theory second-order energy component for negative ions using systematically constructed basis sets of primitive Gaussian-type functions. *Advances in Quantum Chemistry*, 31:283–311, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601938.

Sugihara:2003:AWP

[SYIY03] Sunao Sugihara, Masahiro Yamamoto, Takamasa Isobe, and Yukio Yutoh. Analysis of wetting property of electrode metal on A1N at their interface using discrete variational-Xα. *Advances in Quantum Chemistry*, 42:465–474, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420698.

Shinzato:2008:NEC

[SYM+08] Yoshifumi Shinzato, Hiroshi Yukawa, Masahiko Morinaga, Takeshi Baba, and Hiromi Nakai. New expression of the chemical bond in hydrides using atomization energies. *Advances in Quantum Chemistry*, 54:145–160, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000123.

Silkowski:2021:CTA

[SZP21] Michał Siłkowski, Magdalena Zientkiewicz, and Krzysztof Pachucki. Accurate Born–Oppenheimer potentials for excited Σ^+ states of the hydrogen molecule. *Advances in Quantum Chemistry*, 83:255–267, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000149.

Tapia:2004:GED

[TA04] O. Tapia and Gustavo A. Arteca. Generalized electronic diabatic ansatz: a post-born–oppenheimer approach to electronuclear dynamics in external fields. *Advances in Quantum Chemistry*, 47:275–291, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470166.

Takahashi:2019:HDV

[Tak19] Kaito Takahashi. How does vibrational excitation affect the X-ray absorption spectra of monohydrated halide and alkali metal clusters? *Advances in Quantum Chemistry*, 78:57–81, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327618300315.

Trsic:2004:GCM

[TAM04] Milan Trsic, Wagner F. D. Angelotti, and Fábio A. Molfetta. The generator coordinate method for atomic and molecular systems: Revision and further developments. *Advances in Quantum Chemistry*, 47:315–329, 2004. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S006532760447018X`.

Tanaka:2000:ADX

[Tan00] Isao Tanaka. Application of DV-Xα calculations in ceramics science. *Advances in Quantum Chemistry*, 37:213–227, 2000. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327600370150`.

Tapia:2001:TRB

[Tap01] O. Tapia. Towards a rigged Born–Oppenheimer electronic theory of chemical processes. *Advances in Quantum Chemistry*, 40:103–131, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327601400116`.

Tapia:2009:QLS

[Tap09] O. Tapia. Quantum linear superposition theory for chemical processes: a generalized electronic diabatic approach. *Advances in Quantum Chemistry*, 56:31–93, 2009. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608004024`.

Tapia:2011:QSQ

[Tap11] O. Tapia. Quantum states for quantum measurements. *Advances in Quantum Chemistry*, 61:49–106, 2011. CODEN AQCHA9. ISBN 0-12-386013-X. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780123860132000024`.

Tapia:2017:SQC

[Tap17] Orlando Tapia. State-quantum-chemistry set in a photonic framework. *Advances in Quantum Chemistry*, 74:227–251, 2017. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327616300429`.

Toulouse:2017:IVD

[TAU17] Julien Toulouse, Roland Assaraf, and Cyrus J. Umrigar. Introduction to the variational and diffusion Monte Carlo methods. *Advances in Quantum Chemistry*, 73:285–314, 2017.

CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327615000386`.

Tergiman:2001:TSC

[TBM01] Y. S. Tergiman and M. C. Bacchus-Montabonnel. Theoretical study of charge transfer mechanism in N^{4+} + He collisions at keV energies. *Advances in Quantum Chemistry*, 39:163–170, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605390101`.

Tew:2021:CFP

[Tew21] David P. Tew. Principal domains in F12 explicitly correlated theory. *Advances in Quantum Chemistry*, 83:83–106, 2021. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327621000162`.

Editors:1996:A

[The96] The Editors. Apology. *Advances in Quantum Chemistry*, 27:viii, 1996. CODEN AQCHA9. ISSN 0065-3276. It has come to out attention that substantial portions of the paper

Yi Lao, Hans Ågren, Poul Jørgensen, and Kurt V. Mikkelsen (1995).
Response theory and calculations of molecular hyperpolarizabilities
Adv. Quantum Chem. **26**, 168–237.

were taken nearly unaltered from

Henne Hettema, Hans Jørgen Aa. Jensen, Poul Jørgensen, and Jeppe Olsen (1992).
Quadratic response functions for a multi-configurational self-consistent-field wave-function.
J. Chem. Phys. **97**, 1174–1190.

and republished without proper copyright permission. The Editors regret this breach of courtesy and offer their sincere apologies to the authors of the *Journal of Chemical Physics* paper and to the *American Institute of Physics* for any resulting inconvenience or embarrassment.

[See [LÅJM95].].

Tu:2010:IQM

[TL10] Yaoquan Tu and Aatto Laaksonen. Implementing quantum mechanics into molecular mechanics: Combined QM/MM modeling methods. *Advances in Quantum Chemistry*, 59:1–15, 2010. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327610590014`.

Takahashi:1997:BST

[TLOK97] Masao Takahashi, Gao-Chao Lai, Katsuhiro Ohta, and Fumikazu Kanamaru. Bond strength and thermal stability of transition metal nitrides. *Advances in Quantum Chemistry*, 29:253–268, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602737.

Thakkar:2013:EEP

[TM13] A. J. Thakkar and S. P. McCarthy. Electron and electron-pair number and momentum densities for low-lying states of He, H^-, and Li^+. *Advances in Quantum Chemistry*, 67:19–54, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000029.

Tucholska:2021:CTM

[TM21] Aleksandra M. Tucholska and Robert Moszynski. Molecular properties from the explicitly connected expressions of the response functions within the coupled-cluster theory. *Advances in Quantum Chemistry*, 83:31–63, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000113.

Tomanek:2021:CSF

[TMK21] Magdalena Tomanek, Monika Musiał, and Stanisław A. Kucharski. Fock space coupled-cluster method for potential energy curves of KH and its cation. *Advances in Quantum Chemistry*, 83:125–138, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000101.

Takahara:2003:STT

[TMM03] Wataru Takahara, Hiroshi Maeda, and Fumiyoshi Minami. Superconducting transition temperature of Laves phase V_2Zr compounds with alloyed magnetic elements. *Advances in Quantum Chemistry*, 42:275–281, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420558.

Torrontegui:2010:QDL

[TMMS10] E. Torrontegui, J. G. Muga, J. Martorell, and D. W. L. Sprung. Quantum decay at long times. *Advances in Quantum Chemistry*, 60:485–535, 2010. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600093.

Takahashi:2010:DQC

[TMN10] Hideaki Takahashi, Nobuyuki Matubayasi, and Masayoshi Nakano. Development of a quantum chemical method combined with a theory of solutions: Free-energy calculation for chemical reactions by condensed phase simulations. *Advances in Quantum Chemistry*, 59:283–351, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610590099.

Tokesi:2019:ELC

[Tők19] Károly Tőkési. Energy loss of charged particles in collision with atoms and surfaces. *Advances in Quantum Chemistry*, 80:87–125, 2019. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327619300383.

Toschek:2008:SQS

[Tos08] Peter E. Toschek. A single quantum system: Evolution, prediction, observation. *Advances in Quantum Chemistry*, 53:7–26, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607530029.

Tregenna-Piggott:2003:AER

[TP03] Philip L. W. Tregenna-Piggott. Analysis of the EPR and Raman scattering of copper(II) doped CaO. *Advances in Quantum Chemistry*, 44:461–481, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440306.

Thorsteinsson:1998:PCP

[TR98] Thorstein Thorsteinsson and Sten Rettrup. Parallelization of the CI program PEDICI. *Advances in Quantum Chemistry*, 31:267–282, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601926.

Taylor:2014:QIM

[TR14] DeCarlos E. Taylor and Betsy M. Rice. Quantum-informed multiscale M&S for energetic materials. *Advances in Quantum Chemistry*, 69:171–219, 2014. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780128003459000052.

Trickey:1990:I

[Tri90] Samuel B. Trickey. Introduction. *Advances in Quantum Chemistry*, 21:1–5, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605882.

Thanopulos:2010:CEL

[TS10] Ioannis Thanopulos and Moshe Shapiro. Coherence effects in laser-induced continuum structure. *Advances in Quantum Chemistry*, 60:105–161, 2010. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327610600032.

Tanaka:2000:RAO

[TSON00] Kumiko Tanaka, Rika Sekine, Jun Onoe, and Hirohide Nakamatsu. On role of the $3d$ atomic orbital in the chemical bonding of sulfur fluorides. *Advances in Quantum Chemistry*, 37:375–383, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370277.

Takai:2003:NPB

[TSTH03] K. Takai, M. Seike, K. Tanaka, and Y. Hayafuji. New pseudo-binary titanium silicide systems for lowering phase transformation temperature. *Advances in Quantum Chemistry*, 42:239–261, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420534.

Tokesi:2004:FFC

[TTLB04] K. Tőkési, X.-M. Tong, C. Lemell, and J. Burgdörfer. Friction force for charged particles at large distances from metal surfaces. *Advances in Quantum Chemistry*, 46 (part 2):29–64, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760446002X.

Turecek:2007:CSR

[Tur07] František Tureček. Computational studies of radicals relevant to nucleic acid damage. *Advances in Quantum Chemistry*, 52:89–120, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520052.

Tanaka:1985:ESC

[TY85] Kazuyoshi Tanaka and Tokio Yamabe. Electronic structure of conductive conjugated systems and their physicochemical properties. *Advances in Quantum Chemistry*, 17:251–284, 1985. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603044.

Uda:1997:CR

[Uda97] M. Uda. Concluding remarks. *Advances in Quantum Chemistry*, 29:467–469, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602841.

Uda:2000:EAS

[Uda00] Masayuki Uda. Extended analysis of satellite structures in particle induced X-ray emission spectra using molecular orbital calculations. *Advances in Quantum Chemistry*, 37:31–55, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370034.

Uchida:2003:DSC

[UJYU03] Yoko Uchida, Tomoko Jimbo, D. Yamashita, and M. Uda. Density of states of Cu with stacking faults. *Advances in Quantum Chemistry*, 42:453–463, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420686.

Urban:2005:STR

[UK05] M. Urban and V. Kellö. Some trends in relativistic and electron correlation effects in electric properties of small molecules. *Advances in Quantum Chemistry*, 50:249–269, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500121.

Ueda:2008:SXR

[UMD08] Satoshi Ueda, Yasuji Muramatsu, and Jonathan D. Denlinger. Soft X-ray emission spectral analysis of graphite fluoride $(CF)_n$ using the DV–Xα calculations. *Advances in Quantum Chemistry*, 54:219–226, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000172.

Uda:1997:ROR

[UYT97] M. Uda, T. Yamamoto, and T. Takenaga. Resonant orbital rearrangement during F 1s ionization or decay process. *Advances in Quantum Chemistry*, 29:389–419, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602804.

Valdemoro:1998:FOC

[VdLCPT98] C. Valdemoro, M. P. de Lara-Castells, E. Pérez-Romero, and L. M. Tel. The first order contracted density equations: correlation effects. *Advances in Quantum Chemistry*, 31:37–52, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601823.

Vos:2022:MDF

[VG22] Maarten Vos and Pedro L. Grande. Model dielectric functions for ion stopping: the relation between their shell corrections, plasmon dispersion and Compton profiles. *Advances in Quantum Chemistry*, 85:??, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000156.

Vilkas:2001:RMM

[VI01] Marius Jonas Vilkas and Yasuyuki Ishikawa. Relativistic multireference Møller–Plesset perturbation theory calculations for the term energies and transition probabilities of ions in the nitrogen isoelectronic sequence. *Advances in Quantum Chemistry*, 39:261–293, 2001. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605390162.

Visscher:2005:MBE

[Vis05] Lucas Visscher. Magnetic balance and explicit diamagnetic expressions for nuclear magnetic resonance shielding tensors. *Advances in Quantum Chemistry*, 48:369–381, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480193.

Ventura:1997:DFT

[VKI97] Oscar N. Ventura, Martina Kieninger, and Kenneth Irving. Density functional theory: a useful tool for the study of free radicals. *Advances in Quantum Chemistry*, 28:293–309, 1997.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602221.

vanLeeuwen:2003:DFA

[vL03] Robert van Leeuwen. Density functional approach to the many-body problem: Key concepts and exact functionals. *Advances in Quantum Chemistry*, 43:25–94, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603430025.

Vignale:1990:MFD

[VRG90] G. Vignale, Mark Rasolt, and D. J. W. Geldart. Magnetic fields and density functional theory. *Advances in Quantum Chemistry*, 21:235–253, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605997.

vonSonntag:2007:FRI

[vS07] Clemens von Sonntag. Free-radical-induced DNA damage as approached by quantum-mechanical and Monte Carlo calculations: An overview from the standpoint of an experimentalist. *Advances in Quantum Chemistry*, 52:5–20, 2007. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606520027.

Vieyra:2024:CFU

[VT24] Juan Carlos López Vieyra and Alexander V. Turbiner. Chapter five — ultra-compact accurate wave functions for He-like isoelectronic sequences and variational calculus. IV. Spin-singlet states $(1s\ ns)\ n\ ^1\mathrm{S}$ family of the helium sequence. *Advances in Quantum Chemistry*, 89:305–337, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000679.

Veniard:1998:TDQ

[VTM98] V. Véniard, R. Taïeb, and A. Maquet. Time-dependent quantum treatment of two-colour multiphoton ionization using a strong laser pulse and high-order harmonic radiation. *Advances in Quantum Chemistry*, 32:197–205, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604141.

Valdemoro:1997:CSE

[VTPR97] C. Valdemoro, L. M. Tel, and E. Pérez-Romero. The contracted Schrödinger equation — some results. *Advances in Quantum Chemistry*, 28:33–46, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602051.

VanHove:1989:SSS

[VWOS89] M. A. Van Hove, S.-W. Wang, D. F. Ogletree, and G. A. Somorjai. The state of surface structural chemistry: Theory, experiment and results. *Advances in Quantum Chemistry*, 20:1–184, 1989. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606267.

VanMourik:1998:EBS

[VWP+98] Tanja Van Mourik, Angela K. Wilson, Kirk A. Peterson, David E. Woon, and Thom H. Dunning, Jr. The effect of basis set superposition error (BSSE) on the convergence of molecular properties calculated with the correlation consistent basis sets. *Advances in Quantum Chemistry*, 31:105–135, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601859.

Wahl:1970:MOV

[WD70] Arnold C. Wahl and G. Das. The method of optimized valence configurations: a reasonable application of the multiconfiguration self-consistent-field technique to the quantitative description of chemical bonding. *Advances in Quantum Chemistry*, 5:261–296, 1970. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608603421.

Wrighton:2022:CFS

[WD22] Jeffrey Wrighton and James Dufty. Structure and correlations for harmonically confined charges. *Advances in Quantum Chemistry*, 85:39–55, 2022. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327622000077.

Wrighton:2016:FTQ

[WDD16] Jeffrey Wrighton, James Dufty, and Sandipan Dutta. Finite temperature quantum effects in many-body systems by classical methods. *Advances in Quantum Chemistry*, 72:1–11, 2016.

CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000179.

Weinhold:1972:ULB

[Wei72] F. Weinhold. Upper and lower bounds to quantum-mechanical properties. *Advances in Quantum Chemistry*, 6:299–331, 1972. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608605493.

Weiner:2004:AGP

[Wei04] Brian Weiner. Antisymmetrized geminal power coherent states. *Advances in Quantum Chemistry*, 47:107–127, 2004. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327604470075.

Weniger:2021:CTF

[Wen21] Ernst Joachim Weniger. Are B functions with nonintegral orders a computationally useful basis set? *Advances in Quantum Chemistry*, 83:209–237, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000174.

Watabe:2024:CTS

[WHB+24] Hiroshi Watabe, M. M. Haque, M Masum Billah, Mahmudul H Khandker, M. Shorifuddoza, M. N. A. Abdullah, A. K. F. Haque, Malik Maaza, Bidhan C. Saha, Arun K. Basak, and M. Alfaz Uddin. Chapter two — scattering of $e^{\pm}$ with Al, Ni, Cu, Ag, Pt, and Au atoms including the relativistic effect at 1 eV $\leq E_i \leq$ 1 MeV. *Advances in Quantum Chemistry*, 89:61–223, 2024. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000527.

Wilson:1998:Pa

[Wil98a] S. Wilson. Preface. *Advances in Quantum Chemistry*, 31:xv–xvi, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608601781.

Wilson:1998:Pb

[Wil98b] S. Wilson. Preface. *Advances in Quantum Chemistry*, 32:xv–xvi, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604037.

Wozniak:2023:EAL

[WLM23] Aleksander P. Woźniak, Maciej Lewenstein, and Robert Moszyński. Exploring the attosecond laser-driven electron dynamics in the hydrogen molecule with different real-time time-dependent configuration interaction approaches. *Advances in Quantum Chemistry*, 87:167–190, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000023.

Wilson:1997:DGB

[WM97] S. Wilson and D. Moncrieff. Distributed Gaussian basis sets: Some recent results and prospects. *Advances in Quantum Chemistry*, 28:47–63, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602063.

Witkowski:2018:DBA

[WmG18] Mateusz Witkowski, Szymon miga, and Ireneusz Grabowski. Density-based analysis of spin-resolved MP2 method. *Advances in Quantum Chemistry*, 76:279–293, 2018. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327617300412.

Wineland:1998:CQS

[WMM+98] D. J. Wineland, C. Monroe, D. M. Meekhof, B. E. King, D. Leibfried, W. M. Itano, J. C. Bergquist, D. Berkeland, J. J. Bollinger, and J. Miller. Coherent quantum state manipulation of trapped atomic ions. *Advances in Quantum Chemistry*, 30:41–64, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S006532760860502X.

Wladyslawski:2005:AEG

[WN05] Mark Wladyslawski and Marcel Nooijen. Analytical energy gradients for excited-state coupled-cluster methods: Automated algebraic derivation of first derivatives for equation-of-motion coupled-cluster and similarity transformed equation-of-motion coupled-cluster theories. *Advances in Quantum Chemistry*, 49:1–101, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605490012.

Woolley:1998:GIM

[Woo98] R. G. Woolley. Gauge invariance and multipole moments. *Advances in Quantum Chemistry*, 32:167–180, 1998. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604128.

Wormer:2006:AMD

[WP06] Paul E. S. Wormer and Josef Paldus. Angular momentum diagrams. *Advances in Quantum Chemistry*, 51:59–123, 2006. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327606510020.

Weiner:1999:TDV

[WT99] B. Weiner and S. B. Trickey. Time-dependent variational principle in density functional theory. *Advances in Quantum Chemistry*, 35:217–247, 1999. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608604621.

Wybourne:1997:GHF

[Wyb97] B. G. Wybourne. Guesses — hunches — formulae — discoveries. *Advances in Quantum Chemistry*, 28:311–318, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602233.

Yablokov:2003:MJT

[YAJHR03] Yurii V. Yablokov, Maria A. Augustyniak-Jablokow, Michael Hitchman, and Dirk Reinen. The mechanisms of Jahn–Teller complex reorientations. *Advances in Quantum Chemistry*, 44:483–496, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603440318.

Yamamoto:2003:FPC

[Yam03] Tomoyuki Yamamoto. First principles calculations of pressure-induced structural phase transition of Co. *Advances in Quantum Chemistry*, 42:199–207, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420492.

Yan:1981:SRG

[Yan81] Ji-Min Yan. Symmetry rules in the graph theory of molecular orbitals. *Advances in Quantum Chemistry*, 13:211–241,

1981. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602944.

Yang:1990:IFD

[Yan90] Weitao Yang. Integral formulation of density functional theory. *Advances in Quantum Chemistry*, 21:293–302, 1990. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608606012.

Yasui:2017:IPE

[Yas17] Jun Yasui. Introducing a polynomial expression of molecular integrals for the algebraic molecular orbital (MO) equation. *Advances in Quantum Chemistry*, 73:161–172, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000222.

Yasui:2023:DAM

[Yas23] Jun Yasui. Definition of the algebraic molecular orbital equation. *Advances in Quantum Chemistry*, 88:75–97, 2023. CODEN AQCHA9. ISSN 0065-3276. URL http://www.sciencedirect.com/science/article/pii/S0065327623000357.

Yeager:2005:MST

[Yea05] Danny L. Yeager. The multiconfigurational spin-tensor electron propagator method (MCSTEP). *Advances in Quantum Chemistry*, 50:289–313, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605500145.

Yamashita:1997:XRA

[YFK+97] Seiichi Yamashita, Manabu Fujiwara, Yuko Kato, Toshio Yamaguchi, Hisanobu Wakita, and Hirohiko Adachi. X-ray absorption near edge structure study and DV–Xα calculations on some square-planar copper(II) complexes with macrocyclic ligands. *Advances in Quantum Chemistry*, 29:357–371, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602786.

Yukawa:2003:LES

[YIYM03] Hiroshi Yukawa, Shigeyuki Ito, Daisuke Yamashita, and Masahiko Morinaga. Local electronic structures of hydrogen and phase stability of vanadium hydride, V_2H. *Advances in Quantum Chemistry*, 42:263–273, 2003. CODEN AQCHA9. ISSN

0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420546.

Yin:2008:SAF

[YKC+08] Ri-Zhu Yin, Yang-Soo Kim, Wanuk Choi, Sung-Soo Kim, and Heejin Kim. Structural analysis and first-principles calculation of lithium vanadium oxide for advanced Li-ion batteries. *Advances in Quantum Chemistry*, 54:23–33, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607000032.

Yamanaka:2012:ESS

[YKS+12] S. Yamanaka, K. Kanda, T. Saito, Y. Umena, K. Kawakami, J.-R. Shen, N. Kamiya, M. Okumura, H. Nakamura, and K. Yamaguchi. Electronic and spin structures of the $CaMn_4O_5$ $(H_2O)_4$ cluster in OEC of PSII refined to 1.9å X-ray resolution. *Advances in Quantum Chemistry*, 64:121–187, 2012. CODEN AQCHA9. ISBN 0-12-396498-9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780123964984000168.

Yokomizo:2000:XSC

[YKY+00] Mitsutoshi Yokomizo, Tsutomu Kurisaki, Toshio Yamaguchi, Hisanobu Wakita, Yoshio Oka-Inagaki, and Kazuchika Ohta. XANES spectral changes for discotic liquid crystals of bis(1,2-bis(3,4-dioctyloxyphenyl) ethanedione dioximato) Ni(II). *Advances in Quantum Chemistry*, 37:57–68, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370046.

Yukawa:1997:NCB

[YM97] H. Yukawa and M. Morinaga. The nature of the chemical bond in hydrogen storage compounds. *Advances in Quantum Chemistry*, 29:83–108, 1997. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602646.

Yukawa:2000:CES

[YM00] Hiroshi Yukawa and Masahiko Morinaga. Characteristics of electronic structures in hydrogen storage alloys. *Advances in Quantum Chemistry*, 37:193–212, 2000. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327600370149.

Yamaguchi:2021:CSI

[YMI+21] Kizashi Yamaguchi, Koichi Miyagawa, Hiroshi Isobe, Mitsuo Shoji, Takashi Kawakami, and Shusuke Yamanaka. Isolobal and isospin analogy between organic and inorganic open-shell molecules — application to oxygenation reactions by active oxygen and oxy-radicals and water oxidation in the native and artificial photosynthesis. *Advances in Quantum Chemistry*, 84:425–564, 2021. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327621000320.

Yamashita:2003:SAC

[YNNU03] D. Yamashita, Y. Nakajima, H. Nakamatsu, and M. Uda. Self-absorption correction for Mn, Fe and Cu L X-ray spectra based on MO calculations. *Advances in Quantum Chemistry*, 42:419–427, 2003. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327603420650.

Yukcu:2013:RSE

[YÖ13] N. Yükçü and E. Öztekin. Reducing and solving electric multipole moment integrals. *Advances in Quantum Chemistry*, 67: 231–243, 2013. CODEN AQCHA9. ISBN 0-12-411544-6. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/B9780124115446000091.

Yurchenko:2005:RVM

[YTC+05] Sergei N. Yurchenko, Walter Thiel, Miguel Carvajal, Hai Lin, and Per Jensen. Rotation-vibration motion of pyramidal XY_3 molecules described in the Eckart frame: The calculation of intensities with application to NH_3. *Advances in Quantum Chemistry*, 48:209–238, 2005. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327605480144.

Yamabe:1978:CEP

[YTF78] Tokio Yamabe, Akitomo Tachibana, and Kenichi Fukui. Complex eigenvalue problems in atoms and molecules. *Advances in Quantum Chemistry*, 11:195–221, 1978. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327608602373.

Yotov:2001:GCK

[YZDM01] P. Tz. Yotov, F. E. Zakhariev, Ya. I. Delchev, and J. Maruani. Gradient corrections to the kinetic-energy density functional stemming from a regular two-component relativistic Hamiltonian. *Advances in Quantum Chemistry*, 39:47–55, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605390046`.

Zapol:2001:ARC

[Zap01] Boris P. Zapol. An attempt to realise the constrained search approach in the density functional theory. *Advances in Quantum Chemistry*, 39:57–70, 2001. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327605390058`.

Zou:1998:TES

[ZBM98] Yaming Zou, Tomas Brage, and Indrek Martinson. A theoretical and experimental study of the quartet system of $B\ I$. *Advances in Quantum Chemistry*, 30:301–310, 1998. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327608605134`.

Zakrzewski:2011:IEP

[ZDZO11] Viatcheslav G. Zakrzewski, Olga Dolgounitcheva, Alexander V. Zakjevskii, and J. V. Ortiz. Ab initio electron propagator calculations on electron detachment energies of fullerenes, macrocyclic molecules, and nucleotide fragments. *Advances in Quantum Chemistry*, 62:105–136, 2011. CODEN AQCHA9. ISBN 0-12-386477-1 (hardcover). ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/B9780123864772000097`.

Zhang:2010:GQM

[ZLC+10] Rui Zhang, Bogdan Lev, Javier Eduardo Cuervo, Sergei Yu Noskov, and Dennis R. Salahub. A guide to QM/MM methodology and applications. *Advances in Quantum Chemistry*, 59:353–400, 2010. CODEN AQCHA9. ISSN 0065-3276. URL `https://www.sciencedirect.com/science/article/pii/S0065327610590105`.

Zhong:2020:ATD

[ZLL+20] Yu-Jie Zhong, Chang-Feng Lan, Bo-Chao Lin, Chong-Der Hu, Yuan-Chung Cheng, and Chao-Ping Hsu. The anisotropy and temperature dependence in the mobility of rubrene. *Advances in Quantum Chemistry*, 81:219–241, 2020. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327620300101.

Zuchowski:2023:PES

[ŻM23] Piotr S. Żuchowski and Katarzyna Madajczyk. Potential energy surface of Li–O_2 system for cold collisions. *Advances in Quantum Chemistry*, 87:209–229, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000321.

Zurowska:2023:ENM

[ŻMM23] Olga Żurowska, Mariusz P. Mitoraj, and Artur Michalak. ETS-NOCV and molecular electrostatic potential-based picture of chemical bonding. *Advances in Quantum Chemistry*, 87:375–396, 2023. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327623000059.

Zientkiewicz:2017:AFT

[ZP17] Magdalena Zientkiewicz and Krzysztof Pachucki. Analytic formulas for two-center two-electron integrals with exponential functions. *Advances in Quantum Chemistry*, 73:103–118, 2017. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327615000180.

Zhao:2008:TIA

[ZZ08] Jun Zhao and Renyi Zhang. Theoretical investigation of atmospheric oxidation of biogenic hydrocarbons: a critical review. *Advances in Quantum Chemistry*, 55:177–213, 2008. CODEN AQCHA9. ISSN 0065-3276. URL https://www.sciencedirect.com/science/article/pii/S0065327607002109.