Title word cross-reference

\[ \! \sum \! \sum \! \sum \! \sum \]
CKL$^{+11}$, DLMH12, GZZM16, HSZ$^{+11}$, KV14, KDS17, MVKS10, MIS$^{+15}$, OOK11, PM18, RF15, SGS15, SDF12, YJN$^{+11}$, Zha11. $\pi \cdots \pi$ [CCCLCGRO14], $pK_a$ [BA11]. $\Psi$ [Lnc14]. $q = 0, \pm 1, -2$ [XhD15]. $r_m^3$ [RCM$^{+13b}$]. $\rightarrow$ [CK10, Chu10, GTK10, HZ11, HBL12, LW1D13, NMLD13]. $S_1$ [KKL$^{+13}$], $\sigma$ [DPSL16, GZZM16, LZZ$^{+15b}$, PM18]. $\sigma \pi$ [CZY11, YWZ14]. $\tilde{\Delta}^1A'[MCLD10]$. $\times$ [SRS14]. $v = 0$ [LWD13]. $x = 1$ [CWT$^{+12}$, LZTV10].

-X-  [SZBM13].  -ZSM-5 [Pon10].

/GIAO  [OPR16].  /GIAO-CCSD  [OPR16].  /metal  [BSF18].  /MgO
[BS16b].  /MM  [CZY11].  /TD  [TS15b].  /X  [BSF18].  /Zn  [GEP.

1  [ZZWX11, CS17, DLZ15, GTK10, NHN16, SYH12, SRS14, TTB+10,
UNT16, XLY12, ZsA10].  1'- [ZZWX11].  1-Methyluracil
[HvM17, HvM16].  1-Octene  [MJLV14a].  1-penten-5-yl
[LXFC17].  1.0  [KJM+17].  1.1  [KYG+15].  1.02  [ZDX11].
11-cis-retinal  [ZLHH14].  13  [LAHS16].  13-13  [LAHS16].
13-dichloropentacene  [ZYG+15].  132b  [RVdMB16].
17  [ZYL15].  1T  [RSK+15].

2  [DPNM11, MWJ+11, DH17, HOM+16, LGW12, Liic14, YZGS14b, Yu12b,
2-benzyne  [FC16].  2'-bipyridyld-3  [MWJ+11].  2-dioxetanone
[RSLML12, dSdS12a, dSdS12b].
2-phenylimidazo  [MWJ+11].  2.0  [Yes15].  2.1.0  [KYG+15].
2.02  [ZDX11].  2H  [RSK+15].  2X  [SIG+15].

3  [MWJ+11, DH17, HPSK12, Spr10, YZGS14b].  3-  [LZL+.  3'-15-crown-5  [MWJ+11].  3.37-34242-9  [Spr10].  3-alternate  [ZWS+10].
3-d  [YZ15b].  3-dihydropyrido  [YZ15b].  3-Dipolar
[YZN13].  3-metal-carbon  [ZYW+16].  3-methyl-7-azaindole
[YYT12].  3-squaraines  [AMQ+14].  3-thienophenic  [NHF+10].
31  [Kne11b, MSK+12].  311G**  [TKN13].  31G  [Mit13].  31G**
[TKN13].  33  [ABB+13, CHR+12b, IC5+13].  35  [SFCCK+15].
36  [SMM15a].  38  [HLXH18].
3c  [KV14, LW16].  3c/4e  [LW16].  3D  [HSB+11, SA10].

4  [YLZ+10, LZTV10].  4'  [YLZ+10].  4-amino-1  [ZZWT12].
4-aminophthalimide  [WHL+10].  4-azaborinine  [RS17a].  4-dihydro-1
[RS17a].  4-hydroxyphenylpyruvate  [DGH+11].  4-substituted
[WHL+10, WHL+10].  4e  [KV14, LW16].  4Fe  [PNI13].  4S  [PNI13].

5  [ZZWX11, cCVG+14, LL10c, Mor15, Pon10, SOvG12].  5-b  [YLZ+10].
5'-bridged  [ZZWX11].  5-nitroiminotetrazolate-based  [ZYL+12].
5-triazine  [WDLG12].  5-triazines  [YPC+10].  5-triethyleniminotetrazolate-based
[ZYL+12].  5-triethyleniminotetrazolate-based  [ZYL+12].
5-triethyleniminotetrazolate-based  [ZYL+12].
5-triethyleniminotetrazolate-based  [ZYL+12].
5-triethyleniminotetrazolate-based  [ZYL+12].
5-triethyleniminotetrazolate-based  [ZYL+12].
5-triethyleniminotetrazolate-based  [ZYL+12].

6  [WDLG12, ABM+15, TKN13].  6-311G**  [TKN13].  6-31G**  [TKN13].
6-bisphosphatase [RAR+11]. 6-fluoroquinolones [MPNS13], 6'-tetra [WDLG12]. 6-trinitrotoluene [SH14]. 6.0 [GLW13a, GLW13b]. 60th [HIS17].

7 [ADF+10, MBR+15]. 7-azaindole [YYT12]. 7-tetraene [ABDGN12].

8 [AAC+16]. 8-formyl-7-hydroxycoumarin [LZHH11]. 8R [BG13].


Absorption [RS17a, ZLL+10, FD13, HNN+17, KB16, LLBO12, LX11, LXZ+10, PMC+17, PDMT10, PDG+16, SGDT10, TYN15, TZ12, Tsi14, WWD14, ZTH+15, ZDX11, QCR12]. abstraction [AAMD+11, BS10b, CSXZ17, GY12, JCG+10, LJW+11b, WLHZ12]. Ac [SNKS10]. Accelerated [MFEM15, MFEM16, AGB13, BDTP11, CVT+11, DWC17, GBL+11, HEMCZE+14, HAP+12, KV13, LL11, REV+17, YLX14, YSG12, ZC14, ZLL+13]. accelerates [HS17b]. Accelerating [HASR+12, LZ12, YWJ+16, HP10a]. Acceleration [BKŠ+11, ON14, SOM+13, UTM11, WSGN11, OOT15]. accelerator [SBV10]. accelerators [KK17a]. acceptance [BB11b, KB11c, NDIW15, dRBO13]. acceptor [Gil11, Lu11, MSV16, MIS+15]. acceptors [uLhY11, TWZ12]. accessibility [LHL+10]. accessible [FZY+12, WX+12, WBF17]. Accessing [JZYM14]. accompanying [HSN14]. according [GM17, LPE+10, YZZ16]. account [EPH+13]. Accounting [XML+15, HH11, MBC11]. Accuracy [DBM+15, FCE15, KFY+13, LLH17, BPB11, GRARO+14, HWLW11, KSR+16, LZ12, LDZW17, NTN15, yOaCG10, RS13, RVCT13, Rob13, TO10, ZYS+10, Gil11]. Accurate [BS16b, CX10, CSXZ17, EFOF13, FLMI11, IN13, KG15, LYG+13, LLH11, LWL+10, MK13a, MFR+11, NWW17, Pol13, PVJ10, Sch12, SRR16, SY11, ŠSB+16, SYZ+17, TH13, WL14, YB16, ZWLX11, AF14, BS10a, BPM15, Ben17, CCLP12, CSOGA17, CRZ+18, DKE+17, GAI13, GBW+14, GWZX12, HRC13, LC17b, LZZ14, MAK+14, ME10, MFR+17, NHH16, yOTn16, dRL11, RB13a, RCR+16, RDDS10, RR14, SH15, SS16b, VAMS14, VDVR14].
WXS^12, WJG^13, WX12, XSZL11, YOMT14, dVZ17, dSAAdSL13.
Accurately [Bow16, LFB14, MA16, Zha12b]. ACE [WCDM11, LH^1+10].
acetaldehyde [AS11, AAMD^1+1]. acetals [YZL^1+15]. acetamides [JSW10].
Aceto [SJD14]. acetoxyhydroxyacid [XLY10]. acetone [RS14]. acetyl
[ZBP11, ZP13]. acetylacetone [SJWE10]. acetylation
[FHK^1+12, IMK^1+16, LHL^10]. acetylcholine [SRA17].
acetylene [GRCL12, HSY^1+11, LT13, Tak10]. achieve [PH17, RAR^1+1].
achieving [NNK^1+16]. Achim [Spr10]. acid
[BLG11, CYY^1+17, CC18b, CM16, CB11d, FD14, FZL^1+15, Fel10, FP17b, FCE15, GRL^1+11, GRL^1+12, HPT16a, HGY^1+17, HCP15, KLS10, KML10, LBC^1+12, LXL^1+11, LF12, LP11b, LPMT17, MLS10, MRO17, NHF^1+10, OXW16, PDH13, SISK10, SZBM13, SBW12, SV11, TL16, VMPS17, WC14, W12, XVN17, ZSB^1+11, ZWP11, ZHHX11].
acid-catalyzed [CYY^1]. acid-water [TL16]. acid/base [VMPS17].
acidic [APY^1+16, YDX16]. acidities [ALK^1+5]. acidity [CRZ^1+18, CPK12].
acids [CCCLCGRO14, DKE^1+17, EHSPT16, FCE15, GREA11, RSL16, XLY10, ZKH^1+10]. ACP [STM^1+15, SJ16].
across [AAC^1+16, GMPB12, MGS^1+16]. acrylate [LZL^1+16]. act [LC10]. actinide
[RKS^1+13]. action [XLY12]. activated [CV12, KSR17]. Activation
[Niz13, AALCM11, DR11, DSM^1+11, FB12, MRR11, MBFG15, TS15a, WC11, XLY10, YXXZ17]. activation-strain [FB12]. activator [BM12]. active
[AIGP15, Cas13, DPB^1+12, LVT10, PDG^1+16, SCSW13]. active-space
[PDG^1+16]. actives [EOO^1+16]. activity [BPC13, DXL^1+10, GAI13, GHL17, GFPSD17, MJLY14a, RCM^1+13b, SLY^1+10, TD10, TTB^1+11, YB13, ZSA10]. acute [TL1^+12]. acyclic [ZH^1+10]. acyl [PS10]. adamantane [EHSPT16].
adamantane-based [EHSPT16]. adapted [FF11, SSSM15, TH13, YKH15].
Adaptive [JSK14, KEMP17, LZZ^1+17, AOW11, BGR13, DSK17, FHMB15, HDF^1+15, MJ14, MBFP15, MJG^1+15, OZ14, PN13, SNS13, WMW^1+10].
Adaptive-numerical-bias [KEMP17]. adaptively [SR18]. adcluster
[IN13]. Adding [XHLH16, Zha12b]. addition [FBW14, KS13b, NDG14].
Additive [XVA^1+16, DPNN11, HM13, TSS^1+16, VHA^1+10, VMPS17].
additivity [ZRL^1+15]. address [LG14]. addressing [cCVG^1+4]. adducts
[LC10, LS11b, ZRCC11]. adenine [BZH14, LTL12]. adenosine
[SRA17, WZQW10]. adiabatic [UD12]. adjacency [GZH10]. adjusted
[HH15]. Adjustment [BLZ^1+3]. ADMA [MA17]. AdNDP [KDS17].
adrenergic [CV12, LLHM16, VKC10]. adsorbate [GBS^1+17].
adsorbate-induced [GBS^1+17]. adsorbed
[MCF10, PXW10, SLL13, SIG^1+15]. adsorbents [HVS16]. Adsorption
[CCJ^1+11, FVP14, HB15, KD10, LH14b, PH12, AS15a, BS16b, CMM18, CR14, cCVC^1+14, He10, LL13a, LPK16, LPLS16, LZ14, LT14, LCM^1+14, NPP13, PG12, PLZ17, RHHN10, SH14, SDB^1+16, SKTT11, SYZ^1+17, VS14, WSZW15, WYGW12, YDR13]. Adsorption-induced [HB15]. Advanced
[WBN^1+13, Yan16]. affect [SV15, UNT16]. affected [OHN11]. affecting
[GMSV14]. affects [CLK11]. affinities [CMD13, CTP13, GRS15, MGWR12].
affinity

After

Ag-nanocluster

against

Age

agents

aggregated

against

Age

against

AgX

AHAS

aimed

Al

Al-hydroxylated

Ala

alanine

AlB

alchemical

alcohol

alcohol-based

aldehydes

Alder-ene

Alderase

aldol

aldosterone

algebraic-diagrammatic

Algorithm

algorithm-artificial

algorithmic

Algorithms

aligned

alignments

aliphatic

alkaline-earth

alkane

alkanes

alkenyl

alkyl

alkylthiols

alkynes

All-atom

all-electron

all-organic

alkene

alkenes

allene

allenes

allocation

allophycocyanin

allosteric

allowing

alloy

alloys

Alpha
alphabets [PHDH13]. AlPO [LL10c], alter [CBTZ16]. alterations [HHT+13a, HHT+13b]. alternate [ZWS+10].
alteration [ASL+11], alternative [MA17, NYN17, TF15, Wei12a].
alumina [SH14]. aluminum [GWJJ12, LK16a]. always [KSC16, MBFG15].
AM [FBY+17]. AM05 [MMJ10]. AM1 [KLS10, KMLS10]. AMBER
[MSK+12, RSR+12, GCW14, MSK+10, MJG+15, OYK+11, PGW+17,
SOYC12, SJ16]. AMBER-compatible [SOYC12]. AmberTools
[RN5F+16]. amide [LJW11a, LW11, NDG14]. amidoborane
[PMT16]. amidoboranes [DLT17]. amination [YZ17]. amine
[AK10, BMB13]. amino [CCCLCGRO14, CFC15, CB11d, DKE
+17, FZL+15, FP17b, GRL+11, GRL+12, HCP15, KLS10, KMLS10,
LXL+11, LP11b, MRO17, PHDH13, RSL16, SISK10, SZBM13,
WC14, ZZWT12, ZKH+10, ZHHX11]. amino-acid
[KLS10, KMLS10]. aminoacid [MC10]. aminophenyl
[LZL+16]. aminophthalimide [WHL+10]. aminopolycarboxylate
[CMD13]. ammonia [BEPM14, CC12a, KT12, SNS16, SJZ+15, VS14].
ammonia-borane [BEPM14]. ammonium [AvKSP16]. AMOEBA
[HLW+17, MBE16, PZCL16, XP13]. among
[KYB13, SH15, TCGNT18, WGL+11]. amorphous [Fom13]. amounts
[FN12]. Amsterdam [FP13, SFG+17]. amyloloid
[I013b, LH11]. analog [JBAM11]. analogs
[DCHL12, LP11b, SISK10, VM11, WBT10]. analogue [PGW+17].
alogues [LPS+13, SGWA17, VVBL17, WS12, YLL11]. analyses
[BSF18, KASH14, KP11, PZBA13, SKGB13, VVJ15, XWW+11]. Analysis
[CDM+15, HAI+16, JCGM18, MOS12, XFG+16, AKMT11, AST+16,
ASL+11, ARRC15, Ano15-58, BK15, BH14, BSPP+13, BBG+18, CLFRO18,
CMM18, CAF+13, CEC015, CCC+11, CAT+13, CH14, DMJ17, DHH+11,
DJ12, DBK17, DSC15, EHSPT16, Fer17, FB12, FHW+11, FHK+12,
GVF+10, GLW13a, GLW13b, GNDA+12, GCP+13, Han11, HCD+10,
HPK12, HHT+13a, HHT+13b, HDHL15a, HDHL15b, HDHL15c, HWW17,
Hug12, Jan16, JHH+13, JJW+14, JZZM14, JCX10, KG13, KGY+15, LL13a,
LCPS13, LMZ+11b, LFMI12, LAHS16, LGKS17, MDTD13, MJ14, Mez10,
MADWB11, MCLD10, MGS+16, MCK17b, NI15, NS17, OXW16, OC14,
PTK11, PSP15, PRY1+17, PTB+15, PPUBGD10, FVS12, PS14, RDT14,
REL17, RLG14, SLY+10, SBB10, SPR+11, SGS15, SNDK16, SS13c,
SPR+13, SH18, TYN15, TC16, TD10, TTB+10, TS10b, UKS11, VDMA13].
analysis [WNP+16, Wei12a, Wei12b, XFG+15, YK13, YNH+17, Yes12,
Yes15, ZCS+15, ZBL16, ZHH2, vSGP10, ZSB+11]. Analytic
[Boz18, MDTD13, SXX13a, SXX13b, MY17b]. Analytical
[CCB15, HNWFO7, HNWFO12, HH17, LBG16, SFG+17, WOH18, CHC+13,
FBY+17, HH16a, KN17, KTSW11, MK13a, Pon11, ZWF15]. analytics
[JZL+17]. analyze [LP11c, OVPK15, QLQ11, RLG14, YKO+11, dVAG16].
analyzer [JJW+14, LC12, PVZ13]. Analyzing
[BD11, MRB14, BCP+10, HPT17, LPS+17, PHT17, SWA13, WES13].
anapole [ZPP+16]. anatase [HRL11]. and/or [KB10, Pog10].
androstenedione [VCM15], angle [CKP10, GBFD12, XML+15], angle-dependent [CKP10], angles [BKLA13, EJ13, FZY+12, GREA11, KTK17, LDH+14, OZ14, YZ16]. angular [BBG+18, ENKK+17], anharmonic [Kow11, SSWX14], anhydride [SSP+13]. anhydrides [RB12], aniline [PLP+16], anion [CG15, LC10, uLhY11, SDF12], anionic [SSP+13]. anhydrides [RB12], aniline [PLP+16], anion [CG15, LC10, uLhY11, SDF12], anionic [GZZ12, GWPJ11, HPL13, JCP14, OZ14, YZ16], anion [CG15, LC10, uLhY11, SDF12], anionic [GZZ12, GWPJ11, HPL13, JCP14, OZ14, YZ16], anions [PVS12, RDT14, RJS17, ZWY+10b, ZYL+12], anisotropic [Ano10a, CAT+13, EPH+13, ENKK+17, NLP+16, SLX+15, SN10]. anisotropy [CGP12, LPLB16, ZLZ14], ANN [XWW+11], annealing [RHJ11, SHMO11, SHL+11, ZC14, LMZ11a], annihilation [BL12], annulated [RS17a], Anomerization [SM17], anomers [HH11], antisense [ICS+12, ICS+13], antitrypanosomal [PSdPE+10], antitubercular [TD10], AO [YOPB16], AOFORCE [vW11], API [LAS+14]. Applicability [MAK+14, DI11, GHL17, GKR13, HH15, JZZM14, Ray13, RKG11]. applicable [CL16, WGL+11]. Application [AFBR17, BAMR13, BPE16, GCCM15, HTS15, LDG+15, MBA11, MH10, OL13, PAK15, RVP+11, SMP17a, SRS14, SC17, SDL14, SMM+18, VKTRJ15, WH11, ZsA10, vSGP10, CSAdOM17, DGPMM14, Elk16, GLB16, GFG11, GCW16, IUK+11, KFY+13, KSK11, LHLM16, LP11a, LLL+10, LLLC11, LvG13c, MTD13, PCH13, RZG+13, RCM+13b, SN16a, SLX+15, SYH12, VV14, VKC10, WCDM11, You10, AFP13, BD11, CZNA11, Fer13b, Fer13a, FCOGM12, GAI13, HYUS11, KUDG12, MCC11, Pet11, PW12, TSZQ12]. Applications [KGHC15, LCPS13, LCA17, APK14, CGP11, Feli10, GBFD12, HZY+10, HCD+10, IO13b, KKO+16, uLhY11, LJR+12, MG11, SSSM15, SGM+13, ISP+10], applied [BLG11, CTP13, GKR13, KKR+13, LTT16, Ray13, RKG11]. Applying [KB11a, ZSLL17, CC11], approach [ACD+13b, BPE16, BVHI17, BGR13, CCLP12, CRZ+18, CHC+13, CXS10, DK11, DGPM14, DVPV14, DFF+15, DHE+12, FRSA14, Fer17, FNSF+11, FCPF17, FD16, FSD+18, GPE13, GZ14, GH16a, HRC13, HDH12, HNN+17, HBY10, HZS17, JCX10, KV12, KV13, KSK11, KT10, LTL12, LHI14a, LG14, MZZ11, MGWR12, ME10, Mor15, NO16, OT12, PRP15, PMC+17, PSdPE+10, PH10b, PBE16, PPUBGD10, PLP+16, RKG10, RB12, RVP+11, SLT14, SEF+16, SH11b, SY16a, Sti15, SLLL13, SGH+16, SM17, TAG16, TSR+16, VVLG17, XZ11, YKO+11, ZSLL17, ZLJ10, GFG11, ACD+13a]. approaches [BH13, CME11, DBM+17, ECZWD17, HBI+17, LSH+11, RLDJ17, RSRR15, VLB+10, YJ11]. Appropriate [LZLC13], Approximate
GBVA11, HRK+10, HM13, JYC+16, JGS+17, Jor17, KV14, LC10, LZZ14, MZZ11, Niz13, OCW+15, ST11, SM14b, SYH12, Tsi17, VIT+15, VHA+10, VKAM12, VI17, VDVR14, YPKB12, YHCS11, dLC17, dVZ17, YMP14.
atom-typing [YPKB12]. Atomic [BMFG16, EPD+10, KGM12, AYYO17, BLDK+13, BB11a, CP15, EKH14, Elk16, EP12, EV14, HS12, JMLL13, JXSW15, KOP+14, KR12, Lar11, LZGS11, MK13a, MPA10, MPA12, Mat10, MPBJ11, NPG17, NOKJ16, OBW12, OV14, Pol13, RB13a, SS16b, SE14, SMP17b, VSA11, WWCL15, YOMT14]. Atomic-resolution [BMFG16, NPG17]. Atomistic [BH13, CHKR10, MBA14, SE14, BLKP12, CZNA11, DDP16, HDPM14, LZ12, MK13a, MPA10, MPA12, Mat10, MPBJ11, NPG17, NOKJ16, OBW12, OV14, Pol13, RB13a, SS16b, SE14, SMP17b, VSA11, WWCL15, YOMT14].


12
[FMG12]. balls [CVT+11, KRSC12, OV14]. band [QZI0b, QB10, QB11, SH11a, VLGK+17]. bang [KPF+15, MPA12].

Baoshan [JW12]. bare [SM17]. barrel [LJR+12, yOnCG10, WXL+12].

Barrier [BS10b, ZW17, GAJ+17, HRRD16, KG15, MSBF16, Yu12a]. barriers [HH10, MJLV14a, SFD14, XLYZ10, dALdS+15]. basal [LL13b]. base [BH13, BZH14, DKT13, FD14, HwM12, LZh+11, LW11, ONTTL16, SZZS16, VMPS17, WXY14, YKH+10, ZLL+10, ZLHH14]. base-catalyzed [WXY14].

Based [CSM16, SN16b, AMGB10, ALK+15, AM10, AO10, BSCCJ+13, BARM13, BPE16, BMPML+13, BHR15, CGPP11, CDS16, CH10, CGBK13, CB11b, DK11, DVPF14, DH14, Dil15, DJX+11b, DJX+11a, DFF+15, DPB+12, DXL+10, DCS15, DMM+15, EFAC13, EHSPT16, EV14, EBP13, EP15, EBPK17a, FCL+10, FCOGM12, FCPJM14, FMG12, Fra15, Fra16, GLB16, GH17, Gar12, GJMPAM+14, GBVA11, GV+10, GS13, GBSE11, GZ14, GKB15, HKRS11, HS11, HLS12, HTS15, HZY+10, HKR12, HB14, HEMCZE+14, HSB+11, HYUS11, HM13, HLWD15, ISN13, JWW+14, JLCA17, KGHC15, KZ+16, KNE11a, KC14, KP11, LFB14, LZ11, LDB+17, LMZ+11a, LMZ+11b, LWL+11, LLZ+12, LSH+11, LZS+17, LTA+11, LGKS17, MDTD16, MZZ11, MMM+16, MC10, MA16, MS13, MPNS13, MMZW14, MFR+17, MO15, MNNK10b, NC12, NC13, NC14, NJX+10, NG10, OVPK15].

based [OZLSBH12, PRP15, PLZ17, PCI11, PBBP11, PN13, PKIC11, PP14, PLH16, PBE16, PPUBGD10, RLD17, RZG+13, RV+11, SMI14b, SFG+17, SL+12, SLX+15, SFDE16, SLC+17, TYZ+16, Tak14, TTB+10, TS14, VGV+11, VVJ15, VKC10, VSA11, Vor10, WXL+12, WCDM11, Wei12b, WL14, WS13, WDHZ13, YJN+11, YZ16, YWJ+16, YZZ16, YDL+10, YJ11, YN15, YS13, YS15, YS10, YZZ+17, ZSLL17, Zha12b, Zha12a, ZY14, ZM10, ZY+12, ZT14, dCLFGL13, dSVdM+16, dVZ17, NKJ16].

based-on [CDS16]. bases [CWZB10, KASH14, MSLS10, SBW12, ZLL+10, Zha12a, ZBMZH15]. Basic [CMTvG10]. basin [JLH+14, RDRC16]. basin-hopping [JLH+14]. basins [SNB13a, SNB13b]. Basis [BLF14, BRLS08, BRLS12, PHK14, SN16b, TKN13, ACD+13a, ACD+13b, BLFZ13, BLL13, BLBG+13, BS10a, BLG10, CC11, DBM+15, DLZ15, Fer13a, HSN14, Hii13, HBL12, KK17a, KNP+12, LBH+11, LCW12, Leh15, LYC+13, Mit13, OAN15a, PML+12, PGdO+16, PO13, Pla11, PD11, RLD12, SWM10, SG10a, Sea10, SNKS10, Sun15, SG13, TH13, WX12, ZPP+16, ZLT13]. Batch [WHJH13, TJB12]. bath [CSEMB+16, MO15, Vor12, WAM17]. BaTiO [BE12, EB12, EBK13]. bay [QCR12, WvrSM14]. Bay-type [WvrSM14].

Bayesian [Fer17, GZ14, VZ14]. BayesWHAM [Fer17]. BD_BOX [DZT11].

Be [LDJ+10, EPH+15, IMSR18, KV15b, LWZ+11, NG14, SMGB11, TH13, TCPFC14, Zha12b, BWKW10a, CCM15, CM16, ZLY+16]. Becke [FPV13].

BeH [ZLY+16, ZLY+16]. behavior [AVHB18, BVY+12, CME11, CSAdOM17, FCD10, FTR15, KRTB10, LZY+12a, PD11, TDG+12]. belief [GFPSD17]. Benchmark [WSZW15, AF14, ANH+11, CSXZ17, cCVG+14, GAI14, KG15, RS13, ZWGO16, IKN13]. benchmarked [XYW+14].
Benchmarking [Ben17, GAJ+17, Hug12, LCM+14, GP11b, HRJ+14, HRJ+15, HZ13, JRSHP14, KSM17, RSG14]. benchmarkings [GPdC+16].
bonding-induced [YLZ+10]. bonding/back [PKK17].

Bonding [WFZ+18, DGB+13, ED15, FPRSI4, Gra18, HH15, Jab14, JJJ16, LZH+11, LZY+15b, LDG+15, OOK11, Rob13, SM16a, SK13, SJ16, YLL11, YKH15, YJ17, ZY14, ZYW+16, vSGP10, EHSPT16].
catechol [PBLdS12]. catechol-O-methyltransferase [PBLdS12]. Catenanes [LAHS16].
cathespin [ETLS17]. cation
[CCCLCGRO14, CGPP11, DLMLH12, DDM+15, RMGB11, SSGS15, ZYL+12].
Cationic [HJ13, W.JX+10]. cations [CC18b, KGR+16, LCL+10, LdSRR16, PVS12, SBD+17, Tac17, THP+15, ZWY+10a, ZWS+10].
cations/nucleobases [CC18b]. caused [GDV17]. cavitand [CC18a].
cavities [HRB+17, ZSB+16]. cavities/vacancies [HRB+17]. cavity [ZWS+10]. CAVS [SDZ17]. CB [BTMS12, CC18a, ILKR11]. CBS [KG15].
CBS-QB3 [KG15]. CC [Gil11, LLTC12]. CC2 [SGWA17]. CC3 [LZ14].
ccCA [RJWW12]. CASSD [BG17]. CBB [BTMS12, CC18a, ILKR11]. CBS [KG15].
CBS-QB3 [KG15]. CDOCKER [GLB16]. C enumerates [CROB16]. Ce [Ibr17, YOPB16]. cefotaxime [MFM+12]. cell
[ACS12, CGBK13, Elk16, Fom11, Gon12, JMS14, SRL+15, VÅA14, dACP12].
Cells [FPV13, ACS12, DZA11, DGL+13, JYS+12, LCL+15a, SV11, SLC+17, TZ12, YJN+11]. cellular [VBD11]. cellulose [GS12, LHT15, GS12].
Cellulose-Builder [GS12]. cementite [VED10]. cementite-type [VED10].
cementitious [TZ11]. CENCALC [SDMS13]. census [PPUBGD10].
CEPA [Sch12, SB14]. ceramics [RKB+14]. CERES [CPRS18]. cerium [SRL+15].
CF [JCG+10, NMLD13, RVdMB16, ZLL12, AR10, CROB16, NMLD13, ZZL+10a].
CFCF [NMLD13]. CFCl [JCG+10]. CH
[AR10, LW12, LdG+12, WLH12, ZZL+10b, ZYLL12, ZLL12, BS16b, CK12, CXW14, CY12, HVS16, JCG+10, KBC12, LW12, LGW12, LLTC12, LJG+11, MCU15, OK11, RVCFF13, TCPPC14, VVY17, VDVR14, WLH12, ZZL+10a, DR11]. CH/ [OOK11].
chaff [NMF+14]. Chain [xRWG17, BFI+13, CHK10, HAL14, KV14, KLS10, KMLS10, LP8+13, LZGS11, LP11b, LgV13a, LzLMP16, OZ14, PD12, PS10, QZM11, SA13, SISK10, SZBM13, TSN16].
chains [AFSW16, FP17a, JSW10, LZZ14, NPP13, Pla11, PLH16, TLdG+12, TS15b].
chalcogenides [SPS+12]. chalcone [CPLL11, YZ17]. challenge [SDM+16].
Challenges [HGY15, KHW17, HLvdV13]. challenging [CAP17, VT14, WLF11]. change [EMD17]. changes
[GDV17, GBS+17, HB15, Lk13, MjL14b, M017, RO14b, YZGS14b].
Changing [XVN17, LVG10]. channel
[HYZ13, PVL+13, SFBT17, SY16b, TCX+13]. channels
[KC13a, LL10c, OKIS17]. character
[BMB13, Cas14, Ibr17, RJJ+11, YSSB12]. characteristics
[PSL16, Gav12, LT14, Mat14, RDT14, TZ11]. Characterization
[VT14, XWSW13, CBP+15, DGL+13, GBW+14, GZZ12, Kop15b, MjBM12, MPA10, RNP13, ZYG+14]. Characterizing [LH11, PRSG13, She12, Yu12b]. characters [LSH+11, ZLL+10]. Charge
charge-assisted [SSGS15]. charge-inverted [UT15, YJ17].
Charge-transfer [JM11, ANH+11, EFAC13, YLZ+10]. charge-transport [HLWD15]. charged [BK13, KD10, MRO17, NPP13, RJS17, Tsi14].
Charges [WFZ+18, CCB15, IM17, JMLL13, RB13a, SN15, TBSM12, VSA11, Yan14, ZBG11].
Charles [HIS17]. CHARMM [MSK+12, AKMYB18, BF17, DPNM11, GLB16, GZM11, HBJ+17, HC14, JCL+17, KYB13, LZdlL+10, MSK+10, MMZW14, RR14, VHA+10, WCJ+14, XVA+16, YHVM12]. CHARMM-based [MMZW14].
Chatt [Bac12]. CHCICH [WLHZ12]. CHEM [ABB+13, CHR+12b, HNWF12, HLXH18, ICS+13, Kne11b, MSK+12, RK16a, SFCCK+15, SMM15a, GCC14, GKV+13].
Chemical [BLG10, BCP+10, JCGVPHT17, OM12, SLLL13, VGTI16, ALK+15, ASS+17, AAC+16, APA+14, Bac12, Ben17, Bou14, Cam15, CHP11, DKE+17, DS12a, DJ11, DB12, EOA+11, FB10, FVB10, GH10, GGM+12, GPGSM11, GPSCM12, HPT+16b, HHDC16, HJ13, Ii12, JKS+16, KV12, KASH14, KP11, LK11, LHZ+11, Li14a, Li14b, MDTD13, MDTD16, MN15, MAPB10, MSvG12, MSSP17, MFR+11, MMJ10, MH10, NCV10, NC13, NC14, OKIS17, OSHG17, ONTTL16, OC14, PTK11, PGD+16, Pie14, PBG17, RK15, RSKG14, SRA17, SLC14, SCOJ13, SEF+16, SKMS13, SHB17, TLA10, TG12b, TR12, UD12, VBM13, WBT10, WCT+11, WF16, Wei12b, WL14, Wu10, WDP+12, YZ15a, YB16, ZY14, ZBB16, ZT14, dCDP15, VBD11, Chat10].
chemical-bonding [MDTD13]. Chemically [EFAC13, ZZ12, Zim13].
chirality-based [PBBP11]. Chloride [KJ10, KLN16, Rab12, SG10b].
chlorides [RFP11, YZGS14b]. chlorine [Sán17, ZBMZH15]. chloroform [GC11, WG12]. chloroform-to-water [WG12]. CHOCL [LHHW14]. choice
The image contains a page of a document with text that appears to be a list of abbreviations or references. The text is not clearly legible but seems to involve scientific or technical terms such as "coarse-graining," "cobalamin," "codes," "coefficient," and "cofactors." It also contains names and codes that might be associated with specific references or authors in academic citations.

The text is not legible enough to extract meaningful information in a coherent format. It appears to be a page from a scientific or technical document, possibly an academic paper, report, or reference list.
Complete
[SN16b, CSKH15, LYC+13, OAN15α, SPS+12, SCSW13, TCB16].

Complexity-optimization [Leh15]. Completeness [Leh15].

Complexes [EHSPT16, GPdC+16, SKGB13, AvKSP16, AMK11, ASMS10, AK10, BCSJ+13, BLFZ13, BLDK+13, CSGOA17, CPRS18, CWT+12, ČMD13, CZH12, CGPP11, CAT+13, CMS13, CM16, CB11d, DS12b, DLP11, EPH+13, ED15, FHW+11, FCE15, FPB12, FB14b, GKI5a, GHL17, GPK+16, Gil11, Gra18, HDK+12, HSY+11, HKR12, HLB15, HRJ+14, HGHP14, HRJ+15, HDPM14, HG10, JRSHP14, KTI2, KPL13, KTK17, LS11a, LLC+10, LWL+11, LHHW14, L LZ+15b, LDZW17, LZX+10, LYSS11, LJJ+11, MC10, MFR+11, OSHG17, OOT15, PGCT+12, PHK14, PM13, PZBA13, RRH12, RHPWS13, RLD12, SB10, SLIB12, SPR+13, SDL14, SGH+16, TLY+12, TS15a, Tru18, TS02b, VB+10, VVP12, VYV17, WL14, XMS16, YKH15, ZCK+16, ZRCC12, ZZL+12, ZLZ14, ZDX11, ZYW+10b, ZYW+10a, ZBMZH15, vSGP10].

SGS¹⁶, SNDK¹⁶, SY¹⁶a, Su¹⁰, SDMS¹³, SDL¹⁴, SIG⁺¹¹, SIG⁺¹⁵, TF¹⁵, TLA¹⁰, TRA⁺¹⁶, VZ¹⁴, WDI¹³, WXL⁺¹², WCDM¹¹, WS¹¹, XWSW¹³, YDX¹⁶, ZCK⁺¹⁶, dCLFGL¹³, FHW⁺¹¹, Spr¹⁰]. computationally [JJAB¹⁶]. computations [AGB¹³, BLBG⁺¹³, CC¹²b, SRL⁺¹⁵, VECT¹², VAMS¹⁴, YB¹⁶, dACP¹²]. compute [HDM⁺¹⁵, KK¹⁷a, YAS¹³, dVAG¹⁶]. computed [CCYL¹¹, Fra¹⁵, Fra¹⁶, HJ¹³, JJH⁺¹³, RLDJ¹⁷, UKS¹¹]. Computer [BBG⁺¹⁸, CLC¹¹, BV¹⁴, CBP¹⁴, DSK¹⁷, GP¹², KSH⁺¹⁷, SYN⁺¹²].

Computer [BBG¹⁸, CLC¹¹, BV¹⁴, CBP¹⁴, DSK¹⁷, GP¹², KSH⁺¹⁷, SYN⁺¹²].

Computerized [NYH⁺¹⁷, VBDS⁺¹¹].

Computing [Ano¹⁰a, GK¹⁵a, HJ¹³, JJH⁺¹³, RLDJ¹⁷, UKS¹¹].

Conceptualized [PSP¹⁵].

Concepts [CLFRO¹⁸].

Conceptualizing [LLL¹⁰].

Conceptualization [IPAA¹¹].

Conceptualize [GRL¹¹, GRL⁺¹², dSVdM⁺¹⁶].

Concurrent [HS¹⁴b].

Conduct [SV¹¹].

Conduction [KJ¹⁰].

Conductor-like [KB¹⁴b, SDF⁺¹⁷].

Conductors [MRB¹⁴, NFI⁺¹⁶].

Cone [BKLA¹³].

Confidence [KSM¹⁷].

Configuration [SS¹³a, Cas¹³, CTP¹³, CAP¹⁷, EK¹⁷, FF¹¹, GA¹⁴, GP¹¹a, HPT¹⁷, HBL¹², LCB¹⁰, MIS⁺¹⁵, MCP¹⁸, ZRCC¹¹].

Configurational [RO¹⁴a, WDHZ¹³].

Confinement [CC¹⁸a, TM¹⁶].

Conformational [AD¹⁰].

Conformational-space [AD¹⁰].

Conformationally [AFPI¹³, CP¹⁵].

Conformations [CC¹²b, DJ¹³, LC¹⁶, LZZ¹⁴, NR¹¹, OCL¹¹, PH¹⁰a, RVP⁺¹¹, ZC¹⁴].

Conformers [DBG¹¹, HH¹⁰, HH¹¹, LG¹¹, MS¹⁷, TCGNT¹⁸].

Conjugated [MSV¹⁶].

Conjugation [LBH⁺¹¹, NC¹³, RKGN¹⁰].

Connected [ACD⁺¹³a, ACD⁺¹³b, NR¹¹].

Connectivity [IP⁺¹⁰, ZYS⁺¹⁰].

Conquer [BRP⁺¹², BGR¹³, KKN¹¹, NYH⁺¹⁷, NN¹⁸, NKN⁺¹⁶, WX¹², YN¹⁵].
consensus [DMJ17, SRA17, PLV^{+11}]. consequences [KG15].
conservation [MB16]. Conserving [PH17]. considerable [LLD17].
Consideration [Fom11]. Considering [CSEMB^{+16}]. Consistent [MKO^{+13}, POB13, BKŠ^{+11}, BY11, BK17b, DK11, GBVA11, Hill13, HKR^{+14}, JSXH16, KT10, LBH^{+11}, LCW12, ON14, SPS^{+12}, SMP17b, SCSW13, TYN15, VGV^{+11}, YN15, ZBG11, BLKP12], consistently [IM17].
consolidate [BK17c]. constant [AB16a, CS14, KSK11, KN^{+12}, MK17, PS13, RAGLL11, STM17, Vor12, WOH16, WOH18, dACP12].
constant-distance [dACP12]. constants [AAMD^{+11}, CBH14, CPK12, DSD^{+11}, ECZWD17, FD14, GAI13, GKR13, MG11, OZLSBH12, Ray13, RSG14, RKG11, Rui11, RKK16, SACdG14, TTR^{+12}, Tsi14, WL14, XWW^{+11}, YS13, ZZZ^{+10b}, ZLLL12]. Constraining [SLG15, GREA11, GA12, VBV13b, WBN^{+13}]. Constraints [KB11a, OPBR17, OZS^{+13}], constructing [hh10], constructed [HDL^{+17}, ZLY^{+16}]. Constructing [Che17, HS16b, LG11, SWA13].
construction [AGR11b, JCPC11, KSR17, LZX16, UIW^{+10}, WWD14, YD17].
contact [DBK17, MK13a], contacting [Mau14]. contacts [CCCLCGRO14, Ham11, Kri10, PRP15, SNDK16]. containing [AKMYB18, ACD^{+13a}, ACD^{+13b}, DGL^{+13}, GP12, GPaC^{+16}, HDP14, KLN12, LDZW17, VDVR14, YHVM12, YDX16, ZZZ^{+12}, ZM10].
Continuous [Dry14, PLA13, PBZA13, GFM11, LBGS16]. Continuum [JJJ16, Cam15, CXY11, HZSS17, ISO^{+13}, LFN^{+10}, MC1U15, SK12, SK17, TNG^{+10}, WC13, WRHF10, XZ11]. contraction [HSN14, STM17].
contractions [KK17a]. Contrasting [TS15a], contribution [Pro16].
Contributions [JJH^{+13}, ARRC15, BCNH^{+11}, CGR16, CPN^{+17}, ENKK^{+17}, WS10].
control [BVY^{+12}, DPAB16, Hel13, HH16b, LPLB16, SR10, XYW^{+14}, ZQ14].
controlled [VGTL16]. Controlling [FWB14]. convective [SBN^{+16a}, SBN^{+16b}]. Conventional [SHL^{+13}, BKŠ^{+11}]. conventions [BCJ^{+14}], converged [FLM11, GR10a, KHWB17]. Convergence [GS16, LT13, ZHI12, ASS10, BKŠ^{+11}, GS15, ON14, RFH10, SL17].
converges [SH11a]. Converging [OSR16], conversion [LDB^{+17}, LZZ^{+15a}, LCB10, RVP^{+11}], convex [CLFR18], convolution [SZTSM10], convolutional [LHO17], cooperative [DBG11].
Cooperativity [RS14, AFSW16, JSW10, SM16a], coordinate [AMGB10, HSN14, Hel13, LL15, LL13a, MS10, WBN^{+13}]. coordinates [BK15, LWK^{+14}, NCV10, PH10a, Sch13, VBV13b, You10, ZT14].
coordination [ASMS10, CRC13, HS16b, KJ10, Mor15]. copper [JRSHP14, KKP11, SBC^{+11}, SPR^{+13}, WC14, ASMS10, CPK12, HRJ^{+14}, HGHP14, HRJ^{+15}, XSW13]. coprocessors [WS13]. Copyright
[Ano16-94, Ano16-89, Ano16-95, Ano16-96, Ano16-97, Ano16-98, Ano16-99, Ano16-100, Ano16-101, Ano16-102, Ano16-90, Ano16-91, Ano16-92, Ano16-93].


coupled-cluster/Kohn [VV14]. coupled-electron [SB14]. coupling [AMQ+14, BLZ+13, FD16, GP11a, KSK11, KNP+12, Kos16, LLB+12, LSH+11, LWD13, MG11, MCP18, PS17, Rui11, RRK16, SACdG14, Wu10, YB11, ZTH+15, ZLZ14, ZYvIZ14]. couplings [CSEMB+16, LK11, LZH+11, dVAG16]. covalency [HS14a]. Covalent [WT10, FCCP17, HAI+16, KAR12, MR17, OZS+13, RS13, SFA17]. CovalentDock [OZS+13]. covalently [CZA11]. Cover [Ano12a, Ano12b, Ano12c, Ano12d, Ano12e, Ano12f, Ano12g, Ano12h, Ano12i, Ano12j, Ano12k, Ano12l, Ano12m, Ano12n, Ano12o, Ano12p, Ano12q, Ano12r, Ano12s, Ano12t, Ano13a, Ano13s, Ano13t, Ano13u, Ano13v, Ano13x, Ano13y, Ano13l, Ano13i, Ano13c, Ano13z, Ano13-27, Ano13-28, Ano13-29, Ano13-30, Ano13-31, Ano13b, Ano13c, Ano13d, Ano13e, Ano13f, Ano13g,

D [LWD13, OZLSBH12, RSKG14, UT14, YZ15b, AKMT11, BWKW10a, BWKW10b, Chn10, DVVP14, ETLS17, GMMH*+16, GSS13, GPK12, KTT16, LTT16, MA16, MYT*+14, MH11, MSSP17, MH10, PSS14, PZBA13, RSKG14, TFQ*+10, UT15, YJN*+11, YDL*+10, ZLY*+16, TS15b, YOPB16]. D-
dance [JW16]. dancing [LL10b]. Dancoff [HH17]. data [BRGN12, BCP+10, FNA12, Fom11, HPT+16b, HM13, JZL+17, JS17b, LAS+14, MMB+17, MCC12, RO14a, REL+14, RCM+13b, SB10, XW15].
Decoding [MBT14]. decoherence [CSEMB+16]. Decomposition [DBGO+17, AMAA+11, MBMJ11, FFA14, GS14, GCW16, ISN13, KNE11a, KRSC12, NJX+10, PS17, RSLML12, SSXS15, STM17, SKGB13, WWU12, WES13, dSD12a, dSD12b, dLC17]. decomposition-based [KNE11a].
deficient [YLL11]. defined [JJAB16, GY10]. definitions [JY+16].
Definitive [TCGNT18]. Deformation [WYL+15, Gav12, MRB14, WCY+11, WCT+11, dLC17]. deformations [HRMAL+13]. Deformed [CSAdOM17, TFQ+10]. degree [Clo15].
delocalization [BK11, FVB10, HSB+11, Jan16, Mat14, SS13b, SSA+17].
delocalized [Alg17, HSH15, dLC17]. DelPhi [DLSA14, JLC17, LLZA12, LPLA13]. DelPhiForce [LCA17]. deltahedra [LK16b].
Densities [ATM18, HGCG10]. LP11c, MA16, REL17, dLC17]. Density [AMK11, CD13, CWH11, FPV13, FD16, GNGC10, GWJP11, INT18, JYS+12, KKPT11, LBGS16, LGW12, LBTV12, LPM17, MWJ+11, Oht16, PPH+14, RB12, RSLML12, TS10b, WDLG12, WGN+16, YJ11, ZLZ14, ZYG+14, ZWY+10b, ZYW+10a, dS812a, ALK+15, Ano15-59, AG12, ASS10, BY11, BBLG+13, Ben17, Boz18, BBI+11, BZB+13, BG13, CHG+16, CRZ+18, CDB10, CR14, CAA10, CSEO15, CGR16, CKH17, CSXZ17, CC11, CAP17, CNK97, CPL11, CB11d, DH17, DWC17, DIL15, ED15, EPI12, FED17, FCPJM14, GAI14, GHL17, GZL+12, GWJR18, GMG+10, GSS13, Gra15, GEG11, GAY+17, Han11, HNWF07, HNWF12, HPT17, HEMCZE+14,
HLBLCCG15, HRMAL+13, HH16a, HH17, Hii13, Höf14, HG10, HOK17, IKN13, IM17, JCP14, JLH+14, JW16, KD10, KB10, KSH13, KOP+14, KGHK12, KB13, KZZ+16, KLN12, KYG+15. density [LL15, LCW12, LBT11, LHKS12, LWGW12, LH14b, LLH17, LZS+17, LKi16a, MAK+14, Mat14, MEZ10, MKM+17, MFR+17, MMJ10, NF17, NN18, NO16, NKK+16, NFI+16, NS17, ORZ11, OM12, OVPK15, PAK17, Pie14, Pil17, PW12, PZM15, QZi10b, RJJPB12, RS13, RB13b, RSG14, Rod13, RPWS13, RHT+15, REV+17, Rui11, RSKG14, SPS+12, SGJP+17, SH15, SS16a, SDF+17, SFG+17, Sea10, SCW11, SDM+16, SEF+16, SE14, SH14, ST13, SHL+13, SPR+13, SZX13a, SZX13b, SMM15a, SMM15b, SMM+18, SKTT11, SSZ16, STS15, SK11, TLdG+12, TN10, VCV+11, VAR12, VECD12, VV14, Viki11, VLI17a, VIII7, VED10, Vy16, WKC10a, WHL+10, WGL+11, WCWW11, WWU12, WWCL15, WHX+10, WL14, WTH+16, XYW+14, YLZ+10, YS13, Yu12b, ZTH+15, ZXS+10, ZSWL12, ZKE+17, ZDX11, ZLHH14, ZGS+10, dSdS12b, dSdLBNB17, dLC+17, CDM10]. density-based [LZS+17]. density-density [SS16a]. density-fitting [Boz18, Hil13]. Density-functional [Oht16, CHG+16, HNWF07, HNWF12, IM17, JCP14, KZZ+16, MFR+17, NF17, NN18, NO16, NKK+16, RHPWS13, SP5+12, VED10]. density-peaks [LZS+17]. deoxy [VM11]. deoxyribonucleoside [XVN17]. deoxyribonucleosides [RJWW12]. dependant [PNG10]. dependence [BRLS08, BRLS12, FE14, GZ12, KKO+16, LG12, LFE+10, LLTC12, MP17b, PZA15, PBE16, PS10, SGPS+17, SY16b, AD10, MGWR12]. dependences [SMM+18]. dependency [DKT13, PHDH13]. dependent [AALCM11, BS16a, CHG+16, CP15, CKP10, DP15, EP+10, GTK10, HNWF07, HNWF12, HG10, HYUS11, JYS+12, KCPMG12, LPLS16, LZ12, LGS11, Mat10, NS10, PAK17, PPJ14, PVJ10, RHPWS13, REL17, SY16a, SFBT17, Viki11, WHL+10, WHX+10, YLZ+10, ZXS+10, ZDX11]. deposition [SE14]. derivation [SCMA+17, VVV+15b]. derivative [MY17b, TPL+10]. Derivatives [KTSW11, CWHH11, CZH12, CBTZ16, CROB16, HSZ+11, JS17a, JYS+12, KG11, KPL15, LWGZ15, LWGW12, MFR+11, MIS+15, NS10, PC14, RV+12, RFN15, REH13, SBR13, SZX13a, SZX13b, VVJ15, VVY18, VSD10, WGL+11, WRG+17, WDP+12, ZsA10, ZW11, ZZ12, ZZWX11]. derive [RVP+11]. derived [CIKT13, GMMH+16, KSR+16, LZGS11, MCLD10, OSS10, PLZ17, REL17, SOYC12, SE14, TBSM12]. Deriving [CCYL11]. descent [MS16]. describe [RHRCH16, RS13]. described [BM12, CCB15, KDS17]. Describing [MKGA10, JCP14, JBSQG11, MY17b, VBD11]. Description [FD16, MR17, BD12, BE16, Cam15, CRZ+18, LZLC13, MFR+11, PM13, PLH16, PVAM16, SRF+17, SSA+17, TKNN10, WvRSM14, WL14]. descriptor [DFF+15, MA16, PRTY+17, TMJ15, WMW+10, Yap11]. descriptor-based [DFF+15]. descriptors [FCL+10, FZL+15, GJMPAM+14, MH10, NKJ16, PKIC11, RB13b, TTB+10,
Wei12b, YLCX10, Yap11, YDX16, ZWX16. **Design**

[LCM16, Tak14, TZ12, VBD11, AM10, AFBR17, BAMR13, BEPM14, BPC13, CBP14, DPB+12, DPOS16, DGL+13, GS14, GMZ12, HHEY10, ISP+10, KSD+12, LABSG17, LBS10, MS16, PC11, SYDS11, SGM+13, Sli15, TKXT13, TRA+16, VVY17, VMPS17, XHLH16, ZSB+11, ZWP11, ZYW+16, ZWS+10]. **designed** [BL13]. **Designing** [BL13]. **desolvation** [BK17a]. **detailed** [ABB+12, ABB+13, GPdC+16, MP13, MO15, MC10]. **determined** [CHP11, IM17, YK13]. **Determining** [DSD+11, SGPJS+17, SDB+16, WOH16]. **detonation** [LWWG12]. **developers** [GKV+13]. **Developing** [CK17, DSK17, LPS+13]. **Detection** [CBP+15, BV14, CLX+10, ZLM+15]. **detectors** [SK13]. **Detection** [LB13]. **detailed** [ABB+12, ABB+13, GPdC+16, MP13, MO15, MC10]. **detected** [TCPPC14]. **Detecting** [DVVP14]. **Detection** [CBP+15, BV14, CLX+10, ZLM+15]. **detectors** [SK13]. **Detection** [CBP+15, BV14, CLX+10, ZLM+15]. **detectors** [SK13]. **Determination** [KLS10, KMLS10, AFPI13, BLS10, FSC+14, KR12, Kne11b, LPS12, CK11, LAT10, LAT11, MS13, NHN16, PG14, PBG17, SS16b, SPR+13, WAM17, WOH18, XLYZ10, YKO+11]. **determine** [VDVR14]. **determined** [CHP11, IM17, YK13]. **Determining** [DSD+11, SGPJS+17, SDB+16, WOH16]. **detonation** [LWWG12]. **developers** [GKV+13]. **Developing** [CK17, DSK17, LPS+13]. **Development** [GLB16, GMMH+16, LLJ12, MMB+17, MMZW14, MCP18, RZG+13, RLD12, SC17, TNYN16, WPM+15, ZA15, CYG+15, GMASBF16, GCP+13, LPLA13, PZA15, PPM15, WDHZ13, YWZ14, ZA10, ZSYH12, CRC13, WCM10, WCM11]. **developments** [YWJ+16]. **Deviation** [CSAdOM17]. **deviations** [HDL+14, KG15]. **devices** [DJX+11b, DJX+11a]. **Dewar** [Bac12]. **DF** [Chu10]. **DFT** [BRLS12, CLFRO18, SIG+15, YJ17, ZZZ+16, AALCM11, AR10, AF14, ASMS10, BTMS12, BRLS08, BIL10, BTB+11, CLFRO18, CMM+18, CCB15, CH10, cCVG+14, CVS10, DJD12, EFAC13, FVP14, FPRS14, GMASBF16, HSH15, HRJ+14, HRI+15, HBI+17, JRSHP14, KG15, Kar17, KT12, KKL+13, KM13, KP10, LEDDOLdV17, LRBB12, LZX+10, LZHH11, LZX+10, LSH+11, LYSS11, LZCL13, LH41a, LLSW14, LCM+14, MMS16, MDTD16, MG15, Mat10, MS11, MVKS10, Mor15, MCK17a, MCK17b, NKJ16, NC12, NMLD13, PTK11, PHK14, QLYL10, RS17a, RDF+11, RS14, RRC+15, RN17, REL17, RK3+14, RK15, SRF+17, SWM10, SRL+15, SDL14, TSNC+17, TG12b, Tsi14, TSI15b, Tsi17, VVJ15, VECT12, VAMS14, WKLC12, WYG12, YZGS14a, YSRSS10, YZ15b, XZZ17, ZCK+16, ZWGO16, ZWWT12, dSDdAR10]. **DFT-based** [NKJ16, NC12]. **DFT-derived** [REL17]. **DFT-MD** [GMASBF16]. **DFT-predicted** [WKLC12]. **DFT/MM** [RN17]. **DFT/MD** [GX116]. **DFT/PP** [LXZ+10]. **DFT/TPD** [LXZ+10]. **DFT/TDDFT** [MS11]. **DFTB** [SA10, FHT+15, MR17]. **DFTB/MM** [RN17]. **DFTB3** [KW15]. **DGeCl** [MCLD10]. **DH** [SGPJS+17]. **DH2** [SBW12]. **di-mannose** [VM11]. **di-tetrazine-tetroxide** [MCAG+16]. **Diabetic** [DHOG13]. **diabetes** [PC11]. **Diagnosis** [MC12, TDKT10]. **diagonal** [BMBJ11, KTK17]. **diagonalization** [BK+11, HRK+14]. **diagonalization-free** [BK+11, HRK+14]. **diagram** [OV14, VED10, ZY14]. **diagrammatic** [WWD14, YD17]. **diameter** [AS15a, KGHK12]. **diamond** [JWO15, WGN+16, WGLG+16, ZSL+11]. **diamond-like** [ZSL+11]. **dianion** [DP11, GRD+10, YZGS14a]. **diarylalkyl** [NS10]. **diarylalkyl-imidazole**
diarylalkyl-triazole [NS10]. Diarylbenzofuranone [SFA17].
diaryl dichalcogenides [ZWGO16]. diastereoselectivity [AARP17].
Diatomic [ATM18, LS11b, Tsi14]. diatoms [TG12b].
diatropically [CPN + 17]. dicarbide [Kop16]. dichloropentacene [ZYG + 15].
dichroism [HNHR13, SB13, SB15]. Dickerson [IPAA11]. dicopper [RHPWS13].
dielectric [DOM + 11, DSF17, JLCA17, KCPMG12, PS13, WXL17, YHW17].
Diels [BJSI12, CC18a, FB14a, GNDA + 12, LZH16, ORZ11, ST13, dSVdM + 16].
difference [LLH17, WL10, Yon16, ZRCC11]. difference-dedicated [ZRCC11].
differences [BVC13, GO13, HDL + 17, KHWB17, LGL11, PM18].
Different [PH15, BRGN12, Di15, FZL + 15, GO13, GR11, GFPSD17,
MCS11, MC12, MPA12, NMLD13, NOKJ16, RHNN10, Rao11, SLP + 12, SIG + 15, TSNC + 17, UT15, VVY18, ZR10].
Differential [HHT + 13a, HHT + 13b, CJL + 13, MY17a, MY17b].
difficult [RJS17, VDVR14]. diffuse [YCGA10].
diffusion [CPV + 12, CC12a, GC11, RSLS13, ZW17, WH11].
Diffusive [SM16b]. digitized [YNH + 17].
dihedral [CYG + 15, OZ14, SZBM13, WES13, ZRL + 15]. dihedrals [LDH + 14].
dihydro [RS17a]. dihydrofolate [RKDM14].
dihydrogen [PM13, UT14, WHX + 10].
dihydrogen-bonded [UT14, WHX + 10].
dihydrogen/hydride [PM13].
dihydropyrido [YZ15b]. diimide [MCC11].
diiodide [AARP17].
diiodide-induced [AARP17]. diketopyrrolopyrrole [HLWD15].
diketopyrrolopyrrole-based [HLWD15]. dilanthane [ZLZ14].
dilute [KVR10].
dimension [HKRS11].
dimensional [BPLL12, KYT + 17, KRSC12, KTO13, MB16, PJ13, SG10a, TYN15, TCX + 13, TKC + 11, ZWX16].
dimensionless [MS10].
dimensions [CHC + 13, HAL14, SRL + 15].
Dimer [LWL + 16, ARRC15, ANH + 11, BPPS17, CBTZ16, FCL + 10, FMNC11,
KCB + 12, LCB10, PD11, SKY + 11, Tac17, WWKS16, YCGA10].
dimeric [PS14].
dimerization [DSD + 11, KAR12, TLA10, WJX + 10].
dimerization/oligomerization [KAR12].
dimers [BCNH + 11, BWKW10a, BWKW10b, CLFRO18, CK10, JKS + 16, LJVW11a,
LMI + 14, PVS12, RS13, SZSS16, VT14, Zha11].
Dimetallic [ZYG + 14].
dimethyl [GC11, WLC12, ZSWL12]. dimethylaminoazobenzene [KP10].
dimethylaminophenyl [YLZ + 10].
dimethyl nitrosamine [FFA14].
dimyristoylphosphatidylcholine [ML14].
dinitrophenol [MIS + 15].
dinuclear [OS10, QLYL10].
dioxide [GM17].
dioxetane [KCN + 16].
dioxide [SC17, Kop17b, QZ10b].
dioxygen [DSM + 11].
dioxygenase [DGH + 11].
dipeptide [EJ13, IO13b].
dipeptide [DHF + 11, RSL16].
diphenyl [GKR13, Ray13, RKG11].
diphenyldimethane [KLN16].
dipidium [KT12].
Dipolar [YIZ13, CSS17, LKI11].
Dipole [GH16b, LIRL + 16, ZBG11, AS15b, BLB + 13, DHOG13, GH16a, HBKL10,
KCB + 12, LHHW14, MNNK10a, MNNK10b, PC14, Yan11].
dipped [IN13].
Dipole [JKS + 16].
diradical [YSSB12].
Direct
[LS11b, WM17, FF11, FSSW17, JCG + 10, RSB + 13, Yu12a, LLHM16].
directed [CH14, HHBY10]. direction [PAK17], direction-dependent [PAK17], directionality [CRC13]. disaccharides [GMSV14]. disconnectivity [SOJ14], discover [Hsu14]. Discovery [AKMT11, Aki16, FMG12, HYYZ13, Ibr11, IGK16, PVJ10, Zim13]. Discrepancy [Yan11], discrete [EJ13, MCUJ15, WAM17]. discretization [AD10, LLFH16], discriminate [UCFR16], Discriminating [FZL+15]. discrimination [YL13], discriminative [KS12], discussion [CDB10], disjoint [BK13], dismutase [GEP+14], disorder [LLL+12]. Disordered [MYT18, GP12, LC16, LC17a, NDLW13, SJZ+15, ZC14]. dispersion [AG12, BCNH+11, CLFR08, cCVG+14, GEG11, Han11, Has14, HGHP14, ITIN15, KB10, KSSH13, LCM+14, RJPB12, STS15, SBB11, SSB13, TG12a, WM17]. dispersion-corrected [CLFR08], Dispersive [TG12a, SDB+16].

dispersion [AG12, BCNH+11, CLFR08, cCVG+14, GEG11, Han11, Has14, HGHP14, ITIN15, KB10, KSSH13, LCM+14, RJPB12, STS15, SBB11, SSB13, TG12a, WM17].

discussion [CDB10], disjoint [BK13], dismutase [GEP+14], disorder [LLL+12].

dissection [BMFG16], dissimilarity [HS17a, YDL+10], dissipation [VVG13], Dissipative [PH17], dissociation [CCJ+11, GCCM15, Gil11, LBC+12, LL10c, MH11, Rob13, WSH10, YPvD13, ZWLX11].

dissociative [HBL12, RIJ+11], dissolve [SG10b].

dissolved [SIG+15], distance-dependent [KCPMG12], distances [BLDK+13, SSWX14, SMGB11].

distance-dependent [KCPMG12], distance [PHDH13, DCˇS15, Hug14, JMS13, KCPMG12, LZ12, PPUBGD10, RPNP10, RH12, UT14, Yon16, ZT14, dACP12].

distance-dependent [KCPMG12], distance [PHDH13, DCˇS15, Hug14, JMS13, KCPMG12, LZ12, PPUBGD10, RPNP10, RH12, UT14, Yon16, ZT14, dACP12].

divergence [PNG10], diverse [KSM17, LLC+10], diversity [WF16], Divide [NNK+16, BRP+12, BGR13, BK17c, KKN11, NYH+17, NN18, WX12, YN15].

Divide-and-conquer [NNK+16, BRP+12, BGR13, KKN11, NYH+17, NN18, WX12, YN15].

divide-and-conquer [NNK+16, BRP+12, BGR13, KKN11, NYH+17, NN18, WX12, YN15].

divide-expand-consolidate [BK17c]. Dividing [SLT+15], division [WWW+18].

dropping [CH14, HHBY10]. direction [PAK17], direction-dependent [PAK17], directionality [CRC13].
Pro16, RTP+13, SA13, SPL+18, SHL+11, SKKS13, TO10, VSD10, Vor10, WdVN12, WZ17, XML+15, ZL11, ZWL13, ZSB+16, dVZ17. **docking** [LZ11], **docking-rescoring** [BMR11]. **DockoMatic** [JBAM11]. **Does** [MBFG15, MIS+15, SV15]. **DOI** [Ano15-59]. **Domain** [KNE11a, AC11a, IMK+16, MBT14, RZ16, SFBT17]. **domains** [FCPJ14, OOK11]. **dominant** [Hua16]. **done** [LRvE17]. **donor** [DGL+13, Gil11, Lu11, MSV16, MIS+15]. **donor**- [MIS+15]. **donors** [LC10, TZ12]. **dopant** [SRL+15]. **doped** [GAMAC+14, LLC17, PGC12, TN12, VS14, WMW11]. **doping** [HYL+11, LLD17, WMW11]. **DOT2** [RTP+13]. **dots** [DPAB16, WAB17]. **double** [Alg17, BE14, CCB15, CGR16, CC11, FC16, KM13, LBH+11, LYC+13, LLL+12, SGPSJ+17, SP13, Sea10, YYT12, ZLY+16]. **double-Hybrid** [CGR16, LBH+11, SGPJS+17, Sea10]. **double-wall** [BE14]. **doubly** [CSXZ17, SZX13a, SZX13b, ZWLX11]. **Douglas** [YS13]. **DOX** [RCR+16]. **DPO** [WGL+11]. **DPPC** [LBDP12, oRWGS17]. **DPT** [BH13, BZH14]. **Dramatic** [MLY+13]. **Draw** [LBB+15]. **drawback** [BRGN12]. **Drew** [IPAA11]. **driven** [BSL11, BG17, DSM+11, HXM+16, KC13b, LLL+12, REL17]. **driving** [RN17, YZ17]. **Drude** [LRvdSM15, Ric16, SM14b, ZM10]. **Drug** [GSHM10, MBA14, FLM11, GMASBF16, Ibr11, ISP10, PC11, PVJ10, VHA+10]. **drug-like** [VHA+10]. **druggability** [LG14]. **drugs** [PPUBGD10].
LH11, LJR+12, LL13a, LRvdSM15, LCH10, LYC+13, LMI+14. **dynamics**

[LPE+10, LLTC12, LZS+17, LPLB16, LLT12, LBDP12, MBT14, MKS+12, MSC+10, MJJC14, MN15, MCR17, MFEM15, MADWBI1, MKM+17, MB16, MHRR11, MO17, MIOM13, NPTS16, NST14, NFPD13, NFG+13, NKN+16, NHK+13, NTNY15, Obt16, ON14, OGL10, OCL11, OLY17, OT12, OCW+15, PMC+17, PSS14, PAK15, PH17, PL14, PM13, PD12, PHT17, PVZ13, PS10, PVAM16, RS12, Ras17, RO14a, RO14b, RFN15, RR14, RdA12, RVdB16, RLG14, REL+14, RJRR15, RSB+13, SHMO11, SLT+15, SWM10, SSWX14, SOM+13, SJ17, SR18, SYN+12, SM16b, SK13, SKMS13, SFLG+17, SLLL13, SJ16, SV11, SBvG14, SAvG15, Tac17, TNYN16, US11, Vor10, VM11, WKLC12, WBN+13, WAM17, WC11, WHL+10, WH11, WWKS11, WLC12, WES13, WG14, Wu10, WBVE16, YPvD13, YJXZ13, Yon16, Yu12a, ZZY+16, ZX11, ZDKM12, ZBP11, ZP13]. **dynamics** [dCLFGL13, dSVdM+16].

**dynamics-based** [Vor10]. **DynamO** [BSL11].

**E-I** [GM17]. **EA** [MLCD11]. **EADock** [GZM11]. **early** [CBP+15]. **earth** [Ano11, JHMB+09, JHMB+11, WD10]. **easy** [TKT11, VVV+15b, Yes12].

**Ebola** [OLY17]. **economic** [PN13]. **Ecoupling** [dVAG16]. **edge** [DWZ+17, DJX+11b, PDG+16]. **edge-modified** [DJX+11b]. **editing** [You10]. **Editor** [GKR13, GPGLM12, JW12, Ray13, RSLML12, WM12, vLBBR12, Ih12, BCJC+14, Cor17, KR14, Man13, SFLG+17, VVB13]. **Editorial** [Ano16-56, Ano16-103, Ano16-104, Ano16-105, Ano16-106, Ano16-107, Yan16, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-111, Ano16-112, Ano16-114, Ano16-116]. **Editorials** [BEFS13]. **Effect** [AB10, CSKH16, CD11, CXS10, DKT13, DJX+11b, DLW12, FCGM12, FHK+12, GFGS18, HLBLCCG15, JWO15, JYS+12, KTT16, KCL+14, KL16, LLvG10, RWR+13, SLT14, SBC+11, SY16a, UT15, VLGK+17, WDLG12, ZJZM13, ZLL+10, BLG10, CC11, IYK11]. **Effective** [GKV+13, IM17, YZ16, AASP18, DMN15, CVG14, DR11, DMN14, GA12, KS13a, KS15, LCM+14, PHC13, PRY+17, PS13, RLD12, SB+16, UCFR16, WX5+12, YZ16, YZ15b, ZKH+10]. **Effects** [CS14, JAH+17, LGOM+15, LCH+15, Mor15, SEM12, Tac17, YCK16, AS15a, AK10, AS18, BB1+11, EP+13, RA15, FD16, GMG+10, HS16b, HLBLCCG15, INT18, JMX+16, KG11, KYCL11, LGVA14, LHT15, LWD13, MKGA10, MBC11, MRK11, MLY+13, MUC15, MGS+16, NAS15, ORZ11, OS17, OCW+15, PDM+10, PC14, RMGB11, RRS16, SSWX14, SMP17a, SFLG+17, TM14, TYN15, UT14, VKAM12, WXY14, YIN17, YJ11, ZPP+16, Zha11, ALW+10, THP+15]. **Efficacy** [LC17a]. **efficiencies** [RO14a]. **Efficiency** [AC11b, BB11b, BB11c, FE14, GBSE11, XFG+16, AC12, GSHM10, LY10, LWL+11, LZ15a, MKGA10, RO14a, XFG+15, vLBBR12]. **Efficient** [AB16a, BC13, BSA14, Cas13, DMAH15, DBF14, EP10, GCWS15, GPK12, Ham11, HNS16, HDL+14, HIW17, JMS13, LZ11, LGKS17,
MKS+12, NYN17, PSS14, PAK15, Ran12, RJS17, SS16b, TJBJ12, WHAS+16, WM12, ZZ14, ZKE+17, AM10, BW11a, Boz18, CBP14, CHG+16, CY09, CY13, CMS13, DS15, DGL+13, GREAl1, GWZX12, HDL+17, ISK14, JZ17, KB11a, KV15b, LFBl4, LPK16, LLZA12, LZL+15a, LZS+17, LAS+14, NPTS16, NN18, OK16, PW12, PBG17, Ran13, RR14, Rod13, RSL16, SCOJ13, SA13, SSMW09, SCW13, SWB+12, Sun15, TO10, WJG+13, WOH18, ZWP11, Zha12b, Zha12a, vLBBr12, WHAS+10]. Efficiently [WES13, ASMS10, DDK14]. EFP [CBG17]. egg [Pla11, ZP13]. egg-box [Pla11]. EGRAD [vW11]. Ehrenfest [Dil15, FED17]. eigensolver [KZZ+16]. eigensolvers [ZVY+15]. eigenvalue [HLXH17, HLXH18]. eigensolver [KZZ+16]. eigensolvers [ZVY+15]. eigenvalue [HLXH17, HLXH18]. eight [KZZ+16]. either [TCPPC14]. elastic [ECZW17, LBTV11, QB10, QB11, SH11a, XTY+14]. Electric [GH16b, LL13b, BLFZ13, BLBG+13, BS10a, CXS10, GH16a, KZK+12, MRB14, SH15, SLX+15, Yan11, YJ11, YCK16, ZSL17]. electrical [LLL11]. electro [TMJ15]. electro/nucleophilicity [TMJ15]. electrochemical [SIG+11, SGH+16, YJ11]. electrochemistry [DSK17]. electrode [MKO+13]. electrolytes [HAL14]. electrolytic [SV11]. electromagnetic [SEM12]. Electron [BK11, Bar14, BLG11, BWKW10a, BWKW10b, CEB10, HS16a, HRMAL+13, HGGCR+16, KGR+16, Pil17, WWU12, ACD+13a, ACD+13b, ABDG12, BHB12, CDB10, CAA10, CWHH11, CTP13, DaGR15, ED15, EP12, ESM+12, EP15, FRSA14, FED17, FCPJ14, GND412, HSH15, HPT17, HEMCZ+14, HAP+12, HBL12, IYK11, Jan16, JBSQG11, KPL13, KTK17, KYG+15, LW16, uLhY11, LHO17, LY16, LLJ12, LP11c, MKGA10, MRB14, Mat14, MBFP15, MKH+13, MCK17a, NYH+17, NS17, PAK17, PGdO+16, PSC11, PS17, PN13, PTB+15, PHT17, PC16, Ras17, Rod13, REL17, RSKG14, SB14, SHB17, SGL13, SK11, SSA+17, VGV+11, VECT12, VL17a, VI17, Vy16, WLW+10, WMW11, YKH+10, YLL11, ZPP+16, ZSG+10]. electron-correlation [NYH+17]. electron-deficient [YLL11]. electron-hole [PTB+15]. Electron-pair [WWU12]. electron-withdrawing [CWHH11]. Electronegativity [FCPJ14]. Electronic [AMQ+14, ASS10, DAdGR15, GND412, HLW15, Ibr17, KYCL11, KKL+13, LLBO12, LS11b, MAPB10, NIIT15, PMC+17, RLA+11, TN12, TN10, TFQ+10, TS15b, VI17, WRM+12, YW12, ZRCC11, AR15, AK10, AC12, BLZ+13, CPRS18, DKE+17, DHOG13, EH13, EWK+13, EPBK17b, FB10, GTT10, GRAR0+14, GWX+12, GZZ12, HASR+12, HS14a, HSB+11, Hu16, IIF+10, KPT11, KSM17, KG11, Kop15b, Kos16, KP10, LGOM+15, LX11, LBTV11, LBTV12, LZX+10, LSH+11, LLWS14, MC10, MA16, MCF10, Mat10, NC14, NFI+16, OLA15, PHK14, PTB+15, PVAM16, Fyy13, RCM+13a, RML+15, RR12, RNI12, SFA17, SLP+12, SRS14, SB15, SKGB13, TFQ+11, TD10, TS15a, TNG+10, TS11, TG12b, VVP12, VHR16, VARI12, VBMA13, VLGK+17, VGTL16, WHL+10, WGL12, WJG+13, WIO15, WSGN11, WZK+13, YK13, ZJZM13, wZB11, ZBB16, dCDP15]. electronic [dVAG16, vSGP10]. electronically...
electronics [RN17].
electrons [EKH14, WCY+11, WRG+17, XhD15, YCGA10].
electrophilic [MA16].
electrophilicity [YB16].
Electrostatic [CLA16, LP11b, MLZZ12, Sch18, WFZ+18, BCNH+11, BSF18, BK13, CCC+11, CS14, CPK12, CB11c, DLSA14, GBL+11, HOK17, IO13a, KTN10, KYG+15, Lar11, LCA17, LCM16, Mat14, PVJ10, RB13b, TY10, VMRSH+17, VVY18, YKO+11, YWJ+16, YMP14, YZL+15, ZDM13, ZBP11, KG12].
Electrogynics [BSG18, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14].
Electrostatics [BSG18, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14].
element [GPK+16, RMGB11, TG12b, TCX+13, XYX17].
elementary [LPLB16, Zim13].
elements [TKN13, BV14, CWZB10, Hil13, JJJ16, LFB14, SK15a, TDKT10, Tsi14, WS12, XhD15].
elevation [HH10].
ELF [RSKG14].
ELI [BWKW10a, BWKW10b].
ELIA [BWKW10a, BWKW10b].
Electrostatics [BSG18, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14].
Electrostatics [BSG18, CZY11, FGM11, FP17a, KFY+13, LPLA13, MBA11, MBC13, NLP+16, SDZ17, SWPR11, UHH+11, XYX17, YMP14].
Element [BCCO10, GPK+16, RMGB11, TG12b, TCX+13, XYX17].
Elementary [LPLB16, Zim13].
Elements [TKN13, BV14, CWZB10, Hil13, JJJ16, LFB14, SK15a, TDKT10, Tsi14, WS12, XhD15].
Ellipsoidal [DGB+13, LDG+15].
Elongation [OLA15, MKGA10, MKGA10].
Elongation-MP2 [MKGA10].
Elucidating [HNHR13, TDP+12].
Elucidation [CPLL11, TNYN16].
Embedded [DSF17, GMG+10, HSH15].
Encapsulated [EOO+16, STS15].
Encapsulation [YDGZ15].
Energy [AF14, AS14, AG12, BW11a, BLF14, BHV11H, BS16b, BE16, CHG+16, ŠMD13, CH10, CTP13, CB16, DHOG13, DM17, DHF+11, DPOS16, FGM11, GI11, GP11a, GR13, HAGK10, HH10, HH11, HLW+17, HHWL17, IK13, KSH13, Kar17, KSM17, KJDB12, KB11b, KBY13, LJ1W11a, LW11, LHWW14, LH14a, MCS11, MS13, MSK12, MB16, MMJ10, NWW17, NMF+14, OBW12, yOTn16, OAN15a, OSR16, PGT+12, PPJ14, RLDJ17, RDAS10, RAR+11, RO14b, RZ16, RR14, Rob13, RJS17,
SRR16, SK12, SHL+13, SOD+11, STM+15, SGWA17, TS14, TSN16, UD12, VVG13, VECT12, VM11, WBT10, WS10, WJG+13, WG12, WX12, YAS13, YMP14, ZZ14, dALdS+15, dRBO13. **Energy**

[DK11, GS16, IIHY15, JCGVPHT17, LFN+10, LPLB16, SN16b, SSGS15, SKGB13, WM12, AMGB10, AC11a, Aol10a, AK10, AK16, BCSCJ+13, BPM15, B&E16, BH15, BS16a, BRLS08, BRLS12, BACSCJ+10, BG17, Bou14, Boz18, BD11, BWMSM10, BB11b, BB11c, BG12, CM13a, CK10, CDM+15, CLA16, CY09, CX10, CZY11, CY13, CH16, CSXZ17, Che17, CS17, CHR+12b, CHR+12a, CKP10, CMvG10, CPK12, CWZB10, DGH11, DBG11, DS12b, DH14, DWC17, EV14, FMNC11, Fer17, FED17, FCOGM12, FSSW17, FCCP17, FLM11, GS14, GS15, GHK12, GO13, GMO16, HDL+17, Hel13, HDM+15, HH15, HG13, HYMZ16, HYUS11, HJKJ13, HYD10, HDHL15a, HDHL15b, HDHL15c, IMK+16, ISN13, JCPC11, JMLL13, JZ12, JZZM14, JCX10, KCB+12, KTT16, KB10, KNHN16, KN17, KHWB17, KDR+18, KB11a, Kop15a, Kop16, Kop17a]. en

exchange-correlation [HG10, Vyb16].
exchange-coupled [CAT+13]. exchange-repulsion [CGPP11, ENKK+17].
exchanged [LZTV10]. Excitation [KDR+18, CHG+16, EFAC13, PTB+15,
SH17, TG12b, TSN16, UD12, WJG+13]. excitations [ACD+13a, ACD+13b, CMF+17, FE14, IIF+10, PVAM16, WWD14].
Excited [CH10, SGWA17, ZXS+10, BSL+16, EK17, ESM+12, FD14, FAA15,
FD16, HNWF07, HNWF12, HH17, HZSS17, HDHL15a, HDHL15b, HDHL15c,
JCGVPHT17, KB14b, LLBO12, LLW12, LWGZ15, LX11, LSH+11,
LYSS11, MPSG11, NYN17, PH10b, RRCH16, RR14, SFCCK+14,
SFCK+15, SRF+17, SZSS16, TSN17, WHL+10, WHX+10, YD17, YLZ+10,
YB11, YYT12, LZL+10, PGW+17]. Excited-state
[SGWA17, FD14, HH17, HZSS17, LWGZ15, MPSG11, NYN17, PH10b,
WHL+10, WHX+10, YD17, YYT12, LZL+10]. excited-states [LLBO12],
exciton [HRH+17, LSH+11]. EXcitonic [JCGM18, ZMMM12]. excluded
[LWZ+17, Yan14]. exhibited [RWR+13]. Existence [BMB13, WD10].
Exothermic [LWL+16]. expand [BK17c, Car14]. expanded
[MLQ+12, TSNC+17, YSSB12]. Expanding [GMZ12]. expansion
[HAGK10, HSN14, LYM+13, LRER13, NI17, SS16a, SNS13]. expansions
[LZGS11]. Expected [Clo15, AF14]. Expedited [DJD12]. expensive
[LDZW17]. experiment [JAH+17, SA10]. Experimental
[NHF+10, AvKSP16, BRGN12, EOO+16, GPdC+16, HJ13, KP10, DCOD13,
Pog10, RO14a, SB10, SGS+16, SKMS13, VZ14, CYI+10]. experiments
[CBP14, HCB11]. explained [FL15]. Explicit
[WG14, BEM14, COOH14, CBG16, EK15, ENKK+17, GLB16, HDL+17,
KJDB12, LH11, RdA12, SYH12, SKMS13, Zha12b]. Explicitly
[yOTn16, SM17]. Exploiting [HB14, BYE+16]. Exploration
[ZGS+10, LW12, LAW+16, OKIS17, RDRC16, STi15]. explore
[JCPC11, MSC+10, MCC12]. explorer [SYN+12]. Exploring
[BHB12, BPBS17, BCG10, MTM14, PJJ13, Tsi17, ZT14, dSDLB17,
RDRC16, NOKJ16]. explosive [YPC+10]. Exponential [BBOB16, BB11].
expressions [Gav12]. extended
[GWZx12, KUDG12, LRvds15, SSWX14, TSN17, YB16, Pon11]. Extending
[LMZ11a, Man13, VBVI3a, VVBI3, PHH+12]. extensible
[GCW14, JYC+16, LAS+14]. Extension
[HSN14, PFVL14, SDZ17, YHVM12, Cam15, LL11, RLLHL12, Ras17].
extensions [NYH+17]. Extensive [JW12, SLHV09, YB11, CF14, KM13].
extent [GFGS18]. external [GKSS14, SEM12, ZSLL17]. extract [MDTD16].
extracted [HNTS15]. Extraction [CVG14, VVG13]. extrapolation
[CC11, LYM+13, OAN15a, SRR16]. Extreme
[HRH+17, Cam15, DS12a, JBSQG11]. Extremely [ZM11].
LBDP12, MSK+10, MSK+12, MS15, ST11, SEM12, VVV+15b, VHA+10, WKC+10b, WLC12, WG12, YPKB12, ZRL+15]. **fifth** [KM13]. **fifth-rung** [KM13]. **file** [SY16b]. **files** [MK5+12]. **filter** [MH10]. **find** [MN15, RVVK13, SB11]. **Finding** [Ber17, MLC13, GFG11, JZ17, Zim15]. **fine** [Hua16]. **fine-structure** [Hua16]. **fingerprints** [SS13b, Yap11]. **Finite** [ISO+13, BCCO10, BVC13, DJX+11b, EPD+11, Hsu14, LLH17, MLC13, NPP13, SK15a, TD11, TCX+13, WL10, XYZ17]. **finite-difference** [LLH17, WL10]. **Finite-field** [ISO+13]. **finite-size** [DJX+11b, Hsu14]. **FIPSDock** [LZL+13]. **firefly** [FD14, PE11]. **First** [BE12, BE14, CCJC10, DBM+15, EB12, EBK13, EBPK17a, HFSO12, JCG+11, LLLM11, LLB+12, LCWW10, RRK16, TKN13, YPvD13, YR13, wZbZ11, BPE16, BCCO10, BEL+11, EMD17, GD10, GA14, Ibr17, LL10c, Lu11, MCF10, NNS15, PLZ17, RZG+13, SFA17, SK12, TKC+11, TZ11, WX+12, WYL+15, WD10, WZK+13, YHS11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC+14, HYL+11, NG10]. **First-principle** [HFSO12, BE12, BE14, EB12, EBK13, EBPK17a, JCG+11, LLLM11, wZbZ11, BPE16, EMD17, GD10, PLZ17, RZG+13, WYL+15, WD10, ZWMW10, ZZ12, vADC+14, HYL+11]. **fit** [BHNS14, BCG10, GDV17, KGM12, WKC+10b]. **Fitting** [SN16b, Boz18, DGPM14, FN12, Gra15, Hil13, LBGS16, MKH+13, MKM+17, SY11, VYM15, WOH16, WOH18, ZDM13]. **five** [HCD+10, KJDB12]. **five-membered** [HCD+10]. **fix** [WCWV15]. **fixed** [AS15b, FSD+18]. **flakes** [SDF12]. **flash** [AGM+13]. **flavonoids** [PC11]. **Fleksy** [WdVN12]. **Flexibility** [OXBW16, BCG10, FTW12, FMG12, GTZ+18, KL14, LZ11, NPG17, PRSG13, PHH+12, dVZ17]. **Flexible** [GLB16, MKM+17, NG10, SC17, WdVN12, AFPI13, CZNA11, DVVP14, FRLN10, GBW+14, HDM+15, JC16, LS11a, LHS12, PL14, PS13, PJ13, RHJ11]. **flexible-boundary** [PL14]. **Flexible-Monomer** [SC17]. **flip** [ZLHH14]. **FLOODing** [HNTS15, HNS16]. **flow** [TCC+13]. **fluctuating** [CCB15, CMS13, GM17, IHY15, KUDG12, YWZ14]. **fluctuation** [II10, OXBW16]. **fluids** [KGHC15]. **fluorene** [CH10, HXM+16, PH10b, YJN+11]. **fluorene-phenylene** [CH10]. **fluorescence** [CH10, EJ13, ZLL+10]. **fluorescent** [LZL+10, NSO+14, PGW+17, WJG+13]. **fluoride** [LZL+10, MBRC16, NC12, Rab12, SRL+15]. **fluorides** [ASS+17, Sán17]. **fluorinated** [DKE+17]. **fluorobenzene** [KS13b]. **Fluorophilic** [vRWGS17]. **fluoroquinolones** [MPNS13]. **flux** [LGOM+15, Pol13, VGTL16]. **fluxes** [GNDA+12]. **Fly** [PAK15, MIOM13, PL14]. **FMO** [LFN+10, UIW+10]. **FO** [CHu10, GTK10]. **Fock** [ACD+13a, ACD+13b, BY11, CB11d, FRN15, HJKJ13, IYK11, Mat10, PB14, PW12, RRH12, SG13, UIW+10, VL17a]. **Fock-space** [ACD+13b]. **Focused** [MMM+16, CHR+12b, CHR+12a]. **focussing** [CB11c]. **fold** [LK11]. **Folding** [MFEM16, AD10, BPE16, CYT+10, CBG16, DMJ17, DAB16, GRL+11,
GRL+12, HTS15, HTS17, HLH+12, JCX10, KLS10, LKL10, LLvG10, LgV13a, MFEM15, PBE16, WNM17. **folds** [CYT+10]. **folds** [CDS16, CHP11, MV17]. **followed** [AKMT11, Mau14]. **Following** [GS16, MFEM16, XFR+16, Tac17]. **footprint** [BMR11, BAMR13]. **Force** [CYG+15, DBGO+17, DP15, GSD10, LZZ+11, PS10, PNL10, ZSYH12, AKMYB18, AOW11, AS15b, AJR16, BW15, BF17, BVY+12, BMBJ11, BAS14, CCLP12, CRC13, CIKT13, CZAF17, CLC11, CB11b, CB11c, CK17, DPNM11, DGPM14, Di15, DFF+15, DMAH15, DLZ15, FED17, GCWS15, Gar12, GZM11, HH11, HKR12, HDPM14, HLH+12, HJ10, HM13, HJLV16, IHIJ+13, JYC+16, KLY+16, KS12, KSR+16, KLS10, KMLS10, KWL+16, LALH13, LCS+13, LCA17, LZGS11, LN+15, LLvG10, LGL11, LvG13c, LTP11, LDG+15, LBDP12, MHT+18, MSK+10, MSK+12, MRO17, MJC14, MBC11, MSS+13, MTvG12, MBE16, MJG+15, MIOM13, MS15, PHC13, PLZ17, PG15, PZCL16, PLH16, PVM10, RI10, ST11, SM14b, SK17, SZBM13, SIE15, SNK16, SS13c, SR18, SM15, SYZ+17, SBB14, VV+15b, VHA+10, VVEL17, Vor12]. **force** [WKC+10b, WLC12, WOH16, WOH18, WTH+16, WC14, WGD12, WHZ13, XP13, XVA+16, YWZ14, YJXZ13, YPB12, YVM12, ZRL+15, ZL11, ZP13, ZM10, ZCGM11]. **force-constant** [WOH18]. **force-field** [DMAH15, LLvG10, MBC11, WTH+16, ZL11]. **force-fields** [CCLP12]. **force-matched** [KSR+16]. **forcefield** [LDB+17, MMZW14]. **forcefields** [CBP14]. **ForceFit** [WKC+10b]. **forces** [EPD+10, Elk16, Has14, HNWF07, HNWF12, IO13a, RN17, SDB+16]. **ForConX** [LDB+17]. **forest** [WZ17]. **form** [GWX+12, YZ15b]. **formaldehyde** [CYC+17, GNCA10, YPGD13]. **Formalism** [MKGA10, SFCK+14, SFCCK+15, SMP17a]. **formamides** [JSW10]. **format** [LAS+14]. **formate** [CJZS10]. **formate-lyase** [CJZS10]. **Formation** [DWZ+17, BPS17, CD11, ED15, GRCL12, KSM16, KAR12, LH11, LWL+10, MCK17b, OHT16, RVP+11, TDP+12, UCFR16, WNM17, WKC11, WD12, YPC+10, ZSWL12, ZWX16, ZYL+12]. **formations** [HTS17]. **formats** [REL+14]. **formed** [RVB+12]. **formic** [TL16]. **forming** [Car14, ONTTL16]. **FORMS** [RMPAM15, FD14, KG11, PS14]. **formula** [BB11b, Ish12, MA16]. **formulas** [KTSW11]. **Formulation** [BD12, SSSM15, CSKH16, DLMH12, KCL+14, MBA11, SMM15a, SMM15b, WRHF10, ZKE+17]. **formyl** [LZHH11]. **förster** [RCM+13a, Kos16, RML+15]. **forsterite** [DOM+11, DBM+15]. **forth** [PNW+16]. **Four** [PRJ+17, RK15, EB12, HKR+14, JKS+16, LLC+10, LWQ15, WS15, WS12, ZWZ11]. **Four-component** [RK15, HKR+14, JKS+16]. **four-membered** [WS11, WS12]. **Fourier** [YW+16, Ish12, LL13a, SHTSM10]. **fpmb** [CWT+12]. **fraction** [Gil11]. **fractionations** [NASH15]. **Fragment** [GK15b, IF+10, CIKT13, DR11, FMG12, GWF11, GV+13, HB14, KS13a, KS15, LMZ11a, LFP+10, MFR+17, NF17, OOT15, OOK11, RKGN10, VB13b, WCT+11, dLC17]. **Fragment-based** [GK15b, FMG12, HB14, LMZ11a]. **fragmentation**
fragmented [JSXH16]. fragments [CM16, Kos16, KSR17, Sax12].
fragments-rooted [CM16]. framework
[BFH+13, EH13, GPY1a, HPT17, JBB+11, KTNN10, MKGA10, OM12, PHT17, RCM+13a, RML+15, Ñez16, SK15b, SWB+12, WYD13].
frameworks [LSD+10, PLZ17, VVV+15b]. francium [TH13]. Franck
[CHC+13, MCLD10, MLCD11]. Free
[Bou14, CBG16, GS16, GO13, GMD16, MCvdV13, OCW+15, PZCL16, SISK10, AC11a, Ano10a, AK10, AKN16, BKS+11, BSL11, BH15, BS16a, BD11, BB11b, BB11c, BG12, CY09, CX10, CY11, CY13, Che17, CS17, CHR+12b, CHR+12a, CMvG10, DMJ17, DGH+11, DHF+11, DPOS16, Fer17, GS15, GHK12, GMPAM+14, Gri13, HLS12, HH10, HH11, HDK+12, HLW+17, HLD+17, HDM+15, HG13, HYUS11, HKR+14, HHLW17, IMK+16, JMLL13, JCX10, KHWB17, KB11a, KB11b, KYB13, LMZ11a, LGL11, LP11b, LAW+16, MSC+10, MS13, Mau14, MSÁK12, MBE16, MIOM13, OSR16, OK16, PGCT+12, PBLs12, PBBP11, PPJ14, RLDJ17, RDDS10, RAR+11, RO14b, RZ16, RR14, SM14a, SFR+11, SWPR11, SY11, SH11b, SOD+11, SoVG12, SN10, SMM15a, SMM15b, SMM+18, TS11, VLB+10, VG13, VM11, WSH10, WCT+11, WWWW18, WG12, XTG+11, XVN17, YOMT14].
free [YAS13, Yan14, YHH+13, ZZ14, ZPF14, ZWY+10b, ZH12, ZVY+15, dRBO13, WLF11, XYW+14]. Free-energy
[GO13, GMO16, BH15, CY09, HDM+15, HYUS11, IMK+16, JMLL13, JCX10, KHWB17, KB11a, KB11b, KYB13, LMZ11a, LGL11, LP11b, LAW+16, MSC+10, MS13, Mau14, MSÁK12, MBE16, MIOM13, OSR16, OK16, PGCT+12, PBLs12, PBBP11, PPJ14, RLDJ17, RDDS10, RAR+11, RO14b, RZ16, RR14, SM14a, SFR+11, SWPR11, SY11, SH11b, SOD+11, SoVG12, SN10, SMM15a, SMM15b, SMM+18, TS11, VLB+10, VG13, VM11, WSH10, WCT+11, WWWW18, WG12, XTG+11, XVN17, YOMT14].
free-standing [TS11]. freely
[CH16]. frequencies
[LBH+11, LLH17, WX12]. frequency
[BMPML+13, CK10, LCW12, LS11b, yOTn16]. frequency-independent
[yOTn16]. FRET
[RO14a]. Friedel
[CYY+17]. friendly
[DBF14, SFR+11]. frontier
[MGS+16, TZ12]. frozen
[BVC13, Fer13b, Fer13a, HH16a, HH17, HÖf4, SDF+17]. frozen-density
[HH16a, HH17, HÖf4, SDF+17]. fructose
[RAR+11]. fructose-1
[RAR+11]. fuel
[GO13, GMO16, BH15, CY09, HDM+15, HYUS11, IMK+16, JMLL13, JCX10, MIOM13, OSR16, PBBP11].
full-pivoting
[PS17]. fullerene
[GKSS14, KCK+15, KP10, Oht16, TPL+10, TFQ+11, TTB+10, XFTW15, YDGZ15, ZSL+11, ZZ12, SWA13].
fullerene-based
[TTB+10]. fullerenes
[GZH10, GLF16, MCK17a, MCK17b, SWA13, STS15, WTH+16]. Fullrnc
[Aou16]. Fully
[AG12, ZSTI14, FBY+17, GBL+11, KG13, LZZ+13]. function
[ABDG12, AB16b, BLG11, CKP10, GS14, GND+12, GEG11, HH16a, HBL12, HYMZ16, JLC17, JMS13, Kop15a, LL13a, LH11, LCB10, LIRL+16, MB16, yOTn16, ON14, PiL17, PRY+17, RZG+13, RV11, SS16a, SFG+17, TCB16, TO10, UMI3, UCFR16, W015, WDHZ13, YVEI+17, ZLT13, sSGP10].
function-based
[VDHZ13]. function-guided
[YVEI+17]. Functional
[FPV13, AMK11, ALK+15, Ano15-59, AG12, ASS10, BY11, BLBG+13, BK17b, BZB+13, BG13, CHG+16, CRZ+18, CR14, CWHH11, CSKH15, CSKH16, CKH17, CSXZ17, CC11, CNK97, CPL11, CB11d, FD16, GA14, GHL17, GZL+12, GNGCA10, GSS13, GEG11, GAJ+17, GWPJ11, Han11,
HDL+17, HNWF07, HNWF12, HPT17, HG10, HZSS17, INT18, IKN13, IM17, JCP14, JLH+14, JW16, JYS+12, KD10, KKPT11, KOP+14, KGHK12, KB13, KZZ+16, KLN12, LCW12, LBS16, LGW12, LBTV11, LBTV12, LHKS12, LH14b, LLH17, LPMT17, MAK+14, MWJ+11, MFR+17, Mor15, MMJ10, NF17, NN18, NO16, NNK+16, Oht16, ORZ11, OM12, PAK17, PPH+14, Pie14, PD11, QZ10b, RJPB12, RS13, RB12, RSLML12, RHPWS13, RHT+15, Rui11, SPS+12, SH15, SFG+17, SCW11, SBT17, SEF+16, SE14, SH14, ST13, SHL+13, SPH11, SMM15a. functional
[SMM15b, SMM+18, SKTT11, SZSZ16, STS15, TLdG+12, TG12a, TS10b, VV14, Vik11, VL17a, VI17, VLGK+17, VED10, WKC10a, WHL+10, WCWW11, WDLG12, WYT17, WHX+10, WL14, WTH+16, WGN+16, XYW+14, YJ11, YLZ+10, YS13, ZXS+10, ZWXL11, ZSRL12, ZLZ14, ZDX11, ZYG+14, ZYW+10b, ZYW+10a, ZLHH14, ZGS+10, dSdS12a, dSdS12b].

functional/basis [PD11], functionalities [KAG+12], functionalized [KYKR15, LdSRR16], functionals [Ben17, CCB15, CGB16, DH17, DOM+11, DWC17, FPRS14, GWJR18, HG10, HBI+17, KB10, KSH13, KSSH13, Kar17, KM13, LBH+11, LHI4a, LKI6a, PW12, RSG14, Rui11, SGPS+17, Sea10, SDM+16, SPR+13, SXZ13a, SXZ13b, WYT17, Yu12b, ZTH+15, dSdLBNB17].

functions [BLZ+13, CD13, CC11, CVG14, Fer13b, Fer13a, FFA14, Fra15, Fra16, GSHM10, GZ14, KK17a, LRER13, MY17b, Mit13, MLCD11, PHT17, Pro16, RRCH16, SFM14, SYDS11, Sun15, TNY16, WZ17, TKN13].

fundamental [CD16, XLYZ10], furanosides [KRTB10]. Further
[RTS+13, FVB10, PZA15]. fused [CZY11], fusion [OLY17], Fuzzy
[FPV13, SK12, SK17], fuzzy-border [SK12, SK17], FXeOXeF [ARLP13].

G [Ano15-59, BZH14, LWD13, PHK14, ILKR11], g-tensors [PHK14], G2R3 [Gil11], g_membed [WHAS+16, WHAS+10], Ga [UT15, Mit13], Gabedit [Alli1]. GAff [MPBJ11], galactosidase [AKMT11], GALAMOST [ZLL+13], GalaxyDock2 [SKKS13], gallium [YR13], gamepad [HH16b], GAMES [LRBB12, WSGN11], GAMES-UK [WSGN11], GAMPMS [LMA15], gap [QZ10b, RS17a, THP+15, VLGK+17], gaps [TSN16], Garriga [Ihl12], Garriga-Sust [Ihl12], Gas [ATM18, ABB+12, PLZ17, ARLP13, DHE+12, GYX+10, JKS+16, KD10, LPK16, LJW11a, LPLB16, MP13, MFM+12, NIIT15, PGS+15, PMG+16, PSC11, RWR+13, Sea10, SYZ+17, STS15, YHG+11, ZSZ+14, ZYR+15, ZLHH14, ABB+13], Gas-Phase [ATM18, ABB+12, GYX+10, LPPLB16, PSC11, RWR+13, YHG+11, ZYR+15, ABB+13], gaseous [HCBI11, HYWH17], gases [LZ14, DHE+12], gateway [RK15], Gating [SBFT17], GaudiMM [PSC+17], Gauss [MY17a], Gauss-type [MY17a], GAUSSIAN [RSR+12, OYK+11, Bon14, DLL+10, EPD+10, JLCA17, Leh15, MG11, MKB+13, POB13, SPH11, Sum15, TH13, VKTRJ15, ZKE+17], Gaussian-based [JLCA17], gaussian09 [RS13], Gay [SLX+15], GB [OBW12, VM11], GBMV2 [LC17b], GBSA [DSX+11, GR10a, IMSR18, RDDS10, STM+15], GC [GWX+12, YZWC11].


general-contraction [HSN14]. Generalized [GH16b, KCPMG12, AB16b, BSPP+13, DSF17, FCE15, GHI6a, HWLW11, LL10a, MA16, PS13, SZTSM10, SSBW14, VMP17, WHM10, WBVE16]. generate [MPA12]. generated [HWLW11]. Generation [ADF+10, MPA10, RvL11, CAD16, GMSdG15, HGY15, KLJ+17, KSH+17, LTT16, RB13a, TDP+12, WHJH13, ZCGM11]. Generator [MYT18, Gar12, GPM17]. generators [CLK11, GPM17, HMM10].

genes [YS10]. GENESIS [KJM+17]. genetic [AC12, CB11b, FRLN10, LLJ12, NC12, RSL16, SHMO11, WMW+10, YVEI+17, LMA15]. GenIce [MYT18].


geometry-dependent [EPD+10]. Germanium [GSMM15, ALH+10].


glycine [DB12, DP15, FCD10, MC10]. glycoconjugate [LABSG17].

GmbH [Spr10]. GMCT [UU12]. GneimoSim [WK+14]. gold [Auo15-58, BH14, CJC10, FHT+15, GAMAC+14, Li14a, Li14b, LHK12, LH14b, MFR+11, MG14, MBFG15, SRR16, SKTT11, YLGX14].

GPU-accelerated [AGB13, CVT+11, HAP+12, YLGX14, ZL+13].

GPU-based [KGHC15]. GPU-enabled [BK17c]. GPUs
Hexahalogenated [VVJ15]. hexameric [RCM+13a, RML+15].
hexopyranose [HH11, PLH16]. hexopyranose-based [HH11, PLH16]. HF
[BRLS12, LGW12, MCK17a, BRLS08, Chu10, LSH+11, SKGB13]. HF/DF
[Chu10]. HF/DFT [BRLS12, BRLS08]. HFC [AR10]. HFC-263fb [AR10].
Hg [SLIB12, BBI+11]. HgHe [BBI+11]. HGXe [BBI+11].
HH [LGW12]. HI [LGW12]. hidden [DVVP14, LTT16]. Hierarchical
[JYC+16, BCG10, GBFD12, KKN11, RMPAM15, SNS13].
High [MCLD10, MKB+13, RLS13, BACSCJ+10, Cam15, CM13b, CSSB11, DH17,
DLS13, ESB13, EKW+13, GWJP11, IPAA11, JBAM11, JC16, KSM16,
KSM17, LL10a, MJLV14a, MO17, OPB+12, PVL+13, PV10, RVCFF13,
REH13, SC15, WGL+11, WDLG12, ZWL13, dSaSL13]. high-accuracy
[RVCFF13]. high-confidence [KSM17]. High-level
[MCLD10, EKW+13, KSM16, PVL+13]. high-order [REH13].
High-performance [RSLS13, CSSB11, ESB13, EKW+13, LL10a].
high-precision [DH17]. high-pressure [WDLG12]. High-quality
[MKB+13]. high-resolution [CM13b, JC16]. high-temperature [DLSD13].
high-throughput [ESB13, PVJ10]. higher
[NHY+17, PJJ13, VKAM12, WHM10]. higher-dimensional [PJJ13].
higher-order [NYH+17, VKAM12]. Highlighting [BRGN12]. Highly
[CHG+16, HAL14, LLZA12, LWL+16, DBDP16, BWWK10a, BWWK10b,
HYUS11, KOY+12, KZK+12, KV15b, OK16, TFQ+10, TJB12, LZZ14].
hindrance [MP17a]. Hirshfeld
[Man13, VVB13, VGV+11, EV14, GBVA11, OVPK15, VBV13a].
Hirshfeld-based [OVPK15]. Hirshfeld-I
[Man13, VVB13, VGV+11, VBV13a]. histidine [KFY+13, WC14].
histogram [Fer17, HHWL17, SH11b, ZH12]. histone
[GHK12, GH010, GSD10, KC13a]. HIV
[DLZ15, NNN16, OBW12, SYH12, TTB+10, UNT16, XLY12, Zsa10]. HIV-1
[DL15, NNN16, SYH12, TTb+10, UNT16, XLY12]. HIVgp41
HOB [LCL+10]. hole [BSF18, Cas13, CWHH11, EPH+13, GZZM16, GA12,
LZL+15b, PAK17, PTB+15]. holes [PM18]. Hollliday [Ish10, She12].
holo
graphic [CDB10]. Holt [She12]. HOMO [RS17a]. Homocysteine
[AALCM11]. homologated [ZLL+10]. homologation [GRCL12].
Homology [Z11, BFB11, DJ13, KOY+12, XFTW15, YZZ16].
homology-model [KOY+12]. homology/ab [DJ13]. homolysis [SZ17].
homonestable [BWKW10a, BWWK10b]. homopeptides [FC10].
[JLH+14, KV14, LZW+11, RDR16, KRSLO15]. Horizontal [PC16].
hormone [HYYZ13, LLL+10, NS10, OME16]. hormone-dependent [NS10].
hormone-receptor [OME16]. horsetail [MCRL17]. Host
[CC18b, OAN15b, YDGZ15]. hot [RFHG10]. Hou [JW12]. HOX [LZJ+11].
HP [LKL10]. HP-36 [LKL10]. HPt [dSdAR10]. HSE [VLC17]. HSiCl
hydroxyl
[DPNM11, GKR13, JCG+10, KS13b, Ray13, RKG11, TTR+12, ZSZ+14].
hydroxylated [CCJ+11, SH14]. hydroxylation [TLY+12, VCM15].
hydroxylations [MRR11]. hydroxymethyl [HH11].
hydroxymethylfurural [APY+16]. hydroxynaphthaldehyde [MPSG11].
hydroxyphenylpyruvate [DGH+11]. hydroxysteroid [ZX11].
hydroxysulfinyl [TL16]. Hyper [FRN15, BLLB+13, BZB+13, RFN15].
Hyper-parallel [RFN15]. Hyper-parallelism [FRN15].
hyperballs [CVT+11]. hyperboloids [CVT+11]. hyperbonding [LW16].
hyperconjugative [LZH16]. hypercoordinate [BSPP+13]. hyperfine
[CSEMB+16, MG11]. hypermatrices [BMPML+13]. Hypernetted
[HAL14]. hyperpolarizabilities [MLC13, WYT17, YHCS11].
hyperpolarizability [ISO+13, KBC12, TAL12, WXS+12, WZK+13].
hyperpolarizability [KSK11]. hypersurfaces [Ano10a, SN10]. hypervalent
[ASS+17, SLT14, SLT+15]. hypothesized [LLB+12]. hypoxanthine [FF11].
HZSM [cCVG+14]. HZSM-5 [cCVG+14].
Implementing [SCOJ13]. Implications
[CV12, VVY17, CBG16, LP11b, LTP11, RB12]. Implicit
[BEM14, CAD16, Has14, CBG16, EK15, FBEM11, KJDB12, KB11a, KB11b, 
LC17b, ML14, SSBW14, SLX+15, SCMA+17, TCC+13, WWKS11, YL13].
implicit-solvent [WWKS11].

Importance
[APA+14, CPK12, ENKK+17, NMF+14, OOK11, ESM+12, Ham11, 
KTNN10, PBDW11, SDZ17, TNSS17, TKNN10]. important

importing [FN12]. impregnated [GLZ17].

Improved [BS16a, LRER13, CCM15, DPB+12, DSF17, GCCM15, KSR+16, MP11, 
RTP+13, RDC16, SSBW14, YS10]. improvement [GSHM10, NLP+16].

Improvements [JCX10, AB16b, LRBB12, BB11c]. improves [BBOB16].

Improving [DWL11, GS16, LN15, PLH16, SB14, SACdG14, SA11, WZ17, 
ZX16, ZYS+10, GS15, GFPSD17, GZ14, FZY+12, TO10]. impurities
[SBC+11]. IMSPeptider [dCLFGL13]. In/Si [LGKS17]. inactive [CV12].

include [PZA15]. includes [HBKL10]. Including
[KL14, SFLG+17, BL12, FA15, FD16, LH14a, SPH11, TG12a, WC14, YB11].
inclusion [CGR16, LZ11]. Incorporating
[LHO17, Yan14, CSKH16, GCCM15, ZBP11]. Incorporation
[BT10, DDP16]. incremental [DCS15, LTA+11, SR18]. increments
[MS15]. independence [LC17a]. independent
[BVY+12, FVB10, GR11, yOTn16, ŠB15, ZBB16]. index
[CMF+17, OXBW16, RRC+15, TS14]. Indexing
[GPGSM11, GPGSM12, lili12, JZL+17]. indicator [BLG11]. indicators
[Bar14, BWKW10a, BWKW10b]. indices
[BK11, BMPML+13, BVC13, EFAC13, FVB10, GSHM10, HSB+11, MMS16, 
PRSG13, Pon11, SBR13, YB16]. indispensable [BF15]. individual
[LYZ12b, WS10]. indole [AARP17, YHCS11]. indole- [AARP17]. induce
[ASK18]. Induced [ATM18, AB10, AARP17, AKK+16, AS15b, BHNS14, 
BLFZ13, BCG10, CC18a, CPN+17, DH11, DLZ15, GDV17, GBS+17, 
HLBLCCG15, HB15, IMK+16, KL14, LCB10, MTM14, MHT+18, PD12, 
Tru18, WDP+12, YB13, YLZ+10]. induced-fit [BHNS14]. induction
[BCNH+11, DWR17]. inefficient [GMO16]. Inequivalence [MPSG11].
inexpensive [AC12]. infantum [VSD10]. inference [BFH+13, VZ14].

Infinite [CC11, GK15b]. Influence
[BSL+16, CSS17, CSKH16, HLH+12, KCPMG12, LvG13a, AKK+16, 
HGP14, LdSR16, OSHG17, SBD+17, SRL+15, HRK+10, HKRS11, HS11].
influenced [JXSW15, LLT12]. Informatics [SN16b, KSD+12].
Informatics-Based [SN16b]. Information
[ATM18, Ano16-75, Ano16-80, Ano16-94, Ano16-89, Ano16-81, Ano16-95, 
Ano16-82, Ano16-96, Ano16-83, Ano16-97, Ano16-84, Ano16-98, Ano16-85, 
Ano16-99, Ano16-86, Ano16-100, Ano16-87, Ano16-101, Ano16-88, Ano16-102, 
Ano16-76, Ano16-90, Ano16-77, Ano16-91, Ano16-78, Ano16-92, Ano16-79, 
Ano16-93, Ano16-129, Ano16-108, Ano16-109, Ano16-110, Ano16-130,


information-theoretic [CRZ+18, ZLW10]. informed [LZL+13]. infrared [DPAB16, HRH+17, KB16, LBC+12, NHF+10]. ingredients [CMvG10].


initialization [GR11]. initiate [HTS17].

Initio [DHOG13, Kop15b, PAK15, RSR+12, AR10, AG12, BEM14, BLG10, BIL10, BDDx13, BL12, CPRS18, CG15, CLC11, DHL+11, DSLD13, DJ13, EP12, EFOD13, FAA15, FCD10, GKL10, GWZ15, GZZ12, HYD10, KOP+14, KTO11, Kop15a, Kop16, Kop17a, Kop17b, KSR+16, Kow11, KVR10, LLH14, LPK16, LDJ+10, LZJ+11, LPE+10, LX11, LWJ+11b, LLTC12, LTP11, MK13b, MCDL10, MS12, NASH15, NMLD13, NDD+10, OHNK11, OYK+11, ON14, ORP16, OT12, OZLSB12, OOK11, PVL+13, DCOD13, RB13a, RFN15, SL+15, SS13b, SLIB12, SJZ+15, SLLL13, TLG+12, TG12b, US11, VVV+15b, VPR10, WLC12, WXY14, WDHZ13, XZ11, YG12b, YU12a, ZZL+12, ZZ10, ZMM12, ZLT13, ZLZ14, HEM+17, LI13a]. inito [JWST10].


Ano16-118, Ano16-119, Ano16-120, Ano16-57, Ano16-58, Ano16-59, Ano16-60, Ano16-61, Ano16-62, Ano16-63. Issue [Ano16-64, Ano16-65, Ano16-66, Ano16-67, Ano16-68, Ano16-69, Ano16-70, Ano16-71, Ano16-72, Ano16-73, Ano16-74, Ano17a, Ano17b, Ano17c, Ano17d, Ano17e, Ano17f, Ano17g, Ano17h, Ano17i, Ano17j, Ano17k, Ano17m, Ano17n, Ano17o, Ano17p, Ano17q, Ano17r, Ano17s, Ano17-36, Ano17-37, Ano17-38, Ano17-39, Ano17-40, Ano17-41, Ano17-42, Ano17-43, Ano17-44, Ano17-45, Ano17-46, Ano17-47, Ano17-48, Ano17-49, Ano17-50, Ano17-51, Ano17-52, Ano17-53, Ano17-54, Ano17-55, Ano17-56, Ano17-57, Ano17-58, Ano17-59, Ano17-60, Ano17-61, Ano18a, Ano18b, Ano18c, Ano18d, Ano18e, Ano18f, Ano18g, Ano18i, Ano18j, Ano18k, Ano18l, Ano18m, Ano18n, Ano18o, Ano18p, Ano18q, Ano18r, Ano18s]. Issues [GS16, MFEM16, XFG16]. iteration [SBB10]. iterative [Gra15, HLXH17, HLXH18, ZVY15, PGL15]. IV [EH13, MLGB16, VBMA13]. LV [HLXH18, HLXH17].


Lagrangian [FXC+13, HGCCGR+16, LRvdSM15, RHJ11, SDF+17]. 
Lamarckian [FRLN10]. lambda [ISK14]. Landau [SA11]. landscape 
[HDM+15, IMK+16, ZSB+16]. landscapes 
[BRE16, CDM+15, JCP11, PJ13, RDRIC16, SOJ14, SH11h, WSH10]. 
Langevin [OCL11, SSWX14, WBVE16]. language [LMR14]. 
lanthanide [CPRS18, DBF14, Hua16, TS11]. 
lanthanides [JXSW15]. lanthanoid [BCSCJ+13]. 
Large [JBSQG11, XFG+15, XFG+16, AF14, AGR11a, CSGOA17, CHG+16, 
CEBO15, CSSB11, DZA11, DDM+15, FN12, GRS15, GBW+14, GP11b, 
GWXZ12, HLXH17, HLXH18, JSXH16, JS17b, KG15, KNE11a, LS11a, 
LCPS13, LZX16, LWL+10, LCM+14, MK11, MDT10, NYN17, NFG+13, 
OPB+12, RLL+10, RS12, RSB+13, SCQ13, SAGC16, Sch12, SRR16, SG13, 
SMM17, TSR+16, WLW+10, WX12, XhD15, YHCS11, ZWL13, ZLL+13]. 
Large-Scale [XFG+16, JBSQG11, XFG+15, DDM+15, LCM+14, MDT10, 
RSB+13, XhD15, ZLL+13]. large-time-step [RS12]. 
LaSrVMoO [SWMW10]. lateness [MS10]. 
Lattice [RSLS13, EFOD13, Pon10]. layer 
[MBA11, PP10, SE14, YZZ+17]. layer-layer [YZZ+17]. lazy [LLL+10]. 
LCgau [SPH11]. LCgau-B97 [SPH11]. Lck [AC11a]. 
LDA [DOM+11]. leading [SJD14, TCPPC14]. LEAP [LZZ14]. learned [FP17a]. Learning 
[HJG09, Aou16, FZY+12, FSD+18, GHV17, LHO17, LTA+11, YLCX10]. 
least [BCCO10, Bow16]. least-squares [BCCO10]. leave [WMW+10]. 
leave-one-out [WMW+10]. leaving [KV15b]. lectins [MS˚AK12]. legacy 
vWI11]. Leishmania [VD10]. length [ASL+11, KSC16, RAR+11]. lengths 
[GREA11]. Lennard [DPSL16, DH11, KGHK12, NW17]. Lennard-Jones 
[DPSL16, DH11, KGHK12, NW17]. Less [SA10]. Letters 
[BCJC+14, Cor17, GKR13, GPGSM12, Ihl12, JW12, KR14, Man13, Ray13, 
RLSML12, SFLG+17, VVB13, WM12, dSdS12b, vLBBR12]. LEUS [BH15]. 
level [BVH17, DMJ17, EWEK+13, FFA14, HJKJ13, JGC+10, KSM16, 
KSM17, KNN11, MSc+10, MCLD10, OSR16, PVL+13, PTK11, PML+12, 
PBI4, VAMS14, WWD14, ZMM12]. levels 
[AC12, BCSCJ+13, BY11, BACSCJ+10, HYD10, Hua16, KHWB17, Kop15a, 
Kop16, Kop17a, Kop17b, MK13b, dSAdSL13]. leveraged [EPH+15]. Lewis 
[EHSPT16, KASH14, Lüc14]. Li [DDM+15, JW12, RLA+11, YCGA10, 
YHCS11, BWKW10a, RLA+11, TN12, YCGA10, SBW12]. Libcint [Sun15]. 
LIBEFP [KS13a, KS15]. libKEDF [DWC17]. Libra [Aki16]. libraries 
[LG11, RLL+10, WF16]. Library 
[KSD+12, AK16, DWEK17, EWEK+13, FRN15, KS13a, KS15, LRvE17, 
LMZ11a, LAS+14, MZZ11, RFN15, SC15, Sin15, VAR12, Yes12, Yes15]. 
library-based [MZZ1]. LICHEM [KWL+16]. LiCN [LLL+11]. LIE 
[CZY11, VLB+10]. life [RHT+15]. lifetimes [CH10]. Ligand 
[DPOS16, KCI3a, MNNK10a, VKC10, ABD11, AG12, BKLA13, BPD11, 
BCG10, BBG+18, BS10c, CMD13, CIKT13, CHR+12b, CHR+12a, DFF+15, 
FTW12, FBEM11, FRLN10, GHK12, GDV17, GS11, GZ14, HKR12, HG13, 
...
ligand-based [RVP+11].
ligand-binding [GDV17, MGWR12, OSR16, RO14b].
ligand-field [BBG+18].
ligand-induced [KL14].
ligand-receptor [FRLN10, VKC10].
ligand-sized [OGL10].
ligands [CS17, GPdC+16, HRC13, LL10b, LXZ+10, LS11b, SSP+13, TS10b, ZRCC12, ZWY+10b].
ligated [EH13, WC14].
LigDockCSA [SHL+11].
light [HXM+16, KDR+18, PE11, REL17].
light-driven [HXM+16, REL17].
light-harvesting [KDR+18].
lighter [WD10].
Lightweight [RLG14].
lke [AASP18, Che17, EPH+15, KOY+12, KB14b, MP17b, OAN15b, SDF+17, SM15, UCFR16, VHA+10, VVY18, WFZ+18, WKCI16, WGN+16, ZSL+11, VVY18].
Limit [SN16b, Fra15, Fra16, LW16, LYC+13, OAN15a, SLT14, WTH+16].
Limitations [LvG13a].
limited [SLT+15].
limit [II18].
Linear [BG12, YN15, ZLY+16, ARLP13, CPV+12, EP12, FBY+17, FCE15, GZZ12, JZZM14, JMS13, LP11b, MA17, MSAK12, NYH+17, PH17, RS17a, RLA+11, RR11, SS16a, Tak14, VBDS+11, WL10, YDX16].
linear-combination-based [Tak14].
Linear-scaling [BG12, YN15, NYH+17, RR11].
Linearity [IKN13].
linearized [Fra15, Fra16].
Link [ANO12u].
Linkage [HH11, OZS+13].
linked [Fom11, dACP12].
linked-cell [Fom11].
linked-lists [dACP12].
linker [NPG17].
lipid [BPPS17, MOS12, PGCT+12, ST11, WAS+10, WHAS+16].
lipids [HM16, ML14].
lipopolysaccharide [DLA14].
lipopolysaccharides [HBJ+17].
Liquid [WLC12, AASP18, APY+16, BDTP11, CC12a, EK15, GWJR18, IM17, KGHC15, Lar12, MG15, NTNY15, RSJ17, SBvG14, SAvg15, WCWV15, ZZT14].
liquid/lithium [EK15].
lipids [AFPI13, CG15, CFC15, CVG14, DASA15, EDOLdV17, SCM+15, SHF11, You10].
lists [Gon12, dACP12].
lithiated [KZK+12].
lithium [EK15, GMG+10, KOP+14, KYC11, LLL+11, MBRC16, NDG14, NFI+16, PGCI12, PMT16, SKY+11, TN12, ZZL+12].
lithium-doped [PGC12].
load [Fom11].
LOBSTER [MDTD16].
Local [CHP11, GH16a, GH16b, HJK13, ITIN15, CPN+17, DPP16, Fer13a, HH10, KSSH13, KDT+12, KGM12, Lar12, LLL+10, LZS+17, MKH+13, PH17, PRSG13, PRY+17, PW12, Sch12, SEF+16, SB15, WM17].
localizability [Bar14, BLG11, BWKW10a, BWKW10b].
Localization [Sax12, ABDGN12, BLK11, BLG11, GNDA+12, HJJ13, Mat14, Pill17, vSGP10].
localized [ANO15-58, BH14, SB15, ZM11, dLC17].
locate [AMGB10].
location [PTB+15].
locked [XVN17].
locking [XVN17].
locus [NR11].
logarithmic [MIOM13].
LOL [BSPP+13].
lone [BSF18, BSG18, ENKK+17, SSGS15, WCY+11].
lone-pairs [ENKK+17].
Long [BCNH+11, KSH13, KSSH13, AO10, BLBG+13, BZH14, JBSQG11,
KB10, KV14, MMS16, MBC13, PNG10, SMGB11, ST13, SPH11, SSA+17, TSN16, VI17a, Rui11. long-bond [KV14]. long-chain [TSN16].

Long-range
Low-density [BBI+11]. low-cost [TF15].
Low-energy [BPM15, DH14, MPA10, MPA12]. low-index [RRC+15]. low-lying [AC12, TSN17].
Low-memory [Gra15]. low-resolution [SM11, Vor10, BS10c, BBI+11]. lowest [GFG11].
Luminescence [DBF14].
M [LDJ+10, LLL+11, MCK17a, Rab12, TLdG+12, WWKS16, YW12, YHCS11, JJAB16, CCLCGR014, MCK17a, TLdG+12, YHCS11, JJAB16].
machines [GTZ+18, RLL+10, ZWL13]. macrocycles [CMM18, GMASBF16]. macrocyclic [ZRCC12]. macrolide [PG15].
macromolecular [Kne11b, LCA17, LAT10, LAT11, PG14, UW12, RTP+13].
macromolecules [DGC14, DZA11, FXC+13, OHPR17, RZ16, ZKE+17].
macrotetra cyclic [ZHY+10b]. magnetic [BCSCJ+13, BACSCJ+10, CPRS18, CPN+17, FNSF+11, GTT10, HAI+16, Ibr17, JCG+11, KNP+12, LLM11, LLB+12, SACdG14, SB13, SB15, Vik11, wZbZ11, ZLZ14].
Magnetically [ATM18]. magnetizabilities [ZPP+16]. magnetoresponsive [TDKT10, TS11]. main [ACD+13a, ACD+13b, JJJ16, XhD15].
managed [LMA15]. manganese [GHL17]. manganese-based [GHL17].
many-core [KNHN16]. map [MKM+17]. mapper [BJP15]. mapping [EMD17, MMM+16, RNSF+16, TD10]. maps [GMPAM+14, YRSR10].
Marburg [OLY17]. marker [JAH+17]. Markov [BFH+13, LTT16].
Martini [HBJ+17, SM15]. MARTINI-like [SM15]. mass [NPTS16, PGY15]. massive [GP11b, TNY16]. Massively [KNHN16,
KZZ$^{+16}$, MYT$^{+14}$, BWMSM10, KN17, NNK$^{+16}$, OPB$^{+12}$, WHK$^{+12}$.
master [RSLS13]. match [TZ12, YPKB12]. matched [KSR$^{+16}$]. matching
[AW11, GPS10, HS12]. Material [JW12, DGL$^{+13}$, HLWD15, JBSQG11,
LL13b, MCAG$^{+16}$, NGAS17, SLHW09]. materials [BSL$^{+16}$, CD11, DLT17,
ECZWD17, EMD17, Man13, NDD$^{+10}$, SYZ$^{+17}$, VB13a, VVB13, VVY17].
MATLAB [DDK14]. matrices [Car14, LHO17, Mat14, Yon16]. matrix
[CAP17, CWZB10, Kne11b, LAT10, LAT11, PW12, RPNP10, RNP13, RR11,
SS13a, STM17, TCPPC14, UIW$^{+10}$, VGV11, VKNT15, VKNT16, ZVY$^{+15}$].
matrix-based [VGV$^{+11}$]. matrix-free [ZVY$^{+15}$]. matter
[HRB$^{+17}$]. Maxima [L¨uc14]. maximum [MLC13]. may
MC-XQDPT2 [KKL$^{+13}$]. MCN [LLL$^{+11}$]. MCQDPT [LLSW14]. MD
[DDK14, RSR$^{+12}$, BM12, FB14b, GMASBF16, LJL$^{+11}$, MTvG12,
OYK$^{+11}$, RAR$^{+11}$, SISK10, SMP17a]. MDAnalysis [MADWB11]. MDLab
[CCW$^{+10}$]. MDTRA [PVZ13]. Me [KKR$^{+13}$]. mean [HDL$^{+14}$, KERY$^{+16}$,
KT10, KS12, KLS10, KMLS10, MIOM13, MP17b, RI10, VBDS$^{+11}$, Vor12].
mean-force [MIOM13]. meaning [PSP15]. Means
[Sch18, KSM16, TTB$^{+10}$]. measure [TZCK18, WF16]. measurement
[MPSG11]. measures [CDB10, CAA10, Dry14, MK11, PZBA13]. mechanical
[AC11a, APY$^{+16}$, ACS12, ALH$^{+10}$, BTT10, BEL$^{+11}$, CXW14,
DR11, DLW12, ECZWD17, FL15, GMMH$^{+16}$, HYUS11, Ibr11, JW015,
JSXH16, KVR10, LPE$^{+10}$, MHRR11, NKK$^{+16}$, NDD$^{+10}$, OR16, PML$^{+12}$,
PGW$^{+17}$, PVAM16, SBD$^{+17}$, TZ11, VPR10, WKC$^{+10b}$, WCAH10,
YKO$^{+11}$, ZSTI14, ZWMW10, ZKH$^{+10}$]. mechanical/effective [DR11].
mechanical/molecular [BEL$^{+11}$, YKO$^{+11}$]. mechanically [SOYC12].
mechanics [AS10, AGB13, AS15b, BGR13, CGPP11, CXW14, Chu10,
CHKR10, Cor17, CB11b, CB11c, DDM$^{+15}$, EPH$^{+13}$, ENKK$^{+17}$, Fer13b,
Fer13a, GEP$^{+14}$, GPdC$^{+16}$, HWLW11, KGHK12, LAHS16, LTP11, L¨uc14,
MS12, NLP$^{+16}$, NHK$^{+13}$, PSC11, PGW$^{+17}$, SFLG$^{+17}$, VYM15, WOH16,
WOH18, WCDM11, YPKB12, HWLW11]. mechanics-based [WCDM11].
mechanics/dynamics [DDM$^{+15}$, EPH$^{+13}$, GPdC$^{+16}$].
mechanics/generalized [HWLW11]. mechanics/molecular
[FB14b, Fer13a]. mechanics/Poisson [HWLW11]. Mechanism
[GZL$^{+12}$, SLY$^{+10}$, VKNT15, WCW11, BHNS14, BMFG16, BEL$^{+11}$,
CPV$^{+12}$, CPLLI1, FB14b, GYX$^{+10}$, GRCL12, HYZZ13, HDHL15a,
HDHL15b, HDHL15c, JCG$^{+10}$, JLS$^{+10}$, JW16, KV14, KT12, KS13b,
LZL$^{+10}$, LZHH11, LLB$^{+12}$, LWWC16, LHT15, LPM17, NJX$^{+10}$, Oht16,
PMT16, RLGI11, RSK$^{+15}$, SLL13, SBW12, VMTL10, WQZW10, WCL$^{+11}$,
XLY12, YPC$^{+10}$, YHG$^{+11}$, YXZZ17, ZSWL12]. Mechanisms
[WJX$^{+10}$, ZZWT12, DWZ$^{+17}$, GG10, KCI13a, MH11, MLY$^{+13}$, PPH$^{+14}$,
SLT14, SLT$^{+15}$, YB11]. Mechanistic [CYY$^{+17}$, LZZL$^{+16}$, TSJ$^{+10}$, YZ17,
ABB$^{+12}$, ABB$^{+13}$, GDNA$^{+12}$, NGD14, WLVHW12, WHDL11, YZGS14b].
mechanochemical [QB16]. mediated [MRR11, RVP$^{+11}$, XYW$^{+14}$].
medium [FE14, IPAA11, LRvE17, RK15, WWD14]. medium-size [FE14].
[PSC11, PKIC11, PPJ14, PLV+11, Pon10, QLQ11, QB10, QB11, RHRC3H16, RKG10, RLS13, Rod13, RKB+14, RFHG10, SS13a, SCM+15, SBB10, SSWX14, SBN13a, SBN13b, SB15, STM17, SG13, SSAS10, Tk14, TKNN10, Tak10, TSZQ12, TSNC+17, US11, UIW+10, VLB+10, VDVR14, Vor10, WXS+12, WJG+13, WMH10, WTH+16, YWJ+16, Yun10, YN15, YHH+13, ZDZM13, ZMM12, Zha12b, Zha12a, ZLM+14, RFHG10, SSWX14, SBN13a, SBN13b, SB15, STM17, SG13, SSAS10, Tk14, TKNN10, Tak10, TSZQ12, TSNC+17, US11, UIW+10, VLB+10, VDVR14, Vor10, WXS+12, WJG+13, WMH10, WTH+16, YWJ+16, Yun10, YN15, YHH+13, ZDZM13, ZMM12, Zha12b, Zha12a, ZLM+14, RFHG10, SSWX14, SBN13a, SBN13b, SB15, STM17, SG13, SSAS10, Tk14, TKNN10, Tak10, TSZQ12, TSNC+17, US11, UIW+10, VLB+10, VDVR14, Vor10, WXS+12, WJG+13, WMH10, WTH+16, YWJ+16, Yun10, YN15, YHH+13, ZDZM13, ZMM12, Zha12b, Zha12a, ZLM+15, ZW17, ZH12, ZA15, Zim15].

**Methodological** [VKNT16]. methodologies [Rob13]. methodology [Aki16, FF11, GAI13, GMASBF16, HPT17, OHPR17, RJWW12, HCD+10]. methods [Ano12u, Ano15-59, ASMS10, BG13, CLFRO18, CSGOA17, CXS10, CNK97, DKE+17, DBM+15, EWK+13, ESM+12, EV14, Fer13b, Fer13a, FB10, FSSW17, GAI14, GFPSD17, GD10, GSS13, GMSBF16, HCB11, HSB+11, HÖf14, HWLW11, JJH+13, KSM17, KB13, KHWB17, LEDOLdL17, LZLC13, LLSW14, MS13, MY17b, MR17, MVKS10, MOS12, NYH+17, NASH15, NC13, NC14, NTNY15, OSHG17, DCOD13, PN13, PVAM16, RZG+13, RRH12, SFR+17, SS+16, SACdG14, STM+15, SGWA17, TG12b, TS15b, Tsi17, WBT10, WX12, YLCX10, YAS13, YJ17, ZGS+10, dSDLBNB17].

JCL+17, KSD+12, LABSG17, LLH14, LZGS11, LT13, LN15, MBA11, MJLV14b, MA17, MBA14, MPBJ11, NSO+14, NW17, PHC13, PSS14, PGM+17, PHT16, RJS17, SN16a, TTR+12, VKNT15, VAA14, VCM15, WLX17, WPM+15, WLO+17, XDL+10, XLY12, YJ11, ZX11, DHE+12].

modelling [DBM+15], models [BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DI11, DGC14, EK15, EPD+10, GMPB12, GMMH+16, GMG+10, GKR13, GCP+13, GCC14, GAJ+17, HS16b, HGY15, JCP14, JGS+17, KJDB12, KKO+16, KB11b, KSR+16, KSW16, LTL16, LKL10, LZ12, LLWS14, MPSA17, MSAK12, MCIJ15, MKB+13, NNS15, OL13, PCH13, PGY15, PL18, Ray13, RTP+13, RKG11, SCMA+17, SFLG+17, SAvg15, TH13, TTB+11, TTT+12, VKC10, VMPS17, VZ14, WS10, WW14, YJ11, YL13, ZsA10, dSLBNB17].

modelling [DBM+15], models [BEM14, BLKP12, BPB11, CD11, Cor17, CBG16, CK17, DDP16, DSM+11, DI11, DGC14, EK15, EPD+10, GMPB12, GMMH+16, GMG+10, GKR13, GCP+13, GCC14, GAJ+17, HS16b, HGY15, JCP14, JGS+17, KJDB12, KKO+16, KB11b, KSR+16, KSW16, LTL16, LKL10, LZ12, LLWS14, MPSA17, MSAK12, MCIJ15, MKB+13, NNS15, OL13, PCH13, PGY15, PL18, Ray13, RTP+13, RKG11, SCMA+17, SFLG+17, SAvg15, TH13, TTB+11, TTT+12, VKC10, VMPS17, VZ14, WS10, WW14, YJ11, YL13, ZsA10, dSLBNB17].
LZL⁺13, LWXC16, LZS⁺17, LJL⁺11, LP11c, LAS⁺14, MRB14, MKS⁺12.

**molecular**

[MSC⁺10, MJC14, MCRL17, Mat10, Mat14, MSvG12, MWJ⁺11, MFEM15, MADWB11, MPNS13, MKM⁺17, MBA14, MHRR11, MCC12, MFR⁺17, MO17, MS12, NPTS16, NSO⁺14, NLP⁺16, NST14, NPG17, NFPD13, NFG⁺13, NF17, NNK⁺16, NHK⁺13, NS17, NTNY15, Oht16, OHNK11, ON14, OGL10, OHPR17, OCL11, OLY17, OT12, OME16, OVPK15, OOT15, OW15, OWX17, OW16, OW15, OW14, OW13, OW12, OW11, OW10, OW9, OW8, OW7, OW6, OW5, OW4, OW3, OW2, OW1, OW10, OW9, OW8, OW7, OW6, OW5, OW4, OW3, OW2, OW1, OW10, OW9, OW8, OW7, OW6, OW5, OW4, OW3, OW2, OW1, OW10, OW9, OW8, OW7, OW6, OW5, OW4, OW3, OW2, OW1, OW10, OW9, OW8, OW7, OW6, OW5, OW4, OW3, OW2, OW1.

**Molecular networks** [MCC12].

Molecule

[KR12, vRWGS17, DHOG13, DGL⁺13, ETLS17, FAA15, GAI14, GCWS15, GBVA11, HH17, ISG13, IHI15, KB11b, LIRL16, MCC12, PCLL11, RLL⁺10, SG10b, VGV11, WF16, XYW⁺14, XMSZ16].

molecule-mediated [XYW⁺14].

Molecule-specific [KR12].

molecule-transcription [XMSZ16].

Molecules

[ATM18, AIGP15, ARAG17, AGR11a, BLBG⁺13, BS10a, BTMS12, BSF18, Ben17, BS16b, BL12, CHG⁺16, CQFC10, CYG⁺15, CCOH14, CXS10, CZNA11, FE14, GWF11, GP12, GPGSM11, GPGSM12, GAJ⁺17, HRB⁺17, HSB⁺11, Hug12, Hl12, Kan15, KLJ⁺17, KYG⁺15, LPS12, LHSH12, LgV13b, LI4b, LJ⁺11, LG14, MA16, MS13, Mat10, MSS⁺13, MH17, MBE16, MPBJ11, NIT15, OGL10, OT12, PZBA13, Pyy13, RSG14, RK15, SFCCK⁺14, SFCCK⁺15, Sch13, SG10b, SFLG⁺17, SY16b, SM17, TZCK18, TSR⁺16, UNT16, VVV⁺15a, VHA⁺10, VVY18, VDVR14, WC13, WSZW15, WWD14, WX12, You10, YKHI5, YHW17, ZPP⁺16, Zha12b, ZLX⁺13, ZBB16, ZCGM11].

Møller [FSSW17, Hll13, KKKN11, KN17, MCC11, YKHI5].

**MOLSIM** [JP15].

molSimplify [IGK16], MolTPC [WHJH13].

Molybdaticarbaboranes [LK16b].

**molybdocene** [PM13, SDL14].

**Moment** [SS16a, JCG⁺11, KCB⁺12, Yan11].

**Moments**

[GH16b, BLDK⁺13, CP15, CTP13, DHOG13, GH16a, Lar11, NOKJ16, Tru18].

momentum [EP12, GWF11, PH17].

monazite [RKB⁺14].

monazite-type [RKB⁺14].

monoxanion [YZGS14a].

monoboronyl [VVBL17].
[GA14, SP13, CCM15, CF14, GCCM15, MCC11, MC12, SSSM15].

multiresolved [DGC14]. Multiscale
[BLKP12, FXC+13, LC16, LZ14, JBB+11, MBC13, SYN+12, WLO+17].
multisite [CK17, HS14b, MMB+17]. Multistart [MS16]. Multistate
[TM16, AM10]. Multistep [DWZ+17, FZY+12, WDZN16]. Multistructural
[SMM17]. Multisubstate [PBLdS12]. Multithreading [TO10, ZWL13].
multivalent [AS14, FVP14]. Multiwfn [LC12]. Mus [WZQW10].
muscarinic [SRA17]. musculus [WZQW10]. mutagenic [BZH14].
mutant [FHK+12, LMA15]. Mutantelec [VMRSH+17]. mutants [RKDM14].
mutation [BA11, VMRSH+17, ZJZM13]. mutations [BH15, GMO16, KYT+17, SL10, SY16a, WC11].
mMVPack [BACSCJ+10]. MX [Sch13]. mycobacterium [MPNS13].
MyMolDB [XTG+11]. myoglobin [SHB17].

N [Ano15-59, BLF14, BCNH+11, KBC12, KCL+14, LPLB16, NDG14,
PV+13, BCNH+11, BWK10b, BMB13, BSDP16, CWT+12, CCM15,
DCHL12, DLW12, GMASBF16, GZL+12, HLH+12, KV14, KCL+14,
LZL+15b, MLGB16, MS15, OZLSBH12, PVL+13, RHN10, RWR+13,
SB+17, SGHL13, TSJ+10, VM11, WS10, WGL+11, WCL+11, WYGW12,
WS12, Yu12b, YXZZ17, ZP13, HPSK12]. N- [BMB13]. N-heterocyclic
[BSP16, CWT+12, SGHL13, WS12]. N-methyl-N-phenyl-hydrazine
[GZL+12]. N-methylacetamide [HLH+12]. N-substituted [DCHL12].
NABs [SBW12, SBW12]. NABs-Li [SBW12]. NaCl [HB15]. NaI
[OCW+15]. Naiyang [Ano12u]. nano [Ano15-58, BH14, QZ10b].
nano-clusters [QZ10b]. nanobiotechnology [Fel10]. nanochannels
[TM16]. nanocluster [AS15a, RVKV13]. nanoclusters [AASP18, LLJ12].
nanocrystal [KC13b]. nanographene [DWZ+17]. nanographenes
[TSN17]. nanolayers [EBK13]. nanoparticle [CCJC10, NS15].
nanoparticle-PMMA [NS15]. nanoparticles [EOO+16, LZZ+11].
nanopore [SM16b]. nanopores [DMN14, MJ14, SM15]. nanoribbon
[DJX+11b, DJX+11a, RRK14]. nanoribbon-based [DJX+11b, DJX+11a].
nanoribbons [LWZK13]. nanorings [TS15b, YDGZ15]. nanorods
[LHKS12, LH14b]. nanoscale [Hei10, SWB+12]. nanosecond
[Bow16, MCRL17]. nanosheets [wZbZ11]. nanostructure [LLD17].
nanostructures [YZZ+17]. nanosystems [Tia12]. nanotube
[AS15a, FTR15, JWO15, OCW+15, RHN10]. nanotubes
[ASL+11, BE14, BPE16, DI11, Den12, DZAI11, EBK13, EP15, EBPK17a,
EBPK17b, GBS+17, KGKH12, LPLS16, LL10c, LT14, NDD+10, PBE16,
naphthalenediimides [MGS+16]. naphtho [ZLL+10].
naphtho-homologated [ZLL+10]. naphthodianthrene [DGL+13].
naphthol [CY+17, GZL+12]. native [DJ13, HYL+11, UCFR16, YL13].
native-like [UCFR16]. Natural [LCPS13, MBFP15, Wei12a, Wei12b, AO10,
GMZ12, NC14, Sch12, GLW13a, GLW13b]. naturally [XVA+16]. Nature
[ABDGN12, MJM1+15, WFZ1+18, GPK1+16, HBR17, Kri10, LZJ1+11, LYL16, LdSRR16, MLGB16, PKK17, RKDM14, YK13, YJ17, ZRCC12]. navigation [SLG15]. NBe [UT14]. NBO [GLW13a, GLW13b, WvRSM14]. NBS [YZ17]. NCCH [MLGB16]. NCI [REV1+17, VVJ15]. NCY [LZL1+15b]. near [DJ13, SISK10, Yan11]. near-native [DJ13]. near-solute [Yan11]. near-native [Hug14, YS15]. Necessity [JC16]. necks [CC12a]. negative [KV13]. neighbor [AGR11a]. neighbors [Hug14, YS15]. NEMO [HBKL10]. Net [RO14b, CS14]. netropsin [HDK1+12]. network [AD10, GFPSD17, GGM1+12, HNHR13, HAI1+16, IIHY15, LDH1+14, OC14, PC11, PPUBGD10, RKDM14, WMW1+10, XTY1+14]. network-based [PC11, PPUBGD10]. networks [AGM1+13, Clo15, Kan15, KUDG12, LHO17, PPM15, PPUBGD10, TD11]. neural [AGM1+13, HNHR13, LHO17, LDH1+14, PC11, WMW1+10]. neutral [GC11, GWPJ11, JM11, KD10, Tsi14]. new-type [HLWD15]. News [AIGP15, Aki16, APK14, AAC1+16, BTA1+13, BBH12, BCSCJ1+13, BSZ1+12, Ber17, BJP15, DNN15, BBG1+18, CBBH14, CSEM12, ZCZF17, CAT1+13, DDJ12, DVVP14, DDK14, DWC17, DSK17, ESB13, EWK1+13, FN12, FSC1+14, GMSdG15, Gar12, GJMPAM1+14, GLW13b, GS12, GCP1+13, GCC14, GH16b, HG13, HYMZ16, HKR1+14, HBJ1+17, HL14, HC14, IKG16, JHH1+13, JJW1+14, JPCA17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15, KB16, KDR1+18, KKM1+17, KDT1+12, Kos16, KG13, KL1+16, KK17b, KWG15, KYG1+15, KAG1+12, KSW16, KPF1+15, LPS12, LJR1+12, LSH12, Lh15, LRvdSM15, LRvE17, LDB1+17, LLZA12, LBB1+15, LWW1+17, LC12, LAc1+14, MHT1+18, MDT16, MBR1+15, MYT18, MSSP17, MB14, MB16, NKJ16, OV14, OPB1+12, OZS1+13, OC14, PSS14, PGL1+15]. News [DBDP16, PSC1+17, PW12, PPM15, PHH1+12, PVZ13, PG14, RLLHL12, RNSF1+16, RZ17, RX16, RR14, RdA12, RSR1+12, RCM1+13b, SM14a, SFG1+17, SK15b, SW13a, SM14s1+17, She12, SC15, Sie15, SJ17, SW12+12, SDMS13, TNY16, TSC1+13, TTR1+12, TTL1+12, UU12, VMRS1+17, VVV1+15b, VAR12, VBV13b, WDvN12, WDI13, WPM1+15, WF16, Wei12b, WHK1+12, WHJH13, WG14, WC1+14, XCM1+15, XY17, YWJ1+16, YZ16, Yes12, Yes15, YHH1+13, ZDKM12, ZLL1+13, dVAG16, KKR1+13]. Next [ADF1+10, HGY15]. next-generation [HGY15]. NF [ABB1+13, ABB1+12]. NGuaS [WGN1+16, WGLG1+16, WRG1+17]. Nguyen [Ano15-59]. NH [CG12, KS11, LBV12, VVY17, CCJ1+11, Kop15a, LYT1+13, LYT1+11, ON1+16, UT14, Yu12a]. NH-... [MVKS10]. NHH [LZH1+11]. NHOC [LHH1+14]. Ni [ib17, TLdG1+12, Tsi17, WWKS16, MMB1+17, SSX1+14, TLA10, ZRCC12]. Ni-NO [Tsi17]. nickel [ED15, FCW1+14]. nicotine [PMC1+17]. NICSz [AVH18]. nitrate [OSS10]. nitric [BS16a]. nitride [GLF16, LT14]. nitrides [TS11]. nitrilotri [CM16]. nitrilotri- [CM16]. nitrilotriaconic [CM16]. nitro [YPC1+10, ZWZ11]. nitro-substituted [YPC1+10]. nitroaldol
nitroaniline [ZTH+15]. nitroaromatic [PSC11, TD10]. nitrobenzenes [ZGS+10]. nitrocompounds [SIG+15, SGH+16].
nitrophenylbenzofuran [DPB+12]. nitroethane [YZL+15].
nitrogen [LLC17, BEPM14, KV14, ZZWX11, ZYL+12]. nitrogen-atom [KV14].
Nitrogen-doped [LLC17]. nitrogen-rich [ZGS+10, SGH+16].
nitrodibenzofuran [DPB+12]. nitroethane [YZL+15].
Nitrogen [LLC17, BEPM14, KV14, ZZWX11, ZYL+12].
nitrosothiol [TKXT13]. NMR
[Ben17, CHP11, EOA+11, HJ13, HBI+17, HM13, KASH14, LK11, OPR16,
PTK11, PGd0+16, PC14, Pie14, RK15, SEF+16, SKMS13, WL14, YS13].
NNO [WGL+11]. NO
[MCUJ15, Tsi17, ZZ10, WYGW12, BS16a, GY12, OSHG17].
nitrogen-doped [LLC17]. nitrogen-rich [ZZWX11, ZYL+12].
nitrogen-substituted [BEPM14]. nitroiminotetrazolate [ZYL+12].
nitromethane [MCUJ15]. nitrosamine [dALdS+15]. nitroso [TDP+12].
nitrosothiol [TKXT13]. NMR
[Ben17, CHP11, EOA+11, HJ13, HBI+17, HM13, KASH14, LK11, OPR16,
PTK11, PGd0+16, PC14, Pie14, RK15, SEF+16, SKMS13, WL14, YS13].
NNO [WGL+11]. NO
[MCUJ15, Tsi17, ZZ10, WYGW12, BS16a, GY12, OSHG17].
nitrogen-doped [LLC17]. nitrogen-rich [ZZWX11, ZYL+12].
nitrogen-substituted [BEPM14]. nitroiminotetrazolate [ZYL+12].
nitromethane [MCUJ15]. nitrosamine [dALdS+15]. nitroso [TDP+12].
open-ended [RJR14]. open-shell [BG13, ISO\( ^{+} \)13]. Open-source [HLS\( ^{+} \)13, Aki16, APK14, FBY\( ^{+} \)17, HPT17, KSD\( ^{+} \)12, PHT17, Yes12]. open-shell [GMBX\( ^{+} \)16, WCL\( ^{+} \)11, ZQ14]. OpenMM [HLW\( ^{+} \)17]. OpenMP [JMS14, KS15, KN17]. operation [Bac12]. operational [MA16]. operations [WS13]. operator [LMR14, SNS13]. operators [Car14]. Oppenheimer [BLZ\( ^{+} \)13, LCH10, RSB\( ^{+} \)13]. opportunities [KHWB17]. opposed [WWKS16]. opposite [´SSB\( ^{+} \)16]. opsin [RLG11]. Optical [WGLG\( ^{+} \)16, ARLP13, BLL13, BLS10, GTT10, HB15, HRJ\( ^{+} \)14, HRJ\( ^{+} \)15, JRSHP14, KRTB10, KOP\( ^{+} \)14, LLBO12, LLD17, MLQ\( ^{+} \)12, MIS\( ^{+} \)15, MGS\( ^{+} \)16, MCK17a, TFQ\( ^{+} \)10, TFQ\( ^{+} \)11, TS15b, YB13, YCGA10]. optics [Tia12]. Optimal [DBK17, VSA11, HS12, Kne11b, LTT16, LAT10, LAT11, MLC13, SM17, Tak11, TTB\( ^{+} \)10]. optimally [SZZS16]. Optimization [AG11, CB11b, CB11c, HOK17, LC17b, MY17b, TKN13, WM12, BW11b, BHR15, BW15, BS15, BC13, CY09, CY13, CJL\( ^{+} \)13, DS15, DH11, DMAH15, Elk16, HKR12, HJKJ13, LvDH13, Leh15, LZL\( ^{+} \)13, LLJ12, Ponn10, SA13, SZBM13, SKKS13, SMMW09, SLG15, SR10, SM17, TSZQ12, TO10, Vor10, VBVI3b, YS15, ZWP11, ZsA10, vLBBR12, PGL\( ^{+} \)15]. optimization-based [YS15]. optimizations [RR12, WX12]. optimized [Boz18, CX10, GA12, HH10, LZZ14, SD17, SB14, WO15]. Optimizing [SYDS11]. optimum [KTNN10, SB11, TKN10]. ORAC [MSC\( ^{+} \)10]. orange [LWL\( ^{+} \)11]. orbit [AMQ\( ^{+} \)14, FAA15, FD16, GP11a, JKS\( ^{+} \)16, MG11, MCP18, PS17, YB11]. Orbital [WM12, ASL\( ^{+} \)11, Boz18, BVC13, CIKT13, CPN\( ^{+} \)17, CGPP11, DHF\( ^{+} \)11, FE14, GFW11, GLW13a, GLW13b, IIF\( ^{+} \)10, IKN13, KTN10, LCP13, LFN\( ^{+} \)10, LTP11, MFR\( ^{+} \)17, MGS\( ^{+} \)16, NF17, OHNK11, OOT15, OOK11, PRYI\( ^{+} \)17, PH15, RKGN10, SGPJS\( ^{+} \)17, Sch12, SMMW09, SB14, SB15, TKN10, TS14, TSN16, US11, UM13, Wei12a, Wei12b, WCWV15, WM17, ZA15, vLBBR12]. orbital-based [CGPP11, MFR\( ^{+} \)17, Wei12b]. orbital-dependence [SGPJS\( ^{+} \)17]. orbital-optimized [Boz18, SB14]. orbital-weighted [PRYI\( ^{+} \)17]. orbital/local [SB15]. orbitals [AVHB18, CAF\( ^{+} \)13, CCM15, Dil15, EP12, Fer13b, Fer13a, GCCM15, HJKJ13, HJJ13, JXSW15, MRB14, MY17a, MBFP15, MCK17a, Sax12, TZ12, VI17, ZR10, ZM11]. ORBKIT [HPT\( ^{+} \)16b]. ORCA [MG11]. Orchestral [LL10b]. order [BCC10, DCHL12, FSSW17, HIL13, KKKN11, KN17, LCL\( ^{+} \)10, LPS\( ^{+} \)13, MLQ\( ^{+} \)12, MCC11, NYH\( ^{+} \)17, yOTn16, RBOH11, REH13, SK12, SSB\( ^{+} \)16, TAG16, VKAM12, VFAR16, WHM10, ZWF15]. ordered [LPAS11, LC17a, LLB\( ^{+} \)12, SJZ\( ^{+} \)15]. ordering [MNNK10a, MNNK10b]. ordering-based [MNNK10b]. Org27569 [ILKR11]. organic [AH10, Bent17, BE16, CWHH11, CYG\( ^{+} \)15, CLK11, DGL\( ^{+} \)13, ED15, FNSF\( ^{+} \)11, GLZ17, GAJ\( ^{+} \)17, LZ14, LZF\( ^{+} \)15a, LWL\( ^{+} \)10, NDLW13, PLZ17, PNW\( ^{+} \)16, Pog10, PPM15, RSG14, SRR16, SFDE16, SSAS10, SIG\( ^{+} \)11, TTR\( ^{+} \)12, TTB\( ^{+} \)11, VVV\( ^{+} \)15b, VVY17, XWW\( ^{+} \)11, YJN\( ^{+} \)11, YNH\( ^{+} \)17, Zha12a, ZA15, ZCGM11]. organization [AO10, MCC12]. organo [MMS16]. organo-metallic

P [GTK10, HZ11, LCWW10, VT14, BE16, ED15, HAI+16, RVCF13].
P-type [BE16]. P 450 [EH13, MRR11, SLY+10, SOYC12, TDP+12, VCM15].
Pairwise [GS14, Gon12, VMPS17, XTY+14]. pairwise-additive [VMPS17].
palladium \([WCWW11, YHG^{+11}, dCDP15]\). palladium-catalyzed \([dCDP15]\). paper \([GP GSM12, hl12, JW12, WM12, HP10a]\). para \([KYCL11]\). para-substituted \([KYCL11]\). paracyclophe [KGR^{+16}]. paracyclophane-bridged \([KGR^{+16}]\). Paradoxical \([UT14]\). Parallel \([BTB^{+11}, KDB13, NN18, UIW^{+10}, WWKS16, BW11a, BTT10, CEB015, CSSB11, GJMPAM^{+14}, GRARO^{+14}, HP10a, HS17b, HPSK12, KS13a, KNHH16, KN17, KZZ^{+16}, KJM^{+17}, KDT^{+12}, LL10a, LPLA13, MBR^{+15}, MCR17, MYT^{+14}, MJM^{+15}, NNK^{+16}, OPB^{+12}, RFN15, SHMO11, Tcx^{+13}, TJB12, WHK^{+12}, Yes15, ZWL13, ZSS^{+13}, CJL^{+13}, KDT^{+12}, LMR14]\). parallel-generalized \([LL10a]\). Parallel-ProBiS \([KDT^{+12}]\). parallelism \([FRN15, Gon12]\). Parallelization \([AB16b, VDL^{+13}, BWMSM10, IUK^{+11}, JMS14, KS15, KKNN11, LLZA12, RˇSRR15, vW11, ZDKM12]\). parallelize \([vW11]\). parallelized \([DBDP16]\). parallelizing \([BMBJ11]\). parameter \([PFVL14, VVLG17, WDHZ13, LL11]\). Parameterization \([HK18, HJLV16, ILKR11, IHJ^{+13}, MPSA17, PRRT^{+10}, TCC^{+13}, BAS14, CCLP12, DLMH12, KYYB13, LTP11, MSS^{+13}, VLB^{+10}, VBD11]\). parameterizations \([SH15]\). parameterized \([OZS^{+13}]\). Parameters \([CTR13, AG11, AKMYB18, BCSCJ^{+13}, BCJC^{+14}, BW15, BC13, CYG^{+15}, DPSL16, DMAH15, FHT^{+15}, GSD10, HLS12, HM16, HBI^{+17}, HLH^{+12}, KvdV14, GKH12, LvDH13, LPS^{+13}, LLvG10, LSH^{+11}, MRO17, MP11, Pog10, RKB^{+14}, SOYC12, SZBM13, SPB^{+13}, VYM15, VLGK^{+17}, WAM17, WOH16, WOH18, WC14, YWZ14, ZRL^{+15}]\). Parametrization \([PG15, DGPM14, GCWS15, SPS^{+12}]\). Paramfit \([BW15]\). parasite \([FZL^{+15}]\). paratropic \([CPN^{+17}]\). Parrinello \([KCK^{+15}]\). Part \([HRJ^{+15}, CDBM11, CD13, HRT^{+14}, Fer13b, SK13]\). Partial \([HTS17, JMILL13, SMP17b, WOH16, GVP^{+10}, MPBJ11, PL14]\). partially \([UT14]\). particle \([AG11, BK13, Cas13, NO16, PH17, ZDKM12]\). particle-field \([ZDKM12]\). particle-mesh \([AG11]\). partition \([HGCCGR^{+16}, JS13, LRR13, WG12, WDHZ13, YAS13]\). partitioning \([DI11, EV14, FCOGM12, LZS^{+17}, REL17, SS13a, TM15, VGV^{+11}]\). partner \([dVZ17]\). pass \([SR18]\). passing \([CSSB11, ZWL13]\). Past \([GS16, MFEM16, XFG^{+16}]\). patches \([OME16, YSSB12]\). Path \([MA17, VKAM12, CY09, HXM^{+16}, Ish10, JZ17, SRSLO15, SA13, SS13b, SM17, WXY14, ZT14, CY13]\). path-based \([ZT14]\). Path-integral \([VKAM12, WXY14]\). path-search \([Ish10]\). PathOpt \([GPE13]\). Paths \([SH11a, AMGB10, AN13, CX10, NMLD13, RVP^{+11}]\). pathway \([BHB12, HOM^{+16}, LKL10, SJ14, TDP^{+12}, XLYZ10]\). pathways \([CM13a, EFB16, GS11, HNTS15, KGR^{+16}, KDT^{+18}, MTM14, QSW^{+10}, QB16, RCM^{+13a}, RML^{+15}, SJ11, SH18, Tsi17, WSH10, Yon16, BHB12]\). pattern \([CXS10, WGL12]\). patterns \([FZL^{+15}, RS14]\). Paul \([Ano15-60, Ano16-56]\). Pauli \([JH^{+13}]\). PAW \([LGKS17, MDTD13]\). PAW-based \([LGKS17]\). Pb \([MCK17b, PMG^{+16}, vSGP10, FBY^{+17}, OBW12, VM11, vSGP10]\). PB-AM
[SCOJ13, ZWL13]. PH [LZL+15b, dSDdAR10, LZL+15b, AB16a, CS14, CAD16, HS14b, MBA14, PZA15, PS13, SY16a, SOvG12, Vor12].

pH-dependent [SY16a]. pH-responsive [MBA14]. Phage [MP17b].

Phage-like [MP17b]. PHAISTOS [BFH+13]. pharmacokinetics [VBDS+11]. Pharmacophore [HRK+10, HKRS11, HS11, TD10, AKMT11]. Phase [ATM18, ZWMW10, ABB+12, BE12, BG17, DLSD13, DLW12, EMD17, GYX+10, Hsu14, KID10, LJW11a, LPLB16, LGKS17, MFM+12, NIIT15, PSC11, RWR+13, RSLML12, RSJ17, SIZ+15, VKAM12, VED10, YHG+11, YSG12, ZSZ+14, ZWW10, ZYR+15, ZLHH14, dSDs12a, dSDs12b, ABB+13].

phase-change [EMD17]. phases [EB12, LPAS11]. Phen [FD16]. phenol [AAMD+11, AK10, IYK11, PPH+14, WHX+10, YKH+10, AK10].


phenylacetylene-containing [ZZL+12]. phenylalanine [GWF11, PVS12]. phenylaziridines [KYCL11]. phenylene [CH10].


phosphorus [GWX+12, RB12]. phosphorus-containing [YDX16].

phosphorylation [RIJ+11]. Photo [HNN+17]. photochemical [Su10].

photocycloadition [LXFC17]. Photodeactivation [Ant13].

photodetachment [MLCD11]. photodetectors [DPAB16]. photodynamic [ZZ12].

photoelectron [FF11, MLCD11]. photodeossimilation [RJS17].

photoexcitation [RVdMB16]. photoexcited [MS11]. photoinduced [CGP12, MSV16].

photoionization [MY17a, MY17b]. photoisomerization [ZLHH14]. photon [DPB+12, ZTH+15]. photooxidation [LWX16].

photophysical [CWT+12]. photoresponsive [YDGZ15]. photosensitizers [ZZ12].


Physical [CB11d, FCQM12, JJH+13, LHH11, VP12, YJ17, WCT+11].

physicochemical [CCYL11, HZ+10, LHL+10, RI10]. physiological [HM16]. phytochrome [FD13]. piano [FPB12, FB14b, ZCK+16].


pillars [NNK+16]. pilot [SSSM15]. Pimephales [TTL+12]. pinane [BLS10].

pincer [ED15, JJAB16]. pincers [KJDB12]. pinene [BLS10].
[HJJ13]. pivoting [PS17]. PK
[HL51+13, GKL5a, SK15a, SK12, SK17, YDX16, Zha12b, Zha12a]. PLA
[EOO1+16]. Placevent [SYH12]. planar
[BSPP1+13, EV14, XhD15, ZYW1+16, ZLY1+16]. Plane
[Lar11, AS15b, AGM1+13, BHR15, BEL1+11, BTB1+11, EPD1+10, LPS12, LLSW14, OHPR17, SN15, Tac17, TBSM12, Wei12b, YHW17]. points [HDL1+17, HEMCZE1+14]. Poisson
[SCCO10, BD12, CILA16, FBY1+17, FHMB15, FCE15, Fra15, Fra16, GRARO1+14, NWW17, SK15a, WL10, XXY17, YOM1+14, HWW11]. polar
[BK17a, CVD14, GMG1+10, LGL13b, PAT1+10, WWW18]. polar-nonpolar
[WWW18]. polarizabilities
[BLG1+13, BZB1+13, KR12, KNP1+12, LIRL1+16, MLC13, RLA1+11, S16b]. polarizability
[CPK12, EPD1+11, HBK10, KSK11, NNY17, OVPK15, PC14, YB13]. polarizability/reaction [SKS11]. Polarizable
[GE1+14, LPS1+13, NS11, SAVG15, ZM10, BSL1+16, Cam15, CCB15, CPP11, GPM14, DGB1+13, DDM1+15, ENKK1+17, ESM1+12, FPA17a, GR15, GPD1+16, HOK17, HZS17, HCP15, ISO1+13, KFY1+13, KR12, KWL1+16, LRdSM15, LFN1+10, LHH14, LDG1+15, MBC11, MBC13, MBE16, NLP1+16, PMC1+17, PZCL16, Ric16, SM14b, SK17, SBvG14, VV17, WRHF10, WLO1+17, XZ11, XP13, ZRL1+15, ZP13]. Polarization
[MIT13, CD11, JZ12, LCW12, MLZ12, POB13, RF15, TNG1+10, WWID14, YD17, ZJZM13, ZBG11, ZBP11]. polarizable [S16b]. Polarized
[BS10a, BLG1+13, DLZ15, JZM14, NHR1+10, SFM14, YJXZ13]. pole [NNY17]. pole-search [NNY17]. pollutants [GCC14, SIG1+11, TTR1+12]. pollution [LZ14]. poly [CH10, PRT1+10]. polyacenes [KAR12, RS17a]. polyamidoamine [CAD16]. polyatomic [OT12]. polybrominated
Prediction
[Ano12a, CP15, CQFC10, FSD+18, HZSS17, KPL15, LDZW17, MCAG+16, yOaCG10, PRP15, SRA17, SPL+18, WDW12, YHW17, ZYL+12, AGM+13, BLDK+13, Ben17, Bds13, BA11, CZAF17, DWL11, DDP16, EOA+11, FZY+12, GK10, GFPSD17, GTZ+18, HLS+13, HMYZ16, HL14, JSW10, KL14, KT011, LXL+11, LMI+14, LZL+15a, LZZ14, LLH11, LWW+10, LSH+11, MDT10, Man14, MG11, MSK12, PML+12, PN13, PPJ14, PLV+11, RCR+16, RK8+14, SM11, SYH12, TYZ+16, VKC10, WLF11, WH11, WXS+12, WXL+12, WWW+18, XFTW15, YVEI17, YLCX10, YHH+13, YX16, YDGZ15, ZsA10, ZYvIZ14, ZLW10, ZHHX11, VVBL17].
predictions [ALK+15, BCP+10, CLA16, CS17, EOO+16, GAI13, RDDS10, RCM+13b, SHMO11, SA10].
predictive [LLL+10, WKC11].
predictor [CDS16].
predictors [GHK12].
predissociation [YB11].
Preface [GS18].
preferences [FCOGM12, LGL11].
preferential [TKYN17].
preorganized [CM16].
preorganized-interacting [CM16].
preparation [JSD+11].
present [Cas14].
preserving [ZBG11].
pressures [RHN10].
primary [ALK+15, GAI13, VVLG17, KTNN10].
prime [DSX11].
primitive [HAL14].
principal [PSP15].
principle [CCJC10, DBM+15, LLB+12, MCF10, Tsk11, YPvd13].
Principles [HFSO12, BE12, BE14, BPE16, EMD17, EB12, EBK13, EBPK17a, GD10, HYL+11, Ibr17, JCG+11, LLLM11, LCWW10, NNS15, PLZ17, RZG+13, SFA17, TZ11, WYL+15, WD10, YR13, wZbZ11, Zha12b, Zha12a, ZWMW10, ZZ12, vADC+14].
principles-based [Zha12b, Zha12a].
prismane [DM15, VIT+15].
Pro [RB12].
Pro-Tide [RB12].
probe [RN17].
Probing [HH15, KG11, LPK16, TG12b, ZYR+15, BS18].
ProBiS [KDT+12].
problem [BB11a, GA14, KV13].
problems [HLXH17, HLXH18, PNW+16].
procedure [AD10, BK5+11, BY11, CJJS10, HKR+14, MG14, MS12, SA13, dSAdSL13].
procedures [AC11b, CKH17, KSM16, PW12].
process [ABDGN12, BM12, DPAB16, HBL12, NIIT15, ZZ10].
processes [BPLL12, FBEM11, HTS17, JM11, KV15b, LPLB16, PAK17, PTB+15, REL17].
processing [CKKK16, EP10, GBL+11, HASR+12, HEMCZE+14, WSGN11, WS13, YWJ+16, YN15, ZKE+17].
processor [HKR12].
processors [AB16a, AB16b, BDTP11, Fom11].
PROCONS [FHW+11].
produced [LS11a, SIG+15].
Producing [RN17].
product [CC12b, ZQ14].
production [GYX+10].
products [TR12].
profile [AK10, BS16a, GTZ+18, KTT16, XML+15].
profiles [MIOM13, RBOH11, SISK10, Yu12b].
profiling [VMRSH17].
profit [KB11c].
Program [FPV13, GH16b, SWA13, BBG+11, BBG+18, CBH14, CAT+13, FM10, GLW13a, GLW13b, GBW+14, HS16a, HL14, JS17b, KWL+16, KK17b, LHS+12, MHT+18, MSC+10, MSvG12, Mez10, MSSP17, MB14, SFG+17, ...
proteochemometric [NSO+14]. proteoglycans [NPG17]. proteolysis [VKNT15].
Proteus [SGM+13]. protic [RK16a, RK16b]. protocol [KPL13, RCR+16, SDL14, WdVN12, dCLFGL13]. protocols [CLA16, EOA+11, GR11, ZKH+10]. Proton [AK10, IYK11, RJWW12, RK16b, CG15, LPAS11, LZL+10, LWGZ15, MPSG11, RS+13, SRF+17, SB+17, SV11, TM16, VMTL10, Vor12, Wd14, YZGS14a, YKH+10, YTY12, dALdS+15, RK16a].
[HSL+11, QSW+10]. **pyrophyllite** [BHB+17]. **pyrrole** [YCGA10, YHCS11]. **pyruvate** [CJZS10]. **Python** [HPT+16b, LRvE17, PHH+12, Yes15]. **PYX** [LWWG12].

Q [WPM+15, BS10c, GKV+13]. **Q-Chem** [GKV+13]. **QDock** [BS10c]. **Q2MM** [LN15]. **Q5** [REL+14]. **Q5/D5Cost** [REL+14]. **QB3** [KG15]. **QC** [BTA+13]. **QC/MM** [BTA+13]. **QCT** [BLG10]. **QIDH** [SGPJS+17].

QikProp [LP11a]. **QM** [BM12, Lun12, RSR+12, Lun12, PLP+16, AALCM11, BH13, BZH14, CBG17, CJZS10, DSK17, FLMI11, FBP12, FB14b, GRS15, GWZ15, GCW14, HH15, HYUS11, HBR17, JJH+13, JWST10, KTNN10, KWL+16, KG15, LZdL+10, LFM12, LT13, LHT15, LJL+11, MCRL17, MTG12, MJG+15, NO16, OYK+11, PMC+17, PP10, PDMT10, PL14, PLP+16, RR14, RR12, SN16a, SGDT10, SJ14, SCM+15, STN+15, SSAS10, TSC+13, UTN11, VKNT15, VKNT16, VCM15, VKTRJ15, WDP+12, GRS15, RFN15, ZZY+16]. **QM-only** [LT13]. **QM/GRS15, RFN15**. **QM/EFP** [CBG17]. **QM/MM** [BM12, RSR+12, AALCM11, CJZS10, DSK17, FLMI11, FBP12, FB14b, GWZ15, GCW14, HH15, HBR17, JJH+13, JWST10, KTNN10, KWL+16, KG15, LFM12, LT13, LHT15, LJL+11, MCRL17, MTG12, MJG+15, NO16, OYK+11, PMC+17, PDMT10, PL14, RR14, RR12, SN16a, SGDT10, SJ14, SCM+15, STN+15, SSAS10, TSC+13, UTN11, VKNT15, VKNT16, VCM15, VKTRJ15, WDP+12]. **QM/MM-MD** [RSR+12, OYK+11]. **QM/MM-QMC** [UTN11]. **QM/MM-QM** [PLP+16]. **QMC** [UTN11]. **QMX** [KKR+13]. **QSAR** [GKR13, Ray13, AKMT11, BF15, CLX+10, FCL+10, GMMH+16, GCP+13, GCC14, LLL+10, LLL+15a, PKIC11, PPUBGD10, RKG11, TTB+10, TTL+12, WMW+10]. **QSAR/QSPR** [CLX+10, GCC14]. **QSARINS** [GCP+13, GCC14]. **QSARINS-chem** [GCC14]. **QSPR** [CD13, BRGN12, CLX+10, CD13, CD16, GCC14, KKO+16, TTR+12, XWW+11]. **QTAIM** [BH13, BZH14, FCQM12, FCPJM14, GMBX+16, HXM+16, JMX+16, dRL11, Rod13, RSKG14, VVJ15, Wei12b, WvRSM14, XFX+16, ZZE+12]. **QTAIM-based** [VVJ15]. **Quantum** [AKM+13, Ray13, AKMT11, BF15, CLX+10, FCL+10, GMMH+16, GCP+13, GCC14, LLL+10, LLL+15a, PKIC11, PPUBGD10, RKG11, TTB+10, TTL+12, WMW+10]. **Quality** [CLK11, KCK+17, KYB13, MKB+13, POB13, RB13a, RCM+13b, SC15]. **QuanPol** [TSC+13]. **quantification** [Fer17, Ham11, PC14, YNH+17]. **quantify** [LLHM16]. **Quantitative** [DZA11, RDT14, VÀA14, Wei12b, BPC13, CD13, DXL+10, NFG+13, REL17, RCM+13b, XFW15, TTB+11]. **Quantum** [AKM+13, AC11a, APA+14, Chu10, CG12, DDM+15, FRN15, GH10, HHDC16, KASH14, Li14a, Li14b, LWD13, MBRC16, MS12, RFN15, SCOJ13, SAGC16, SBd+17, SOY12, SR10, SHB17, TR12, UD12, WCAH10, WDP+12, Aki16, ASS+17, ARAG17, AAC+16, APY+16, ACS12, ASK18, ALH+10, Bac12, BTT10, BRP+12, BGR13, BEL+11, Cam15, CBH14,}
CDM10, CDB10, CDBM11, CD13, CD16, CXW14, CHK10, CM16, DR11, DKT13, DPAB16, ECZWD17, EV14, Fer13b, Fer13a, FB10, FFA14, FLM11, GPM17, GMMH+16, GTK10, GGM+12, HZ11, HLvdV13, HPT+16b, HGCCGR+16, HMM10, HYUS11, HGY15, JBB+11, JSXH16, KP11, KVR10, LPE+10, Lac14, MP17a, MAPB10, MSvG12, ME10, MSSP17, MHRR11, MFR+11, NC13, NC14, NNK+16, NDD+10, NHK+13, NS17, OKIS17, OSR16, PML+12, PSC11, PGW+17, PBG17, PVAM16, RLLHL12.

reactivities [WS11, WS12].

reach [QZ10b]. Reaching [MCRL17]. Reaction
[DBGO+17, FB14b, HLS+11, LWL+16, NJX+10, QSW+10, QB16, ST13, AMGB10, AS11, Alg17, AR10, APA+14, BK15, CYY+17, CSAdOM17, CXW14, FB12, GYX+10, GZL+12, GTK10, GKR13, GAJ+17, HOM+16, Hel13, HJLV16, IF+10, JZ17, JLS+10, JW16, KV12, KV13, KG15, KB13, KSK11, LGOM+15, LZY+12a, LJW+11b, LZY+16, LWD13, LPMT17, MTM14, MHT+18, MPSG11, MS10, MJLV14a, MJLV14b, MB16, MMJ10, NMLD13, NTNY15, OZLSBH12, PVL+13, PPH+14, QLYL10, RAGLL11, Ray13, RLSL13, RN17, RKG11, RSKG14, RSK+15, SLT14, SLT+15, SJD14, SRF+17, SBD+17, STS+10, SMM17, SM17, Tac17, Tak14, TSJ+10, TDP+12, TCPPC14, Tsi17, VV14, VGTL16, VMTL10, Wu10, WHDL11, WCL+11, YHG+11, YJ11, Yu12a, ZZLL12, ZSZ+14, ZYR+15, Zim13, VBD11].

diffusion [RSLS13]. reactions
[AAMD+11, ABB+12, ABB+13, APA+14, Cam15, CC18a, CSXZ17, Chu10, DSD+11, DS12a, FB14a, FC16, FFA14, GA14, GH10, GNDA+12, GMBX+16, HLS12, HYUS11, HRL11, JZ17, JCG+10, KG15, LHL14, LGW12, LT13, LXFC17, JG+11, MC10, MSV16, ORZ11, OSGH17, RWR+13, RB12, ST13, Su10, SSX+14, TKXT13, TTR+12, Tsi17, VKAM12, VKTRJ15, VGTL16, WHZ12, WCDM11, XLYZ10, YZGS14a, YNH+17, Yu12b, ZZL+10b, ZZL+10a, ZWZ11, ZLLL12, ZW17, dSdLBNB17, dSdVMD+16].

reactive [DMAH15, HJLV16, IHJ+13, LvDH13, MB14, RLLHL12, TDP+12].

activities [WS11, WS12]. Reactivity
[TS14, BCP+10, CRZ+18, DI11, HGY15, JS17a, LZH16, MAPB10, OSF12, OM12, PML+12, PRY1+17, Sti15, YB16, ZYR+15, ZT14]. read [DDK14].

reader [GHK12, JSD+11, KLJ+17]. READY [MB14].

reagents [SLT14]. Re|al [VHR16, JCGVPHT17, MBFP15, RHT+15].


realizes [YHCS11], really [MP17a]. Reannotation [YS10].

rearrangement [ABDG12, BIL10, OPR16]. rearrangements
[BIL10, RSKG14]. reason [SJWE10]. reasonable [Zim13]. ReaxFF
[HJLV16, JW05, LvDH13, YPvD13]. Recasting [HRCHR16]. Receptor
[HK18, CV12, ESB13, FTW12, FRLN10, HYZZ13, ILKR11, LZ11, LLL+10, OME16, PPJ14, SSP+13, VKC10, WC11, YZZ16]. receptor-ligand
[FTW12]. receptors [DR14, SRA17, UU12]. recognition
[CXS10, EPH+15, HS12, Hsnu14, ISP+10, LG14, OME16, OOK11].

recognized [CDS16]. recognizes [uLhY11]. recombination
[DS12a, SLC+17]. Reconsideration [MS11]. Reconstruction
[RSG+10, DWZ+17, MKB+13, MIOM13]. reconstructions [WDZ16].

recrossing [Yu12a]. rectification [LWZK13]. recurrence [HSN14].

recursive [RJR14]. Red [Jab14]. redesign [CGBK13, SL10, PGL+15].

Redesigned [XHLH16]. redistribution [JCGVPHT17]. Redox
[LCB10, GLM+17, INT18, KPL13, LZY+12a, MLQ+12, MKO+13, TN10, Tsi17].

reduction [BS16a, GMPB12, KPL15, LDZW17, PNI13, PSC11, SIG+15, YJ11, ZGS+10].


reference [KGM12, OZLSBH12, SHF11, SMM15a, SMM15b, SMM+18, TYN15, dLC17]. reference-modified [SMM15a, SMM15b, SMM+18]. references [EK17]. Refinement [LVG13c, BCG10, BS10c, CM13b, FLM11, LFM12, LZZ14, LGH11, OCL11, OL13, PNI13, Vor10]. reflectance [DCOD13]. Reformulating [Pro16].

Refraction [MMS16]. regime [CSAdOM17]. region [MTvG12, MNNK10a].

regions [MP17a, Pol13, TZ12]. Regioselective [WDZN16, BCP+10].

reliability [LLSW14]. Reliable [JZ17, LHG11, Kar17, NWW17, OV14, PTK11, RAD+11, RK15, SRL+13, TSR+16, Zha12b, Zha12a].

replacement [YHW17]. Replacing [ZSB+16]. Replica [GS15, GS16, XFG+16, ZC14, CH16, CCOH14, IO13a, IO13b, KCK+17, KTO11, KTO13, LC17a, LMI+14, MS16, OGL10, OLI3, OLY17, OZ14, RFH410, SBN13a, SBN13b, TKT11, XFG+15]. replica-exchange [CCOH14, IO13a, KTO11, KTO13, LMI+14, OLY17, OZ14, SBN13a, SBN13b].

replica-permutation [IO13b]. replicas [LL11]. Reply [Can11, Cor17, GKR13, QB11, VVB13, WM12, LAT11]. representation [CXW14, CWZB10, FFC+13, HZY+10, KCPMG12, KDS17, LLLC11, ME10].
YDL+10, YS10, YHH+13], representations [OVPK15, dVZ17].
representative [KV12, KV13, VLGK+17]. representing [TY10]. repressor
[OHNK11]. reproduced [Zha12b]. reproducibility
[GKR13, Ray13, RKG11]. reproducing [KTNN10, MAK+14]. reproduction
[OPBR17]. repulsion [BBOB16, CGPP11, ENKK+17, HOK17, PS17, PC16].
repulsions [JJH+13]. repulsive [IO13a, SNKD16]. required
[RAR+11, SG10b]. requirement [BF15]. requirements [TS15a]. requires
[LABSG17, BH15, BA11, GMO16, IHHY15, NR11, SL10, SEF+16, WC14,
YHH+13]. Residue-centric [LABSG17]. residues
[FHK+12, KLS10, KMLS10, RKDM14, SK17, WXL+12, WC14]. resistivity
[AB10]. resolution [BMFG16, BS10c, CM13b, DFF+15, Höfl14, JC16, KN17,
NPG17, SM11, Vor10, WNM17, YN15]. resolution-of-identity [YN15].
Resolutions [LMR14]. resolving [AVHB18]. resonance
[EFS16, KNP+12, YB13]. resource [Gil11]. Response
[GPGSM12, dSD12b, BZH14, DHE+12, ESM+12, ITIN15, KSSH13,
KZK+12, LP11b, MRB14, RJR14, RCY+13b, SS16a, SDF+17, WGLG+16].
responses [GWX+12, MLQ+12]. responsive [MBA14]. restrained
[HCD+10, KCK+17, SR18, ZDZM13]. restraining [KOY+12]. restraint
[RO14a]. restraints [SM11]. Restricted [SL10, Cas13, PDG+16, YD17].
restriction [FSD+18]. result [PH15]. results [Ber17, CBH14, CLK11,
GR10a, KERY+16, PLAG11, RAR+11, SHL+13, WDHZ13, KMLS10].
retinal [CG12, SGWA17, ZLHH14]. retinoic [LFM12]. Retracted
[Ano12a, GRL+12]. retro [GRCL12]. retro-imino-ene [GRCL12]. reveal
[MA16, RKDM14]. revealed [ALH+10, PNG10, VKNT15, YZGS14b].
Revealing [VVY17, YW13, YJ17, Bac12, GFGS18]. reveals [NR11, WC11].
Reverse [LWL+16, ASL+11, Aou16, GP12, OPBR17]. reversible [RIJ+11].
Review [DR14, FRS14, GHV17, JCL+17, CMvG10, Sch10, Spr10].
Reviews [HLvdV13, ZZWT12]. Revised [AKMYB18]. Revising [Pla11].
Revision [PLH16]. Revisited
[KR14, ASS+17, CYI+10, Dii15, HZ11, HFSO12, MSBF16, YW13, vSGP10].
Revisiting [OAN15a, Sán17, dSVdM+16]. reweighted [SH11b].
reweighting [Fe17, OGL10]. Rh [SN16a, WJX+10]. rhenium
[TS15a, ZWWMW10]. rhodium [GYX+10, RL12]. rhodopsin [RLG11].
rhodopsins [HRMAL+13]. rhombohedral [BE12]. Rhorix [MSSP17]. RI
[BK17c, BK17c, KNH16, TKN13, RKG10]. RI-MP2
[BK17c, KNH16, TKN13, RKG10]. ribonucleotides [XVA+16].
ribozyme [BJS12]. rich [ZZWX11, ZYL+12, YZWC11]. right [SJW10].
rigid [Aou16, AG11a, CZA11, DBM+17, HBL+14, PG14, dACP12].
Rigid-CLL [dACP12]. Rigidity [NPG17, OX16, PRSG13]. rigorous
[WO15]. ring
[ABDGN12, CPN+17, CB11d, FNS+11, GWT+17, GMBX+16, HH10,
HH11, HCD+10, PCLL11, PLH16, SP13, WCL+11, XV17, YHCS11, ZQ14].

S [CXSO10, GTK10, LWD13, SPS+12, WGN+16, WGLG+16, YZGS14b, ZYG+14, PRRT+10, AS11, Alg17, HOM+16, LGW12, MH11, MLY+13, RWR+13, TKXT13, WJX+10, YZGS14b, Yu12b, Yu12a, YZL+15, ZYR+15].


saccharide [LABSG17]. salicylidene [PLP+16]. Salpeter [KK17b]. salt [EK15, IPAA11, OCW+15, PZA15].


Sampling [AKN16, Yan16, BLKP12, BH15, BG17, CY09, CY13, CS17, DPNM11, DJ13, FM10, FBEM11, FB14b, GFSFD17, GMO16, HH10, HDK+12, HTS15, HNS16, HS17a, HDM+15, HCP15, IMK+16, ISK14, Ish10, KvdV14, KJ+17, KTO11, KB11c, LTT16, LC16, LC17a, LL11, LMT+14, LZZ14, LAW+16, MZZ11, MCRL17, OL13, PBDW11, SEM12, SBN13a, SBN13b, STM+15, TJB12, YZ16, ZZ14, ZC14, DAB16]. sandwich [TS15a, WWKS16]. SAPT [CLFRO18, DWR17, YJ17]. SAR
[AFSW16, CD11]. self-assembly [Hei10, KLN16, uLhY11]. Self-consistent
[JSXH16, BK17b, DK11, GBVA11, HZR+14, IM17, KC13b, KT10, KLN16, MJLV14a,
ON14, OCL11, SPS+12, SCSW13, TYN15, WMW+10, YN15, uLhY11].
[HS17a]. self-metathesis [MJLV14a]. semi [FSSW17, SC15]. semi-direct
[FSSW17]. semi-global [SC15]. semiconducting [VS14, ZSLL17].
semiconductor [LCH+15, SFDE16]. semiconductors [BE16, NDLW13].
Semiempirical [SRL+15, GP11a, HGY15, KTNN10, KB14b, LSD+10,
MGWR12, SPH11, SDL14, TKNN10, TG12a, UCFR16, WCWV15].
semiexperimental [VDVR14]. Seminumerical [PW12], sense
[DR14, ICS+12, ICS+13]. sensing [LZL+10, RRK14]. Sensitivity
[Han11, LL11, LWLG12, PDG+16, Sea10]. sensitized
[ACS12, JYS+12, LZZ+15a, YJN+11]. sensitizer [YJN+11]. sensitizers
[SLC+17]. sensors [DHE+12]. separable [WWU12]. separated
[BK17b, HZSS17, RSG14, SZS16, WYT17]. separation
[CSKH15, DS12a, VLG17, YSG12]. Sequence [TYZ+16, DLL+10, DVL11,
LXL+11, MPP17, Sti15, WXL+12, YZWC11, YS10, ZWP11, HYMZ16].
Sequence-based [TYZ+16, WXL+12]. sequence-reactivity [Sti15].
Sequence-specific [HYMZ16]. sequences [Ano12u, CCYL11, Fel10,
HZY+10, LMZ+11b, LLLL11, LDH+14, OLA15, QLQ11, YDL+10].
Sequential [CBP14]. Ser [LY10]. serial [BB11a]. series
[AC11b, DDM+15, LZZS11, MCK17b, SRA17, SB10, TD10]. serious
[BRGN12]. server [PZA15, XML+15, XXY17, dVAG16]. servers [UHH+11].
services [LP11a, UHH+11]. Set
[SN16b, BLLL13, BLG10, BRLS08, BRLS12, CC11, HZS16b, KNP+12, LS1a,
LLC+10, LCY+13, LZW+10, Mat10, OAN15a, PML+12, PGdO+16, PHK14,
PDL11, Pog10, PFVL14, RLD12, SPS+12, Sch13, SWM10, SG10a, SG13,
VLGK+17, VVLG17, WX12, YOMT14, ZPP+16, FL15]. Sets
[TKN13, BLF13, BLBG+13, BLF14, BS10a, DBM+15, HS14, Hill13,
LBH+11, LCW12, Lec15, Mit13, POB13, Sea10, SNKS10, STM+15, TH13,
UCF16, ZLT13]. Setschenow [XWW+11]. seven [PLAG11]. sextet
[BWMSM10, SSB+16, VV14]. Shao [Ano12u]. Shape [KC14, Zha11, GPS10,
HCS11, Hsn14, MNK10a, OAN15b, XTY+14, YLGX14]. Shape-based
[KC14]. shape-complementarity [GPS10]. shaped [LWK13]. shapes
[CCOH14, Hug12, WS10]. sheets [PL18, WCAH10, YZZ+17]. shell
[Ano15-58, BH14, BG13, GKS14, ISO+13, JCG+11, KSR17, MBA11, MA16,
MS12, SRR16, TBSM12, WW14]. shell-wise [KSR17]. shells
[GPK12, JXSW15]. Sheppard [QB11]. shielding


RS13, SG13, STS15, VT14, WF16, WTH+16, XML+15, XMSZ16, ZCGM11].
small-molecule [ETLS17, WF16]. smaller [MCK17b]. smallest [PMT16].
SMD [ALK+15]. smeared [ENKK+17]. SMILES [TTB+10].
SMILES-based [TTB+10]. Smoluchowski [SG10a]. smooth
[AG11, EFS16, JLC17, ZSB+16]. smoothed [LZ12]. SMPBS [XYX17]. Sn
[MCK17b, PMG+16, RDT14, YW12, ASS10, PKK17]. SnCl [dSDdAR10].
SnO [DHE+12]. Sodium [KLN16]. Soft [SJ11, Ben17, BG12]. Soft-core
[SJC11, BG12]. Software
[AIGP15, Aki16, APK14, AAC+16, BTA+13, BHB12, BCSCJ+13, BSZ+12,
Ber17, BP15, DMN15, BFH+13, BBG+18, CBH14, CSEMB+16, CZAF17,
CAT+13, DJD12, DVVP14, DDK14, DWC17, DSK17, ESB13, EWK+13,
FN12, FSC+14, GMSdG15, Gar12, GJMMP+14, GLW13b, GS12, GCP+13,
GCC14, GBW+14, GH16b, HLC+13, HRB+17, HDH12, HPT+16b, HPSK12,
HHT+13b, HH16b, HG13, HYMZ16, HKR+14, HB17, HL14, HC14, IGK16,
JHH+13, JJW+14, JLC17, JP15, JCGM18, KS13a, KS15, KK17a, Kan15,
K14, KB16, KKR+13, KDR+18, KLJ+17, KJM+17, KDT+12, Kos16, KG13,
KLW+16, KK17b, KWG15, KSD+12, KYG+15, KAG+12, KSW16, KPF+15,
LPS12, LJR+12, LHS12, Lrh15, LRvdSM15, LRvE17, LDB+17, LLZA12,
LBB+15, LWZ+17, LC12, LAS+14, MHT+18, MTD16, MBR+15, MYT18,
MSSP17, MB14, MB16, NKK16, OVI14, OPB+12, OZS+13]. Software
[OC14, PSS14, PG+15, DBDP16, PSC+17, PW12, PPM15, PHH+12,
PVZ13, PG14, RLLHL12, RNSF+16, Rrs17, RZ16, RR14, RdA12, RSR+12,
RCM+13b, SM14a, SFG+17, SK15b, SWA13, SMRM+17, She12, SC15, Sie15,
SJ17, SWB+12, SDS13, TNYN16, TSC+13, TTR+12, TTL+12, UU12,
VMRSH+17, VV+15b, VAR12, VBV13b, WdVN12, WY13, WPM+15,
WF16, Wei12b, WHK+12, WHJH13, WG14, WCJ+14, XML+15, XYX17,
YWJ+16, YZ16, Yes12, Yes15, YHH+13, ZDKM12, ZLL+13, dVAG16,
CCC+11, DBF14, MSvG12, MJG+15, SBV10, SGM+13, Yap11, ZCS+15,
She12]. softwares [All11]. solar
[ACS12, DGL+13, JYS+12, LZZ+15a, SLC+17, TZ12, VAA14, YJN+11].
Solid [RSK+15, ASS10, A11, CL16, HLS12, HBI+17, KLN12, POB13].
Solid-state [RSK+15, HBI+17, KLN12, POB13]. solids
[BK11, HAI+16, MTD13, MS15, dRL11, Pon11, SN16a]. solubility
[KKO+16]. solution [BRLS08, BRLS12, EO+11, TKTL11, YKOP+11, Yan11].
solutes [GC11, PAK15]. solution [AvKSP16, AK10, DR11, DBM+17, DP15,
EOA+11, GA13, GA14, HDK+12, HAL14, HNN+17, KTN10, KVR10,
LVG10, MMB+17, MFM+12, PMC+17, PGW+17, SJWE10, TKN11,
UCFR16, WHL+10, WC13, XTG+11, ZLL+10, ZZ10, vADC+14]. solutions
[Ber17, CFC15, EK15, Kri10, OCW+15, SM14a]. Solvation [RNSF+16,
ZBP11, CBG17, CBG16, FG11, GMMH+16, GPK12, HRC13, JMLL13,
JGS+17, Jor17, KSK11, LP11b, MS13, MPSA17, MBE16, NW17, OBW12,
PL14, RK16a, RK16b, SM14a, SK12, SY11, SM15a, SM15b, SM+18,
TKYN17, TCC+13, WXL17, WWW18, YOMT14, YAS13, Yan14, ZCS+15].
solvation-free-energy [SM15a, SM15b]. solvational [FCL+10].
Solvatochromic [MKH15]. Solvatochromism [TKYN17]. solve [PNW'16]. Solvent [KC13b, AKK+16, BEM14, BRLS08, BRLS12, CAD16, CBG16, EK15, FZY+12, FD16, HDL+17, Has14, HYUS11, KJDB12, KB11b, KCPMG12, LHL+10, LC17b, LZF+16, LWZ+17, MBC11, MBC13, MS11, ML14, MCUJ15, MCC12, MNNK10a, MNNK10b, PDM10, PS13, RdA12, RRK16, SLT14, SBV10, SK17, SLX+15, SYH12, SCMA+17, SKMS13, TYN15, WWKS11, WXL+12, WBF17, YOMT14, Yan14, YJ11, BK17a].


[TCB16, Aki16, APK14, BZH14, CD13, FBY+17, HLS+13, HPT17, KSD+12, PHT17, SMRM+17, XTG+11, Yap11, Yes12]. sources [BK13]. Space [vRGWS17, ACD+13a, ACD+13b, AD10, Cas13, CH16, CXS10, DK11, GA14, GK15b, HB14, HP10b, HSB+11, JCGVPHT17, LMZ11a, LLFH16, LAW+16, MBFP15, PDG+16, SS13a, SHL+11, SCSW13, TJB12, WDHZ13, YD17].


spectrometer [LBB+15]. Spectroscopic [SS13b, GKI10, KDB13, Kp15b, NC13, NC14, T Zack18, Tsi14, ZLL+10]. spectroscopy [HPSK12, LLBO12, NC12, WHK+12].


Spin-flip [ZLHH14]. Spin-orbit [JKS+16, AMQ+14, FAA15, FD16, GP11a, MG11, MCP18, PS17].


KS12, KKL+13, KLS10, KMLS10, LLBO12, LFB14, LKL10, LZJ+11, LMI+14, LYL16, LPE+10, LGL11, LHG11, LWWG12, LLFH16, Mat10, MDT10, Mau14, MAPB10, MV17, NGAS17, OCL11, OL3, OLA15, PSS14, PML+12, PNI3, RLG14, RCM+13b, RR11, SHMO11, SB10, SM11, SLP+12, SLIB12, SRS14, SYN+12, SKGB13, TN12, TTB+11, TG12b, UNT16, VVP12].

structure
[VHR16, VVBL17, VÅA14, VBMA13, VKC10, VI17, VLGK+17, WO15, WRM+12, WSGN11, YY12, YZZ16, ZRCC11, ZHHX11, OSF12, SA10].


studied [Ish10, KRTB10, OLY17, RHPWS13, RI10, TS15b].

Studies [JW12, AALCM11, BLS10, BRGN12, BG10, DMN15, BIL10, DXL+10, GZZM16, GEP+14, JLS+10, KG15, KP11, LXFC17, LCWL10, LJ+11, LW13, RC+13b, SB10, SFA17, SLHW09, TDP+12, VSD10, WCAH10, YK10+10, YPC+10, YDL+10, YXX17, ZZL+12, ZZL+10a, ZYG+15, ZX11].

Study [JLH+14, VL17b, AARP17, AS11, AS15a, AMAA+11, ASMS10, ANH+11, APA+14, APY+16, ALH+10, BEM14, BE14, BHB+17, BEEL14, BJS12, BLG11, BRLS08, BRLS12, BL12, BEL+11, CCLP12, CCLRO14, CWHH11, CBG17, CJC+11, CKL+11, CXW14, CBTZ16, CL16, CSXZ17, cCVG+14, Ch10, CG12, CB11c, CPLL11, CB11d, DASA15, DR11, DI11, DLSD13, DSX+11, EO+11, EV14, FCL+10, FF11, FCD10, FBEM11, FL15, FPB12, FB14b, GAG14, GG10, GYX+10, GVP+10, GD10, GTR10, GWZ15, GNCA10, GGM+12, GKR13, GPWW11, HZ11, HDB15, HHDC16, HRL11, HRB17, HSV16, IB11, II+10, INT18, IN13, IYH15, I10, JA10, JS17a, JCG+10, JAH+17, JJAB16, JW16, JYS+12, KD10, KPF11, KOP+14, KC13b, KB13, KT12, KG11, KNP+12, KS13b, KP10, LC10, LY10, uLhY11, LP11a, LLI3a, LLL+10, LDJ+10].

study
[LZL+10, LCL+10, LZJ+11, LZZH11, LWW+11, Li14a, Li14b, LGW12, LT13, LJW+11b, LBV11, LV12, LTP11, LX11, LHKS12, LH14b, LWS14, LWWC16, LHT15, Lu11, LJG+11, LPM17, MMS16, MC10, MG15, MF10, MLJ14b, MAPB10, MF+12, MH11, MWJ+11, MS11, MPNS13, MHRR11, MBR16, MO17, Mor15, MIS+15, NHP+10, NGAS17, NAS15, NC12, NC13, NC14, NXL+10, NFI+16, OPR16, ORZ11, OSS10, OSH17, OME16, OOK11, PVL+13, PGCT+12, PP10, PGC12, PGS+15, PH12, PPK17, PP+14, QYL10, QZ10b, RS17a, RAGLL11, RAR+11, Ray13, RS13, RS14, RVC113, RSLML12, RKG11, RSKG14, SN16a, SSP+13, SGDT10, SJ14, SCM+15,
tautomers [BZH14, dALdS\textsuperscript{+15}]. Tb [SRL\textsuperscript{+15}]. TD [TS15b, CCB15, CH10, EFAC13, HRJ\textsuperscript{+14}, HRJ\textsuperscript{+15}, JRSHP14, KKL\textsuperscript{+13}, KP10, LZZ\textsuperscript{+10}, LZZH11, LSH\textsuperscript{+11}, LYSS11, RDF\textsuperscript{+11}, SRF\textsuperscript{+17}]. TD-DFT [CCB15, CH10, EFAC13, HRJ\textsuperscript{+15}, JRSHP14, KKL\textsuperscript{+13}, KP10, LZZH11, LZ\textsuperscript{+10}, LYSS11, RDF\textsuperscript{+11}, SRF\textsuperscript{+17}]. TD-DFT- [LSH\textsuperscript{+11}]. TD-HF-based [LSH\textsuperscript{+11}]. TDDFT [CCB15, CH10, EFAC13, HRJ\textsuperscript{+15}, JRSHP14, KKL\textsuperscript{+13}, KP10, LZZH11, LXZ\textsuperscript{+10}, LYSS11, RDF\textsuperscript{+11}, SRF\textsuperscript{+17}].

Temperature-shuffled [HS17b].

Temperature/Hamiltonian [KCK\textsuperscript{+17}].

temperatures [NMLD13, RHNN10]. tempering [LAW\textsuperscript{+16}, MO15, MO17, NPTS16, TKT11]. Template [Mau14, GLF16, KCK\textsuperscript{+17}, ME10, YHH\textsuperscript{+13}]. Template-free [Mau14, YHH\textsuperscript{+13}]. template-restrained [KCK\textsuperscript{+17}].

tension [NFPD13].

tensors [EPD\textsuperscript{+11}, PHK14].

TDDFT [SFCCK\textsuperscript{+15}, CMF\textsuperscript{+17}, LRBB12, MS11, QCR12, SFCCK\textsuperscript{+14}]. Te [SPS\textsuperscript{+12}].

Technique [AMGB10, BG17, LZZ\textsuperscript{+13}, SMM\textsuperscript{+17}, TSR\textsuperscript{+16}].

techniques [BCP\textsuperscript{+10}, BCG10, GVP\textsuperscript{+10}, MCP18, SDF\textsuperscript{+17}, SPL\textsuperscript{+18}, SY11, WBN\textsuperscript{+13}].

Tellurium [RRK16, ZWGO16].

Test [PHC13, BS10b, DPOS16].

tethered [CZNA11].

tetraamines [SB10].

tetracarboxylates [CRC13].

tetracoordinate [XhD15, ZYW\textsuperscript{+16}, ZLY\textsuperscript{+16}].

tetraene [ABDGN12].

tetramer [LYL16, SZZS16].

Tetrazine [JW12, MCAG\textsuperscript{+16}, SLHW09].

tetraaxilvalene [MCF10].

Tetrazine-Tetrazine-Tetraoxide [JW12, SLHW09].

tetrel [YKH15].

tetroxide [MCAG\textsuperscript{+16}].

text [HKRS11, HS11].

text-based [HKRS11, HS11].

tf [XMSZ16].

Th [MCK17a].

Their [ARRC15, Ano11, BG18, CC12a, CBTZ16, CFC15, CB11a, DLT17, DSM\textsuperscript{+11}, GPM17, HJ13, JMLL13, JHMB\textsuperscript{+09}, JHMB\textsuperscript{+11}, KG15, KNE11a, KRSC12, NYH\textsuperscript{+17}, SBR13, TN12, Tak11, TY10, TS11, VVJ15, VVY17, VVBL17, XDL\textsuperscript{+10}, ZWY\textsuperscript{+10a}].

Them [WCWV15].

Theorem [CDB10, KSH13, YB16, ZM11].

Theoretic [CRZ\textsuperscript{+18}, MCC12, ZLW10].

Theoretical [AvKSP16, AMAA\textsuperscript{+11}, BHB\textsuperscript{+17}, BSDP16, CWT\textsuperscript{+12}, DBM\textsuperscript{+17}, DGL\textsuperscript{+13}, FF11, GYX\textsuperscript{+10}, GLZ17, GLM\textsuperscript{+17}, HDHL15c, JW12, KCB\textsuperscript{+12}, KS13b, LCL\textsuperscript{+10}, LWL\textsuperscript{+11}, LLW12, LZY\textsuperscript{+12a}, LWGW12, LWXC16, LXFC17, LJJ\textsuperscript{+11}, MLQ\textsuperscript{+12}, MSV16, NFI\textsuperscript{+16}, OSS10, OAN15b, PKK17, PM13, PE11, RS17b, SB10, SKY\textsuperscript{+11}, STS\textsuperscript{+10}, SZZS16, SLC\textsuperscript{+17}, SGHH13, TPL\textsuperscript{+10}, WMW11, WHDL11, WCL\textsuperscript{+11}, WS12, YJN\textsuperscript{+11},
YPC$^{+10}$, YHG$^{+11}$, YCGA$^{10}$, YYT$^{12}$, YDGZ$^{15}$, ZZL$^{+10b}$, ZZL$^{+10a}$, ZYLL$^{12}$, ZLLL$^{12}$, ZSZ$^{+14}$, ZYG$^{+15}$, ZBZMZH$^{15}$, dSdLB$^{17}$, BL$^{10}$, BE$^{16}$, CZH$^{12}$, CKL$^{+11}$, CB$^{16}$, EV$^{14}$, G$^{10}$, HD$^{15}$, HGHP$^{14}$, LW$^{12}$, LLD$^{17}$, LZW$^{+11}$, MPS$^{11}$, N$^{+10}$, NJX$^{+10}$, PH$^{12}$, Ps$^{+10}$, Po$^{10}$, PH$^{10b}$, RZ$^{+13}$, RVC$^{13}$, RV$^{+11}$, SS$^{+13}$, SJ$^{11}$, SLH$^{14}$, S$^{+11}$, T$^{11}$, WSH$^{10}$, WZQW$^{10}$, YK$^{13}$, YZWC$^{11}$, YZ$^{13}$, YB$^{11}$, Zha$^{12b}$, d$^{13}$, HDHL$^{15a}$, HDHL$^{15b}$, LH$^{15}$, AR$^{10}$, ARAG$^{17}$, ABDGN$^{12}$, AG$^{12}$, ASS$^{10}$, BY$^{11}$, BLBG$^{13}$, B$^{13}$, BG$^{13}$, CHG$^{16}$, CRZ$^{+18}$, CS$^{16}$, CWH$^{11}$, CKH$^{17}$, CCM$^{15}$, CF$^{14}$, CC$^{11}$, DCH$^{12}$, FRSA$^{14}$, FD$^{16}$, GHL$^{17}$, GZ$^{+12}$, GCCM$^{15}$, G$^{10}$, GNGCA$^{10}$, GNDA$^{12}$, GE$^{11}$, GP$^{12}$, Han$^{11}$, HPT$^{17}$, Hii$^{13}$, HNN$^{17}$, HRJ$^{+14}$, HRJ$^{+15}$, HG$^{10}$, IS$^{13}$, IKN$^{13}$, IM$^{17}$, JR$^{14}$, JW$^{16}$, JYS$^{+12}$, KHWB$^{17}$, KL$^{12}$, KM$^{13}$, LC$^{12}$, LBGS$^{16}$, LCL$^{+10}$, LLH$^{17}$, LPMT$^{17}$, MCC$^{11}$, MA$^{+14}$, MW$^{+11}$, ME$^{10}$, NMLD$^{13}$, NO$^{16}$, Niz$^{13}$, ORZ$^{11}$, OZLSB$^{12}$, PAK$^{17}$, PML$^{+12}$, PP$^{+14}$, Pie$^{14}$, Pyy$^{13}$, QZ$^{10b}$, QZ$^{10c}$, QB$^{16}$, RAGL$^{11}$, RJPB$^{12}$, RCM$^{+13a}$, RML$^{+15}$, RB$^{12}$, RSL$^{12}$, RHPWS$^{13}$, Rui$^{11}$, SM$^{14a}$, SFG$^{+17}$, SCW$^{11}$, SSS$^{15}$, SHF$^{11}$, SEF$^{+16}$, SE$^{14}$, SH$^{14}$, ST$^{13}$, S$^{+13}$, SSM$^{16}$, SB$^{14}$, SMM$^{+18}$, SKT$^{11}$, SZS$^{16}$, ST$^{15}$, Tld$^{+12}$].

**Theories**

[OM$^{12}$, WCW$^{15}$].

**Theory**

[IUK$^{+11}$, SZX$^{13a}$, SZX$^{13b}$, WM$^{12}$, AMK$^{11}$, ALK$^{+15}$, AR$^{10}$, ARAF$^{17}$, AB$^{12}$, AG$^{12}$, AS$^{10}$, BY$^{11}$, BLB$^{+13}$, BBZ$^{+13}$, BB$^{13}$, CH$^{16}$, CRZ$^{+18}$, CS$^{16}$, CWH$^{11}$, CKH$^{17}$, CCM$^{15}$, CF$^{14}$, CC$^{11}$, DCH$^{12}$, FRSA$^{14}$, FD$^{16}$, GHL$^{17}$, GZ$^{+12}$, GCCM$^{15}$, G$^{10}$, GNGCA$^{10}$, GNDA$^{12}$, GE$^{11}$, GP$^{12}$, Han$^{11}$, HPT$^{17}$, Hii$^{13}$, HNN$^{17}$, HRJ$^{+14}$, HRJ$^{+15}$, HG$^{10}$, ISN$^{13}$, IK$^{13}$, IM$^{17}$, JR$^{14}$, JL$^{+14}$, JW$^{16}$, JYS$^{+12}$, KHW$^{17}$, KL$^{12}$, KM$^{13}$, LC$^{12}$, LBGS$^{16}$, LCL$^{+10}$, LLH$^{17}$, LPMT$^{17}$, MCC$^{11}$, MA$^{+14}$, MW$^{+11}$, ME$^{10}$, NMLD$^{13}$, NO$^{16}$, Niz$^{13}$, ORZ$^{11}$, OZLSB$^{12}$, PAK$^{17}$, PML$^{+12}$, PP$^{+14}$, Pie$^{14}$, Pyy$^{13}$, QZ$^{10b}$, QZ$^{10c}$, QB$^{16}$, RAGL$^{11}$, RJPB$^{12}$, RCM$^{+13a}$, RML$^{+15}$, RB$^{12}$, RSL$^{12}$, RHPWS$^{13}$, Rui$^{11}$, SM$^{14a}$, SFG$^{+17}$, SCW$^{11}$, SSS$^{15}$, SHF$^{11}$, SEF$^{+16}$, SE$^{14}$, SH$^{14}$, ST$^{13}$, S$^{+13}$, SSM$^{16}$, SB$^{14}$, SMM$^{+18}$, SKT$^{11}$, SZS$^{16}$, ST$^{15}$, Tld$^{+12}$].

**Theory/Configuration**

[HPT$^{17}$].

**Theory/Time**

[JYS$^{+12}$].

therapeutic

[AFBR$^{17}$].

thermodynamically

[DS$^{12a}$, RS$^{12}$, BRE$^{16}$, DMJ$^{17}$, EHSPT$^{16}$, HRC$^{13}$, Kan$^{15}$, WRM$^{+12}$, ZYL$^{+12}$].

thermoelectric

[DS$^{12a}$, RS$^{12}$, BRE$^{16}$, DMJ$^{17}$, EHSPT$^{16}$, HRC$^{13}$, Kan$^{15}$, WRM$^{+12}$, ZYL$^{+12}$].

thermostabilizing

[KYT$^{+17}$].

thermostat

[JWO$^{15}$].

thermostabilization

[PH$^{17}$].

**Thia**

[GMASBF$^{16}$].

**Thia-calix**

[GMASBF$^{16}$].

**Thiaphosphiranes**

[TR$^{12}$].

**Thiazol**

[BMB$^{13}$].

**Thiazol-2-amine**

[BMB$^{13}$].

**Thienylenevinylene**

[TZ$^{12}$].

**Thin**

[MBA$^{11}$].

**Thin-shell**

[MBA$^{11}$].

**Thioacetamide**

[LCB$^{10}$].

**Thioamide**

[KG$^{11}$].

**Thiol**

[GWZ$^{15}$].

**Thiolate**

[EH$^{13}$].

**Thiolate-ligated**

[EH$^{13}$].

**Thiolates**

[FHT$^{+15}$].

**Thiophene**

[PH$^{10b}$, PRRT$^{+10}$, YHCS$^{11}$, ZSLL$^{17}$].

**Thiophene-based**

[ZSLL$^{17}$].

**Thiophenes**

[Su$^{10}$].

**Thiophenic**

[NHF$^{+10}$].

**Thiophenol**

[AMAA$^{+11}$].
 Third-Row [TKN13]. Thole [AS15b]. Thomas [Spr10]. those [SIG+15].
 threading [Mau14]. Three [NR11, NF17, NNK+16, TYN15, TKC+11, HJKJ13, KYT+17, KRSC12, LYSS11, LK16b, MBT14, MS16, SLT+15, TDKT10, TCX+13, UT15, WC14, YLL11, ZZZ+12, ZWX16]. Three-body [NF17]. three-center [YLL11]. Three-dimensional [TYN15, TKC+11, KYT+17, KRSC12, TCX+13, ZWX16]. three-domain [MBT14].
 three-membered [HJKJ13]. three-level [Lar12]. three-membered [HJKJ13]. three-level [Lar12].
 three-body [NF17]. three-dimensional [TYN15, TKC+11, KYT+17, KRSC12, TCX+13, ZWX16]. three-domain [MBT14].
 three-membered [HJKJ13]. three-level [Lar12]. three-body [NF17]. three-dimensional [TYN15, TKC+11, KYT+17, KRSC12, TCX+13, ZWX16]. three-domain [MBT14].
 three-membered [HJKJ13]. three-level [Lar12]. three-body [NF17]. three-dimensional [TYN15, TKC+11, KYT+17, KRSC12, TCX+13, ZWX16]. three-domain [MBT14].
 three-membered [HJKJ13]. three-level [Lar12].
[Ano11, Gav12, GRD+10, JHMB+09, JHMB+11]. **trihalide** [Gra18]. **trihydride** [PM13]. **trimer** [THP+15, YCGA10]. **Trimeric** [PTM16, RCM+13a, RML+15]. **trimetallic** [GLF16]. **trimethylsilyl** [BIL10]. **trinitrotoluene** [SH14]. **tripeptide** [BH15, GMI06]. **triphenylamine** [MSV16]. **triple** [ACD+13a, ACD+13b, POB13]. **triple-zeta** [POB13]. **triplet** [RS17a, THP+15]. **triplets** [EK15]. **tripodal** [SB10]. **tripropylamine** [LL10c]. **tris** [KPI15]. **trivial** [IUK+11]. **tRNA** [LSB10]. **tropocollagen** [PP10]. **Trotter** [VKAM12]. **Trp** [EJ13]. **Trp-Glu** [EJ13]. **TRREAT** [CM13a]. **truncated** [CMI11]. **truncated-CI** [CMI11]. **truncation** [ACD+13a, ACD+13b, CS14, IMR18, MC12]. **trust** [PLAG11]. **trying** [BRGN12]. **trypanothione** [VSD10]. **tryptophan** [EOA+11, PS14, SHB17, VML10]. **Tsallis** [QZ10c]. **TTTO** [JW12, SLHW09]. **tuberculosis** [MPNS13]. **tubes** [TS15b]. **tubular** [uLy11, ZLY+16]. **tularensis** [STM+15]. **tumor** [JAH+17]. **tuned** [BK17b, HZSS17, SSZ16]. **tungsten** [TS15a]. **Tuning** [Ano11, JHMB+09, JHMB+11, BK17b, LWL+11, Mor15, RLG11, WYT17, LZ12]. **tunnel** [KL14]. **tunneling** [CSAdOM17, HS16a, LZW+11, OT12]. **TURBOMOLE** [KK17b, RR14, STH+10, vW11]. **tweezers** [MBA14]. **twelve** [Pog10]. **twist** [KTK17]. **twisted** [YLZ+10]. **Two** [DS12b, Gra18, KKN11, KTO13, SC17, CC0H14, DPB+12, ECZWD17, FRSA14, GAMAC+14, HLH+12, LPAS11, LRER13, NASH15, PS17, PW12, SLT14, SCC11, TCPCC14, VT14, YAS13, YLL11, ZTH+15, SM17]. **Two-Body** [SC17]. **two-center** [LRER13]. **two-component** [NASH15, PW12]. **Two-dimensional** [KTO13]. **two-electron** [PS17, YLL11]. **Two-level** [KKN11]. **two-photon** [DPB+12, ZTH+15]. **two-scale** [FRSA14]. **Two-step** [DS12b, SJC11, TCPCC14]. **type** [BM12, BE16, CYY+17, CRC13, CB11c, Dil15, HLWD15, JYC+16, LH14a, MY17a, MY17b, MKH15, RKB+14, SZX13a, SZX13b, VED10, WvRSM14, ZX11]. **type-II** [CB11c]. **types** [SKY+11, UT15]. **typical** [TZ12]. **typing** [FP17b, YPKB12].

unit-based [WS13]. Unitary [SSSM15]. united [JGS17, Jor17, ST11].
GMO16, GZM11, GRL+11, GRL+12, GBMX+16, GTZ+18, HASR+12, HNS16, HLW+17, HDL+17, HH17, H6f14, HBL12, HYUS11, HJKJ13, HZS17, HHLW17, Hug14, HRH+17, Ish10, HIJ+13, JLH+14, JMS13, KV13, Kan15, KERY+16, KT10, KLOS10, KTN10, KP11, LBGS16, LPK16, LRvdSM15, LZ12, LCH10, LCL+10, LMR14, LHG11, LTA+11, LBDP12, MS17, MZZ11, MB14, MJC14, MN15, MY17a, MSS+13, MKM+17, MCUJ15, MVK10, MKB+13, MFR+17, MIOM13, MMJ10, MS15, NLP+16, NASH15, NH16, OCW+15, PGdO+16, PC11, PG15, Pie14, PJ13, RB13a.

using [RLDJ17, RDDS10, RHJ11, RS13, RRK14, Ric16, REL17, REV+17, Rui11, RFHG10, REH13, SHMO11, SFR+17, SBV10, SA13, SCW11, SEF+16, SHL+11, SKKS13, SY11, SRS14, SZZS16, STS15, TYZ+16, Tak14, TKN10, Tsi17, TJB12, UTM11, VKAM12, VECT12, VI17, WKLC12, WdVN12, WLC12, WZ17, WIX+10, WDHZ13, XTY+14, XYX17, XWW+11, YY+16, Yon16, YD16, ZWX11, ZL11, ZLT13, ZWS+10, ZP13, ZH12, ZHHX11, dLC17, LHL+10].

utility [YHVM12]. utilizing [BVY+12]. UV [GGM+12, KASH14, RDF+11, RvdMB16]. UV-photoexcitation [RVdMB16]. UV/Vis [GGM+12].

vibration [GK10, Kop15a, Kop16, Kop17a, Kop17b, MK13b, Tac17].
vibration-rotation [GK10, Kop15a, Kop16, Kop17a, Kop17b, MK13b].
Vibrational [DB12, LCW12, QZM11, ARLP13, BZB+13, DOM+11, DHF+11, HYD10, KCPMG12, Kow11, LBH+11, LLTC12, LBTV12, LS11b, MCF10, MAK+14, RLA+11, RRK16, SS13a, SSWX14, TZCK18, WX12, XSZL11, dSA13, dSL13, WHK+12].
vibronic [MCLD10, ZTH+15].
vibronic view [DMJ17].
VIII [LMR14].
villin [LKL10].
Vina [TO10].
VinaMPI [ESB13].
vinylidene [HSY+11].
violating [FL15, GZH10].
virial [FED17].
viridis [IIF+10].
Virtual [GRP+12, HDM+15, CCM15, ESB13, GCCM15, HIJ13, JBAM11, KC14, KLS10, KMLS10, LBB+15, MRR14, MMN10b, MHN10, VK10, YZZ16, YD17].
Virtual-system-coupled [HDM+15].
viruses [OLY17].
Vis [GGM+12].
viscoelastic [YS12].
viscosity [BBI+11, GM17].
VISM [ZCS+15].
visualization [CVT+11, HH16b, TKC+11, You10].
Visualize [GH16b, QLQ11].
Visualizing [SOJ14, WM17].
VMD [BBH12, KLOS10].
vmdICE [KLOS10].
VMS [LBB+15].
VMS-Draw [LBB+15].
voids [CC12a].
voltage [ACS12, SFB17].
voltage-dependent [SFB17].

**W4** [KSM17]. **W4-17** [KSM17]. **Waals** [BLF14, BB11a, BC13, CR14, DS12b, DSF17, KBC12, KCK+15, KGHK12, KLN12, LCH+15, SMGB11, SLIB12, SJZ+15, SYZ+17, YZZ+17, ZY14].

**Wales** [DWZ+17, YZN13]. walk [CY09, CY13]. Walking [CH16]. wall [BE14, Den12, FTR15, TSR+16]. walled

[AS15a, PBE16, RHNN10, VS14, WYL+15, YZN13]. **Wang** [Ano12u, JW12, SA11].

**Water** [DBGO+17, HvM17, LWL+16, MCUJ15, RBOH11, UNT16, ZLX+13, AASPI18, AIGP15, AOW11, AF14, BRLS08, BRLS12, CYY+17, CZH12, CXW14, CCOH14, DDP16, GHL17, GM17, HH10, HvM16, Hug12, IUK+11, JCP14, JIS13, JA10, KUDG12, KGHK12, KGHC15, KB13, KJ10, KSR+16, LH11, LK13, LPLS16, LP11b, LIRL+16, LCM+14, LJJ+11, LAW+16, MC10, MKH15, MJM+15, MHRR11, NC12, NC13, OSS10, PAK15, PD11, RTS+13, RZ16, Ric16, RRF11, RSB+13, SG10b, SNS16, SISK10, SMP17a, SY16b, SV11, SIG+15, SM17, Tac17, TM16, TKYN17, TG12a, TL16, US11,
VMTL10, Vor12, WC13, WCW15, WG12, YDR13, YZ17, ZCK+16, Zha12b].

water-fluoride [NC12], water-halide [NC13], water-vapor [SISK10].


Wave-function [HH16a]. wave-functions [Fer13b, Fer13a]. wavefunction [FD16, GSS13, HPT+16b, KSH+17, LC12]. wavefunction-based [GSS13].


REFERENCES


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