Pure & Appl. Chem., Vol. 68, No. 2, pp. 387–456, 1996.
Printed in Great Britain.

INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION
WORKING PARTY ON THEORETICAL AND COMPUTATIONAL CHEMISTRY

ACRONYMS USED IN THEORETICAL CHEMISTRY

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Acronyms used in theoretical chemistry

Synopsis
An alphabetic list of acronyms used in theoretical chemistry is presented. Some explanatory references have been added to make acronyms better understandable but still more are needed. Critical comments, additional references, etc. are requested.

INTRODUCTION

The IUPAC Working Party on Theoretical Chemistry was persuaded, by discussion with colleagues, that the compilation of a list of acronyms used in theoretical chemistry would be a useful contribution. Initial lists of acronyms drawn up by several members of the working party have been augmented by the provision of a substantial list by Chemical Abstract Service (see footnote below). The working party is particularly grateful to CAS for this generous help.

It soon became apparent that many of the acronyms needed more than mere spelling out to make them understandable and so we have added explanatory references to many of them. At present only about 20% of the acronyms are accompanied by explanatory references but we judge that there is the need for many more to be added. However this is a major task and no one person is able to provide anything like all the references required. *We are therefore seeking the help of colleagues to provide additional references.* One of our purposes in publishing the list at present is to stimulate interest, critical comments and, especially suggestions for further explanatory references.

Please note that we prefer explanatory references rather than the historical first reference to the use of the acronym, although sometimes the first reference is also adequately explanatory. However, we have often preferred reference to a suitable monograph or review article. We bear in mind that graduate students and workers from distant fields of science who are trying to become familiar with the theoretical literature will be among the users of our list and will appreciate explanations in many instances.

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Chemical Abstracts Service has supplied acronyms in the area of theoretical chemistry in support of this publication; this contribution was obtained through the work of indexing primary literature, and Chemical Abstracts Service makes no representations as to its accuracy or completeness.

Acronyms used in Theoretical Chemistry

A

AADO	angular (momentum conservation) average dipole orientation (theory for calculation of ion-molecule capture rates) – T. Su and M.T. Bowers, in *Gas Phase Ion Chemistry,* edited by M.T. Bowers, (Academic Press, New York, 1979), Vol. 1, p. 83.
AAFEGE	asymptotically adjusted free-electron-gas exchange (potential)
AAMOM	an approximate molecular orbital method
AAPDI	anisotropic atom point dipole
AAT	atomic axial tensor (in molecular optical properties calcns.)
ABBOT	atomic billiard ball orbital theory
ABC	absorbing boundary condition (Green function)
ABO	adiabatic Born-Oppenheimer (wave functions)
AC	(1) adiabatic capture (theory for association and ion-molecule reactions without energetic barriers) - D.C. Clary, *Ann. Rev. Phys. Chem.*, **41**, 61 (1990) (2) autocorrelation (function) – D.A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976), Chapter 21.
ACC	approximate coupled cluster
ACC-IOS	azimutal close coupled-infinite order sudden
ACCD	approximate double substitution coupled cluster method
ACCDPPA	approximate coupled cluster with double excitations polarization propagator approximation
ACGCSA	adiabatic capture + global centrifugal sudden approximation (theory for association and ion-molecule reactions without energetic barriers) - T. Stoecklin, C.E. Dateo, and D.C. Clary, *J. Chem. Soc., Faraday Trans.*, **87**, 1667 (1991)
ACIOSA	adiabatic capture + infinite order sudden approximation (theory for association and ion-molecule reactions without energetic barriers) - T. Stoecklin, C.E. Dateo, and D.C. Clary, *J. Chem. Soc., Faraday Trans.*, **87**, 1667 (1991)
ACM	adiabatic channel model
ACO	atomic-cell orbital
ACORE	atomic core orbitals
ACP	approximate coupled-pair (method for correlation-energy calcn.)
ACPCSA	adiabatic capture + partial centrifugal sudden approximation (theory for association and ion-molecule reactions without energetic barriers) - T. Stoecklin, C.E. Dateo, and D.C. Clary, *J. Chem. Soc., Faraday Trans.*, **87**, 1667 (1991)
ACPF	averaged coupled-pair functional method -R. J. Gdantiz and R. Ahlrichs, *Chem. Phys. Lett.* **143**, 413 (1988).
ACPQ	approx. coupled-pair (theory cor. for connected) quadruply (excited clusters)
ACPTQ	approx. coupled pair (theory cor. for connected) triple and quadruply excitations
ACQM	arrangement-channel quantum mechanics
ACS	adiabatically corrected sudden
ACT	activated complex theory: also called "Absolute Rate Theory". Name given to early form of transition state theory

	- P.J. Robinson and K.A. Holbrook, *Unimolecular Reactions* (Interscience, London, 1972)
ADC(n)	algebraic diagrammatic construction accurate to order n in the residual electron-electron interaction - J.Schirmer and L. S. Cederbaum, *J. Phys. B* **11**, 1889 (1978); J. Schirmer, L. S. Cederbaum, and O. Walter, *Phys Rev. A* **28**, 1237 (1983)
ADLCM	angle-dependent line-of-centers model
ADO	average dipole orientation (in ion-mol. reactions)
ADRIOS	adiabatic reactive infinite order sudden approximation
ADW	(1) asymptotic distorted wave (2) (rotationally-)adiabatic-distorted-wave (approximation for reactive scattering calculations) - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
ADWIOS	adiabatic distorted wave infinite order sudden
AE-CI	all electron-configuration interaction
AEA-MO	all-electron approxn.-mol. orbital
AEFCA	all-electron frozen-core approximation
AESOP	ab-initio effective spin-orbit operator
AEVO	active electron virtual orbital
AFQMC	auxiliary-field quantum Monte-Carlo
AGCM	adiabatic generator coordinate method (for energy level calcn.)
AGFA	asymptotic Green function approxn.
AGP	antisymmetrized geminal product (wave function)
AHF	approximate Hartree-Fock method
AHM	average hamiltonian model method
AHP	average hole-potential (method for electronic-structure calcns. on molecules)
AI	adiabatic invariance method
AIADC(3)	ab initio third-order algebraic diagrammatic construction Green function method
AIEMP	ab initio embedding model potential
AIM	(1) adiabatic invariance method (in ion-mol. reactions) (2) atoms in molecules method - R. F. W. Bader, T. T. Nguyen-Dang, *Rep. Prog. Phys.*, **44**, 894 (1981)
AIMD	ab initio molecular dynamics
AIMDSA	ab initio molecular dynamics simulated annealing
AIMP	ab initio model potential (for valence-electron mol. calcns.)
AIP	angular-dependent part of the intermolecular potential
AIPM	analytic independent-particle model (in electron-scattering)
AM1	Austin model 1, a computer program for obtaining a semiempirical solution to the electronic Schrödinger equation - M. J. S. Dewar, E. V. Zoebisch, E. F. Healy, and J. J. P. Stewart, *J. Am. Chem. Soc.*, **107**, 3902 (1985)
AMBER	a computer program using molecular mechanics - S. J. Weiner, P. A. Kollman, D. A. Case, U. C. Singh, C. Ghio, G. Alagona, S. Profeta Jr., and P. Weiner, *J. Am. Chem. Soc.* **106**, 765 (1984)
AMO	alternant molecular orbital
AMO MT	alternant molecular orbital Matsubara-Toyozawa method
AMPAC	a computer program for implementing a number of semi-empirical solutions to the electronic Schrödinger equation - M. J. S. Dewar, QCPE Program 506 (1987)
ANA	adiabatic nuclei approximation (in electron-mol. scattering)
ANMO	average-natural molecular orbital

ANO	(1) atomic natural orbitals - J. Almlof and P. R. Taylor, *J. Chem. Phys* , **86**, 4070 (1987) (2) average natural orbitals (3) approximate natural orbital
ANR	adiabatic nuclear rotation (in calcns. on mol. collisions)
AO	atomic orbital.
AOM	(1) atomic overlap matrix (2) angular overlap model
AOVB	atomic orbital valence bond (molecular wave function)
APA	adiabatic perturbation approxn.
APDG	antisymmetrized product of delocalized geminals (wave function)
APDI	anisotropic point-dipole interaction
APG	antisymmetrized product of geminals (wave function)
APGF	antisymmetrical product of group functions (a wave function)
APH	adiabatically adjusting, principal axis, hyperspherical coordinates
APIG	antisymmetrized product (of) identical geminals
APLG	antisymmetrized product of localized geminals (wave function)
APNO	atomic pair natural orbital
APS	adiabatic pseudopotential
APSG	(1) antisymmetrized product of separated geminals (2) antisymmetrized product of spin geminals method (3) antisymmetrized product of strongly orthogonal geminals (variant of multiconfiguration self-consistent field method)
APSGF	antisymmetrical product of strongly orthogonal group functions (a wave function)
APT	(1) analytic perturbation theory (2) atomic polar tensor (in ir spectra calcn.)
APUHF	approximately projected unrestricted Hartree-Fock
APUMPn	approximately projected unrestricted Møller-Plesset nth-order
APW	augmented plane wave
AQO	average quadrupole orientation (theory for calculation of ion-molecule capture rates) – T. Su and M.T. Bowers, in *Gas Phase Ion Chemistry,* edited by M.T. Bowers, (Academic Press, New York, 1979), **Vol. 1**, p. 83
AREP	averaged relativistic effective potential
ARO	analytical radial orbital
ARPA	augmented random phase approximation
ARSCF	approximate relativistic SCF
ARSCFC	approximate relativistic SCF (with) corrections
ART	absolute rate theory (name given to early form of transition state theory) - P.J. Robinson and K.A. Holbrook, *Unimolecular Reactions* (Interscience, London, 1972)
ASA	(1) alternancy symmetry adapted (method for spin-independent hamiltonians for alternant hydrocarbons) (2) atomic sphere approximation
ASBOW	axial spin bond-order wave
ASCW	axial spin current wave (type of Hartree-Fock wave function)
ASDW	axial spin density wave
ASE	augmented secular equation
ASED	atom superposition and electron delocalization (MO)

ASEHF	approximate spin-extended Hartree-Fock
ASF	augmented-space formalism (a generalization of CPA)
ASMO	antisymmetrical molecular orbital
ASO	atomic spin orbital
ASPG	antisymmetrized product of separated geminals approxn.
ASW	(1) augmented spherical wave (2) axial spin wave (type of Hartee-Fock wave function)
ATA	average t-matrix approximation
ATDHF	adiabatic time-dependent Hartree-Fock
ATM	analytic tetrahedron method (for Brillouin-zone integrals and electron spin densities)
AUHF	annihilated unrestricted Hartree-Fock method
AUMP	annihilated unrestricted Møller-Plesset (spin contaminant)
AVCC-IOS	azimuthal (and) vibrational close-coupled (rotational) infinite order sudden
AVDP	analytic velocity-dependent potential (for electron scattering)
AVE	all valence electron
AVO	average virtual orbital
AWM	average wave function method (in calcns. on scattering)
AWP	adiabatic wave packet - E. Deumens and Y. Ohrn, *J. Am. Chem. Soc.* 9**2**, 3181 (1988)

B

B1B	(Coulomb) boundary-corrected first Born (for scattering)
B2B	boundary-corrected second Born (for scattering)
BA	best atom (basis set)
BA + P	best atom + polarization function
BAC	bond additivity correction
BAC-MP4	bond-additivity-corrected Møller-Plesset 4th-order perturbation
BAO	best atomic orbital basis
BAW	bond-order alternation wave (MO)
BBFM	bond-bending force model (for phonon calcns.)
BBGKY	Bogoliubov-Born-Green-Kirkwood-Yvon equations (in kinetic theory of fluids) - P. Resibois and M. de Leener, *Classical Kinetic Theory of Fluids* (Wiley, New York, (1977)
BCA	binary-collision approximation
BCC	Brueckner coupled cluster
BCCD	Brueckner coupled cluster with double excitations
BCM	bond charge model (in force constants calcn.)
BCO	bounded crystal orbital
BCRLM	bending corrected rotating linear model - R.B. Walker and E.F. Hayes in D.C. Clary, ed., *The Theory of Chemical Reaction Dynamics* (D. Reidel, Dordrecht, 1986) p 105
BCRNM	bending corrected rotating nonlinear model
BCS	Bardeen-Cooper-Schrieffer (shell model calculations)
BCSLN	Bardeen-Cooper-Schrieffer-Lipkin-Nogami (model in calcns. on molecules with quantum field theory)
BD	Brueckner (orbitals with) double (substitution) (in electron correlation)
BDE	bond dissociation energy.
BDT	Brueckner (with) double (and) triple (substitutions)
BDTQ	Brueckner (with) double, triple, (and) quadratic (substitution)

BEA	binary encounter approximation
BEBO	bond energy bond order method
BEBO/R	relaxed bond energy-bond order method
BET	bond equilibrium theory
BF	(1) body fixed (see BFF) (2) Buckingham-Fowler potential function - A.D. Buckingham and P.W. Fowler, *J. Chem. Phys.*, **79**, 6426 (1983)
BFBF	body frame Bessel function
BFF	body fixed frame (for quantum scattering calculations) - R.T. Pack, *J. Chem. Phys.*, **60**, 633 (1974)
BFT	bonded function theory
BGK	Bhatnagar-Gross-Krook (kinetic-theory model for reactive collisions)
BH	Barbanis hamiltonian
BHF	(1) broken-symmetry Hartree-Fock (2) Brueckner-Hartree-Fock
BI	bond increment (method in calcns. on large molecules)
BJH	Bopp-Jancso-Heinzinger (potential function)
BK	Brinkman-Kramers (approxn. in ion-molecule collision quantum calcn.)
BKC	Born-von Karman cell (model for electronic-structure calcn.)
BKCM	Burkhardt-Konya-Coulson-March (for electron momentum densities)
BKW	Bobylev-Krook-Wu (method for solving the Boltzmann equation for a mol. system)
BLB	Brillouin-Levy-Berthier (theorem in MO theory)
BLCAO	bilinear combination of atomic orbitals
BLMO	(1) best limited basis molecular orbital (2) Boys localized molecular orbital
BLYP	Becke-Lee-Yang-Parr (density-functional theory)
BMMO	best minimal molecular orbital
BMV	Berthier-Millie-Veillard method (semiempirical MO-SCF)
BO	(1) biorthonormal (wave function) (2) bond orbital (3) Born Oppenheimer (4) Brueckner orbital (5) bond order
BOA	(1) bidirectional orbital approximation (in valence bond theory) (2) bond orbital approximation (3) bond orientational anisotropy (4) Born-Oppenheimer approximation
BOARS	Born-Oppenheimer angular radial sepn. (in molecular complexes calcns.)
BOAW	bond-order alternation wave
BOC	bond-order conservation (model in calcns. on reactions)
BOC-MP	bond order conservation-Morse potential
BOCV	biorthogonality constrained variation method
BODC	Born-Oppenheimer diagonal correction (in molecular calcns.)
BOM	bond orbital model
BOO	(1) bond order orbital (2) bond orientational order
BORT	bond orbital resonance theory
BOVB	biorthogonal valence bond
BOW	bond-order wave

BPDA	Born point dipole approximation
BPFT	Bohm-Pines-Fock-Tani (hamiltonian in calcns. on plasmons)
BQMCT	basis quantum monte-carlo theory (for many electron systems)
BR	Barker and Ridge (model for calculation of ion-molecule capture rates) – T. Su and M.T. Bowers, in *Gas Phase Ion Chemistry,* edited by M.T. Bowers, (Academic Press, New York, 1979), Vol. 1, p. 83
BRNO	best radial natural orbital
BRW	biased random walk (model for collisional energy transfer) – K.F. Lim and R.G. Gilbert, *J. Chem. Phys.*, 92, 1819 (1990).
BS	breathing sphere (approxn. in molecular-scattering calcns.)
BSA	breathing-sphere approxn. (for inelastic molecular collisions)
BSBL	bond strength-bond length (model of atom abstraction reaction)
BSM	breathing shell model
BSO	(1) basic symmetric operator (in second-quantization calculations) (2)Brueckner spin orbitals
BSPT	Blizzard Santry perturbation theory
BSQ	boson second quantization
BSSE	basis-set superposition error
BT	bonded tableaux
BTUGA	bonded tableau unitary group approach
BWEN	Brillouin-Wigner (second-order perturbation theory with) Epstein-Nesbet (energy denominators)
BWPT	Brillouin-Wigner perturbation theory

C

CAB	(1) combination of atomic boxes (MO method) (2) core and bond (molecular partitioning method)
CADPAC	a computer program for solving the electronic Schrödinger equation - Amos *et al.*, University of Cambridge
CADW	converged-adiabatic distorted-wave (quantum calcn. method)
CAFEGE	classically approximated free-electron-gas exchange
CAHF	configuration-averaged Hartree-Fock
CAM	complex angular momentum (for rotationally inelastic scattering)
CAMM	cumulative atomic multipole moment (for mol. charge distributions)
CAOPM	configuration-averaged optimized-potential model
CAS	complete active space - B. O. Roos, P. R. Taylor, and P. E. M. Siegbahn, *Chem. Phys.* **48**, 157 (1980)
CAS-CI	complete active space-configuration interaction
CAS-GEN	computer assisted structure generation - J. Sadowski and J. Gasteiger, *Chem. Rev.*, **93**, 2567 (1993)
CAS-MC-SCF	complete active space-multiconfiguration-SCF - see CAS, MC-SCF, SCF
CASPT	complete active space-perturbation theory
CASPT2	a perturbation method based on complete active space with second-order perturbation theory - K. Andersson, P.-A. Malmqvist, and B. O. Roos, *J. Chem. Phys.* **96**, 1218 (1992)

CASSCF	complete active space self-consistent field theory (a CI-type method - see CAS, SCF)
CASSCF	complete active space self-consistent field theory (a version of multiconfiguration self-consistent field theory for solution of the electronic Schrödinger equation - see CAS, SCF) - B.O. Roos, *Int. J. Quantum Chem. Symposium* **14,** 175 (1980)
CASSCF-CCI	complete active space self-consistent field-contracted CI
CAS-SI	complete active space-state interaction
CASV-MC-SCF	complete active space valence space-multiconfiguration-SCF
CAUGA	Clifford algebra unitary group approach
CB	Coulomb-Born
CB1	corrected first Born (perturbation theory in atom-ion collisions)
CB2	second-order Coulomb Born
CBe	Coulomb-Bethe (for electron-ion scattering)
CBE	Coulomb-Born-exchange
CBEA	constrained binary encounter approximation
CBF	correlated basis function
CBLM	cluster-Bethe-lattice method (for electronic-structure calcns. on crystals)
CBO	(1) corrected Born-Oppenheimer (in calcns. for mol. complexes) (2) Coulomb Born Oppenheimer (3) crude Born-Oppenheimer (wave functions)
CBOA	crude Born-Oppenheimer approximation
CBOX	Coulomb-Born with no exchange
CBS	complete basis set
CBS-FCI	complete basis set-full configuration interaction
CBS-QCI	complete basis set-quadratic configuration interaction
CBX	Coulomb-Born approxn. with exchange
CC	(1) close coupling method (for atom-molecule collisions) (2) coupled channel (method for reactive scattering) - G.C. Schatz, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 1 (3) coupled-cluster (quantum calcn. method)
CCA	(1) channel coupling array (quantum theory for atoms and molecules) (2) close-coupling approximation (3) coupled-cluster approach (4) crystalline cluster approach (in electronic structure calcns.)
CCAM	charge-conserving approxn. method (for quantum calcns.)
CCBA	coupled-channel Born approxn.
CCC	(1) convergent close coupling (2) correlated coupled cluster (quantum calcn. method)
CCCC	complex-coordinate coupled-channel (method in calcns. on rotational and vibrational predissociation)
CCCI	correlation-consistent CI
CCCLC	complex-coordinate coupled-Landau-channel (method in calcns. on autoionizing resonances)
CCD	coupled-cluster method with double excitation
CCDPPA	coupled-cluster with double excitation polarization propagator
CC-DQMC	clamped-coordinate diffusion quantum Monte-Carlo

CCDW	(1) commensurate charge-density wave (2) coupled-channel distorted-wave (quantum method for reactive scattering) - G.C. Schatz, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 1; J.N.L. Connor, *ibid.*, p. 247
CCDZP	correlation-consistent double-zeta (plus) polarization (basis set)
CCF	correlation crystal field
CCFO	charge-charge flux overlap (model in molecular-property calcns.)
CCFOM	charge-charge flux-overlap modified(model in ir spectra calcn.)
CCGF	coupled cluster Green function
CCGM	Cabrera-Celli-Goodman-Manson (atomic scattering theory)
CCI	(1) complete configuration interaction (2) contracted configuration interaction
CC-LRT	coupled-cluster(-based) linear response theory
CCM	(1) complex coordinate method (in calcns. on quantum tunneling) (2) coupled-cluster method (for energy level calculations) (3) cyclic cluster model (in CNDO for deep levels in solids)
CCMC	coupled-cluster method with multiconfiguration reference state
CCMC-T2	coupled-cluster multiconfigurational (double-excitation method with cluster operator approximated by T2)
CCMET	coupled-cluster many-electron theory
CCMGA	core-corrected modified Glauber approxn. (for scattering)
CCO	coupled-channel-optical (potential, for electron-atom scattering)
CCOM	coupled channel optical method
CCPA	(1) cellular coherent-potential approximation (for electronic structure calcns.) (2) cluster coherent-potential approximation (for electronic structure calcns.) (3) constant centrifugal potential approximation
CCPE	charge core potential energy method (for conformational analysis)
CCPPA	coupled-cluster polarization-propagator approxn.
CC-PV(D,T,Q)Z	correlation-consistent polarized (double, triple, or quadruple)-split valence basis set
CCR	(1) close-coupled representation (2) complex coordinate rotation (method for calcns. of resonances in scattering)
CCRM	coupled-channel reactance matrix (in atom surface scattering)
CCS	(1) classical centrifugal sudden (approximation) - T. Mulloney and G. C. Schatz, *Chem. Phys.* **45**, 213 (1980) (2) corrected coupled-states (method for mol.-scattering calcns.)
CCSC	charge and configuration self-consistency
CCSD	coupled cluster method with single and double replacements - G. D. Purvis and R. J. Bartlett, *J. Chem. Phys.* **76**, 1910 (1982)
CCSDPPA	coupled-cluster polarization-propagator approxn. with single and double excitations
CCSDT	coupled cluster with single, double, and triple replacement
CCSDT-1	linearized CCSDT

CCSOP	close-coupling second-order potential (in scattering)
CCST	complex coordinate scattering theory
CCTM	coupled-channel transition matrix (in atom-surface scattering)
CCW	charge current wave (type of Hartree-Fock wave function)
CCWP	close-coupling wave-packet (for molecular scattering)
CCWP-J	close coupling wave packet [in total angular momentum] j [representation] (for collision calcns.)
CD	(1) centrifugal decoupling approximation (for atom-mol.scattering) (2) Coulomb dipole (in electron-atom impact ionization calcns.)
CDAF	continuous distributed approximating function
CDD	charge-density distortion
CDEDW	centrifugally-decoupled exponential distorted wave
CDFT	chemical-density-functional theory
CDOE	charge-dependent orbital exponent theory
CDP	contracted density product (in simplification of MO calcns.)
CDPT	constant denominator perturbation theory
CDW	(1) charge density wave (2) continuum-distorted-wave approximation (3) Coulomb distorted wave (for scattering calcns.)
CDWA	continuum distorted-wave approxn. (for scattering calcns.)
CDW-EIS	continuum distorted wave-Eikonal initial state (in collisions)
CE	(1) correlation energy. (2) configuration energy - L. C.Allen, *J. Am. Chem. Soc.* **114**, 1514 (1992)
CEM	corrected effective medium (for atomic interactions)
CEPA	coupled electron pair approximation
CEPA-2V	coupled-electron-pair approxn. (with) variational (method)
CEPA-SD	coupled-electron-pair approxn. (with) single (and) double excitations
CEPA-VAR	coupled-electron-pair approxn.-variational
CEPM	coupled electron pair method
CEQ	collinear exact quantum (method in reactive-scattering calcn.)
CEQB	collinear exact quantum (with adiabatic) bending (energy) (method for reactive scattering)
CET	collisional energy transfer
CETO	cartesian exponential type orbital
CFF	consistent force field
CFF-SCF-PI-CI	consistent force field-scf-pi-configuration interaction
CFHH	correlation-function hyperspherical harmonic (method for calcn. of wave functions)
CFM	(1) central field model (2) charge-fluctuation model (3) continued-fraction method
CFO	crystal field orbital
CFP	coefficient of fractional parentage (method in quantum calcns.)
CFSO	crystal field surface orbital
CGF	Coulomb Green function
CGO	configuration generating orbital (a type of MO)
CGTF	cartesian gaussian-type function
CGTO	(1) cartesian gaussian-type orbital (2) combination of gaussian type orbitals (3) contracted gaussian-type orbital

CHA	chemical hamiltonian approach - I. Mayer, *Int. J. Quantum Chem.* **23**, 341 (1983)
CHA/CE	chemical hamiltonian approach with conventional energy
CHARMM	a computer program for calculating macromolecular energy and structure - B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan, and M. Karplus, *J. Comp. Chem.* **4**, 187 (1081)
CH-CI	core hole configuration interaction
CHELEQ	charge electronegativity equalization
CHF	(1) Coulomb Hartree-Fock (2) coupled Hartree-Fock
CHFEP	coreless Hartree-Fock effective potential
CHFPT	coupled Hartree-Fock perturbation theory
CHF-PT-EB	coupled Hartree-Fock-perturbation theory-extended basis
CHIRP	core-hole initiated relaxation process (in ionic crystals)
CHMO	constrained Hartree-Fock orbitals
CHO	complex harmonic oscillator (in mol. scattering theory)
CHW	coherent hole wave (quantum excitations in solids)
CI	configuration interaction - E. A. Hylleraas, *Z. Physik* **48**, 469 (1928)
CIBS	corrections to an incomplete basis set (a perturbation theory)
CIC	configuration interaction (in the) continuum (theory in calcns. of atomic resonances)
CID	(1)configuration interaction with double substitution (2) configuration interaction with doubly excited configurations (3) collision-induced dissociation - R.D. Levine and R.B. Bernstein, *Molecular Reaction Dynamics and Chemical Reactivity* (Oxford University Press, New York, 1987)
CIDEP	chemically induced dynamic electron polarization.
CIHT	configuration-interaction Hylleraas-type (wave function)
CI-HY	configuration interaction-Hylleraas
CIMI	configuration interaction from molecular integrals
CINDO	closed shell intermediate neglect of overlap method
CINDORU	(1) cluster INDO restricted-unrestricted (2) unified cluster INDO
CINO	configuration interaction natural orbital
CIOS	(1) classical infinite order sudden (in atom-molecule reaction calcns.) (2) complex infinite order sudden (approxn. in quantum calcns.) (3) corrected infinite-order sudden (approxn in molecular collisions)
CIOSA	classical infinite-order sudden approxn.
CIP	configuration interaction with partner orbitals
CIPSI	configuration interaction perturbing a multiconfigurational zeroth-order wave function selected iteratively
CIPSO	configuration interaction (with) perturbation (including) spin-orbit coupling
CIS	configuration interaction with single replacements
CISA	continuum intermediate-state approxn. (for scattering)
CISC	configuration interaction (with) size-consistency (correction)
CISD	configuration interaction with single and double excitation
CISDQ	configuration interaction with single, double, and quadruple excitations

CISDTQ	configuration interaction with single, double, triple and quadruple excitations
CI-TD-HG	configuration interaction time-dependent Hartree grid
CIVB	configuration interaction valence bond
CLOPPA	contribution from localized molecular orbitals with polarization propagator approach
CM	(1) configuration mixing (2) center of mass
CMC	coupled multiconfiguration
CMC-SCF	complete multiconfiguration self-consistent field
CMO	canonical molecular orbital
CMO	complex molecular orbital method
CMR-CI	contracted multireference configuration interaction
CMS	complete model space (in many-body calcns.)
CMSM	continuum multiple-scattering model
CMX	connected-moments expansion
CMX(2)	second-order connected moments expansion (method for calcg. correlation energies of molecules)
CNDO	complete neglect of differential overlap - a computer program for obtaining semiempirical solutions to the electronic Schrödinger equation - J. N. Murrell & A. J. Harget, *Semi-empirical Self-consistent-field Molecular Orbital Theory of Molecules*, Wiley-Interscience, 1972
CNDO LHP	complete neglect of differential overlap Longet-Higgins-Pople
CNDO SP	complete neglect of differential overlap spin polarization
CNDO/2-FA	complete neglect of differential overlap first approxn.
CNDO/2-FPP	complete neglect of differential overlap with finite perturbation and polarization
CNDO/2-V(N-1)	complete neglect of differential overlap-potential method
CNDO/2D	complete neglect of differential overlap with deorthogonalization
CNDO/2-U	universal CNDO/2 (extended to full periodic table)
CNDO/B	complete neglect of differential overlap / Boyd
CNDO/BW	complete neglect of differential overlap with Boyd and Whitehead parametrization
CNDO/F	complete neglect of differential overlap/force
CNDO/FK	complete neglect of differential overlap/ Fischer-Kollmar
CNDO/IP	complete neglect of differential overlap/ionization potential
CNDO/M	CNDO Mataga approxn.
CNDO/OPTIC	a CI method for electronic transition moments of the optical transition of large molecules based on CNDO/s parametrization
CNDO/S	complete neglect of differential overlap/spectroscopic
CNDO/SW	complete neglect of differential overlap / Sichel-Whitehead
CNDO/SWW	complete neglect of differential overlap/ Sichel-Whitehead-Wratten parametrization
CNDOL(CNDO-l)	complete neglect of differential overlap-azimutal quantum number (of valence ao's)
CNO	canonical natural orbital
CNP	complete nuclear permutation (group, a set of symmetry operations describing the nuclear coordinates) - A.J. Karas, R.G. Gilbert, and M.A. Collins, *Chem. Phys. Lett.*, **193**, 181 (1992)
CNPI	complete nuclear permutation and inversion (group, a set of symmetry operations describing the nuclear coordinates)

	- A.J. Karas, R.G. Gilbert, and M.A. Collins, *Chem. Phys. Lett.*, **193**, 181 (1992)
CO	crystal orbital
COCP	cut-off Coulomb potential
COHSEX	Coulomb-hole (plus) screened-exchange (approxn. in band-structure calcns.)
CONDO	crystal orbital neglect of differential overlap
COPW	complete orthogonalized plane wave
COSCI	complete open shell configuration interaction
CP	chemical pseudopotential
CP	coupled pair (many-electron theory)
CPA	(1) coherent potential approximation - Ning Lu and S. Mukamel, *J. Chem. Phys.* **95**, 1588 (1991) (2) coupled-pair approximation
CPBA	Coulomb-projected Born approximation
CPBE	Coulomb-projected Born approxn. with exchange
CPCC	complex-potential close-coupling
CPCCSD	coupled-perturbed coupled-cluster (with) single (and) double excitation
CPDAM	cumulative potential-derived atomic multipole (calcn. method)
CPDWB	Coulomb-projected distorted-wave Born
CPE	Coulomb wave-plane wave (description with) effective screening
CPF	(1) coupled-pair formalism (2) coupled-pair functional (CI method with energy functional)
CPFD	coupled-pair functional with double excitation
CPHF	coupled perturbed Hartree-Fock
CPIA	Coulomb peaking impulse approxn. (in electron-exchange collision calcns.)
CPMCHF	coupled perturbed multiconfiguration Hartree-Fock
CPMC-SCF	coupled perturbed multiconfigurational SCF
CPMET	coupled pair many electron theory
CPP	(1) charge-perturbation-polarizability (2) core polarization potential
CPSS	Coulomb-repulsion perturbed stationary state
CPSSR	Coulomb-repulsion perturbed stationary state with relativistic effects
CPST	classical perturbation scattering theory
CPT	(1) cluster perturbation theory (2) Coulomb wave-plane wave (description with) truncated (treatment) (3) classical perturbation theory
CRC	coupled-reaction-channels (quantum calcn. method)
CRF	core/core repulsion function.
CRHF	complex-restricted Hartree-Fock
CRIOSA	classical reactive infinite order sudden approxn.
CRPA	correlated random phase approxn.
CRS	coordinate-representation sudden (decoupling method for mol. inelastic collisions)
CS	(1) centrifugal sudden (approximation) - D.C. Clary, *Ann. Rev. Phys. Chem.*, **41**, 61 (1990) (2) configuration space (in wave functions) (3) coupled-states (approximation) - D. J. Kouri in *Atom-Molecule Collision Theory*, edited by R. B. Bernstein (Plenum, New York, 1976), pp. 301-385

CS INDO	conformation spectra INDO
CSA	(1) centrifugal sudden approxn. (in scattering calcns.) - D.C. Clary, *Ann. Rev. Phys. Chem.*, **41**, 61 (1990) (2) charge sensitivity analysis (3) coupled states approxn. (4) coupled static approxn. (in scattering calcns.) (5) coupled-subshell approxn. (in calcns. on inner-shell ionization in collisions)
CSCBS	charge-self-consistent band-structure (method)
CSCF	(1) canonical self-consistent field (2) complex self-consistent field
CSD	correlated single determinant (wave function)
CSDA	continuous-slowing-down approximation (in electron scattering)
CSDW	centrifugal sudden (or coupled states) distorted wave (method for reactive scattering calculations) - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
CSEM	coherent self-energy method
CSE	correction (with the) statistical exchange potential
CSF	configuration spin function (a wave function)
CSF	configuration state function (part of CI wave function)
CSFGH	complex-scaling Fourier-grid hamiltonian
CSGT	continuous set (of) gauge transformations
CSH	centrifugal sudden hyperspherical (coordinate reactive scattering code)
CSM	complex scaling method
CSOV	constrained space orbital variation (in molecular bonding calcn.)
CSPI	coherent state path integration
CSRR	coupled-state rigid-rotor
CSSA	composition-space superposition approxn. (in density-functional theory of mixtures)
CSWP	centrifugal sudden [or coupled states] wave packet method
CT	(1) classical trajectory (2) charge transfer (3) collision theory (bimolecular reactions)
CTA	classical trajectory approximation (in molecular-collision calcns.)
CTCF	collisional time correlation function (in quantum calcns. on molecular inelastic collisions)
CTF	common translation factor (for ion-atom inelastic collisions)
CTIOSA	charge-transfer infinite order sudden approxn.
CTMC	classical trajectory Monte-Carlo (in ion-atom electron-exchange)
CTPGF	closed time path Green function (in many-body theory)
CVA-MO	core-valence approxn.-mo (for at. integral calcns.)
CVBM	conduction-valence-band model (in electronic structure calcns.)
CVM	cluster variation method (in calcns. on semiconductors)
CVM-CI	constrained variational method-CI
CVMO	cluster valence molecular orbital
CVO	canonical virtual orbital
CVPT	canonical van Vleck perturbation theory
CVSEH	correlated valence shell effective hamiltonian

CVT	canonical variational (transition state) theory - D. G Truhlar, W. L. Hase, and J. T. Hynes, *J. Phys. Chem.* **87**, 2644 (1983)
c VT	same as CVT
CVTST	canonical variational transition state theory - D. G Truhlar, W. L. Hase, and J. T. Hynes, *J. Phys. Chem.* **87**, 2644 (1983)
cVTST	same as CVTST
CWBA	Coulomb-wave Born approximation
CWTM	compound Weaire-Thorpe model (in electronic-structure calcns.)

D

DA	diatomic path approximation
DAF	distributed approximating function (in study of quantal wave-packet propagation)
DAIM	deformed atoms in molecules
DBC	detailed balance corrected
DBE	distorted-wave Born exchange
DBHF	Dirac-Breit-Hartree-Fock
DBPHF	Dirac-Breit-Pauli-Hartree-Fock
DCA	(1) direct configurational averaging (in pair potentials for alloys) (2) dressed-cluster approximation (in band-structure calcns.)
DCB	(1) Dirac-Coulomb-Breit (2) distorted Coulomb-Born approxn.
DCBA	distorted-coupling Born approximation
DCBNX	distorted Coulomb-Born no-exchange approxn.
DCBS	dimer centred basis set (in quantum calculations of dimers: *cf.* monomer centred basis set)
DCBX	distorted Coulomb-Born exchange approxn.
DCCI	dissociation-consistent configuration interaction
DCFCI	density-constrained full-configuration-interaction
D-CI	double excitations in configuration interaction
DCM	decoupled cell Monte-Carlo (in simulations on quantum systems)
DCPA	dynamical coherent potential approximation - Ning Lu and Shaul Mukamel, *J. Chem. Phys.* **95**, 1588 (1991).
DDAF	discretized distributed approximating function (propagator, in study of wave-packet propagation)
DDMO	differential density matrix overlap (index, in electron-correlation calcns.)
DD-NRCE	direct dissociative-near resonant charge transfer
DDQRPA	double direct quadratic random phase approximation
DDRPA	double direct random phase approximation
DE	dispersion energy.
DECENT	distribution (among quantum states) of exact classical energy transfer
DEM	distinguishable electron method
DF	(1) density functional formalism (2) Dirac-Fock
DFB	Dirac-Fock-Breit
DFMFT	density-functional mean-field theory

DF-OCE	Dirac-Fock one-center expansion
DFPT	density-functional perturbation theory
DFS	Dirac-Fock-Slater
DF-SCF	Dirac-Fock self-consistent field
DFT	density functional theory
DGB	distributed gaussian basis (molecular wave function)
DHF	(1) decoupled Hartree-Fock (2) derivative Hartree-Fock (quantum theory in calcns. on molecules) (3) Dirac-Hartree-Fock
DHFR	Dirac-Hartree-Fock-Roothaan
DHTF	Debye-Hückel-Thomas-Fermi
DID	dipole-induced-dipole (in molecular polarizabilities calcn.)
DIIS	(1) diatomics-in-ionic-systems (2) direct inversion (in the) iterative subspace (method for optimizing MC-SCF wave functions) - P. Pulay, *Chem. Phys. Lett.*, **73**, 393 (1980)
DIM	diatomics in molecules
DIM-3C	diatomics-in-mols. method including 3-center terms (integrals)
DIMZO	diatomics-in-molecules zero-overlap
DIPP	deformed inverse-power potential
DIRP	direct interaction with product repulsion
DIRP-DIP	direct interaction with product repulsion distributed as in photodissociation
DISEP	difference integrated spatial electron populations
DIVAH	diagonally corrected vibrationally adiabatic hyperspherical (theory in scattering calcns.)
DLA	decoupled *L*-dominant approximation
DLD	decoupled *L*-dominant method (in inelastic-scattering calcns., *L*= orbital angular momentum)
DLMO	density localized molecular orbital
DLVO	Derjaguin-Landau-Verwey-Overbeek model for pair interactions
DMA	distributed multipole analysis - A.J. Stone and M. Alderton, *Mol. Phys.*, **56**, 1047 (1985)
DMBE	double many-body expansion (in potential energy surface calcn.)
DMO	delocalized molecular orbital
DMP	dichotomous Markovian Process (J jumps between two values with the mean frequency)
DNO	delocalized natural orbital
DO	diatomic orbital
DODS	different orbitals for different spins
DOMO	doubly occupied molecular orbital
DOS	density of states (in band structures)
DPCILO	differential perturbative configuration interaction using localized orbitals
DPT	degenerate perturbation theory P.W. Atkins, *Molecular Quantum Mechanics*, 2nd Ed. (Oxford University Press, Oxford, 1983); A. Messiah, *Quantum Mechanics* (North-Holland, Oxford, 1976)
DPUMPn	double-annihilation procedure unrestricted Møller-Plesset nth- order
DQ-MBPT	double and quadruple excitation diagrams in many-body perturbation theory
DQM	diffusion quantum Monte-Carlo (theory) (see DQMC)

DQMC	diffusion quantum Monte-Carlo theory - D. Ceperley, B. Alder, *Science* **231**, 555 (1986); M Quack, *J. Chem. Phys.*, **95**, 28, (1991)
DQMS	dressed quasimolecular - states approximation
DQ-RSPT	double and quadruple excitation diagrams in Rayleigh-Schrödinger perturbation theory
DQT	dissipative quantum tunneling (theory)
DRF	direct reaction field (for intermol. interactions)
DRPA	direct random phase approximation
DR-RWA	dominant resonance-rotating wave approximation
DSA	(1) dynamic simulated annealing (for electronic structure in liq. metals) (2) dynamic simulated annealing (for structure refinement in molecular mechanics) M. Levitt, *J. Mol. Biol.*, **170**, 723 (1983)
DSA-EOM	dynamic simulated annealing-equations of motion (in liq. metals)
DSCCR	diffractive sudden-closed coupled rotation (for molecule-surface scattering calcns.)
DSCF	direct self-consistent field
DSDV	Dirac-Slater discrete variational
DSGE	double Sine-Gordon equation (for describing excitations such as kinks and solitons)
D-SIC	degeneracy-dependent self-interaction correction
DSPB	distorted-wave strong-potential Born (approxn.)
DSW	Dirac scattered-wave (often as SCF-x(alpha)-DSW method)
DTGF	double-time Green function
DTZHD	double-triple-zeta-Huzinaga-Dunning
DVB	diagrammatic valence bond (in study of electronic properties)
DVGR	diabatic vibrational golden rule approximation
DVM	discrete variational method
DVMO	directed-valence molecular orbital
DVR	discrete variable representation (in wave function calcn.)
DVR-REV	discrete variable representation-ray eigenvector
DV-X(ALPHA)	discrete variational-x(alpha) (statistical exchange correlation)
DWA	distorted wave approximation - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
DWB2	second-order distorted-wave Born
DWBA	distorted wave Born approximation (for reactive scattering calculations) - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
DWBA3 (3DWBA)	three-body distorted-wave Born approximation
DWE	distorted-wave (approxn. with) exchange
DWES	distorted-wave energy sudden (for inelastic mol. collisions)
DWFBA	distorted-wave first-order Born approximation
DWIA	distorted-wave impulse approximation
DWIOS	distorted wave infinite order sudden approximation
DWM	distorted wave method
DWP	diabatic wave packet - E. Deumens and Y. Ohrn, *J. Am. Chem. Soc.* **92**, 3181 (1988)
DWPE	distorted-wave (with) polarization (and) exchange
DWPO	distorted wave polarized orbital

DWSBA	distorted wave second Born approxn.
DWTM	distorted wave t-matrix (for electron-atom scattering)
DWX	distorted-wave approxn. with exchange
DZ	(1) double zeta (basis set) (2) Dunning-Huzinaga (basis sets)
DZD	(double zeta)-diffuse (basis set in configuration-mixing mo calcns. on mols.)
DZDP	(double zeta)-diffuse-polarization (basis set in configuration-mixing mo calcns. on mols.)
DZHD	double-zeta Huzinaga-Dunning (wave functions)
DZP	double zeta + polarization (basis set)
DZPP	double-zeta (doubly) polarized (basis set)
DZRS	double zeta Roos-Siegbahn (wave functions)

E

E-2PH-TDA	extended two-particle-hole Tamm-Dancoff approxn. (Green-function method for ionization-energy calcns.)
EAL-MCDF	extended average level-(relativistic) multiconfiguration Dirac-Fock
EAM	(1) effective medium approxn. (2) embedded atom method
EAN	effective atomic number (also called "18-electron rule") - P.R. Mitchell and R.V. Parish, *J. Chem. Educ.*, **46**, 811 (1969)
EB	extended basis (set)
EBA	(1) Eikonal Born approxn. (2) exponentiated Born approximation
EBD	equilibrium brownian dynamics
EBEBO	extended bond energy bond order (quantum calcn. method)
EBIR	energy based integral retention (in electronic-structure calcns.)
EBK	Einstein-Brillouin-Keller (quantization method)- (eg) I.C. Percival, *Adv. Chem. Phys.*, **36**, 1 (1977)
EBO	equivalent bond orbital
EBOM	effective bond-orbital method
EBS	(1) Eikonal-Born scattering series method (2) extended basis set
EBSM	extended breathing sphere model
EBT	extended Brillouin theorem
ECA	equivalent core approximation
ECAMSI	electron configuration analysis for many-system interactions
ECBM	extended classical over-barrier model (in calcns. on inelastic ion-atom colisions)
ECCF	(1) equilibrium charge-charge flux (model in IR spectra calcns.) (2) exchange correlated crystal field
ECCM	extended coupled-cluster method
ECM	(1) embedded cluster method (in electronic-structure calcns.) (2) exchange-charge model
ECOP	electron correlation polarization (potential)

ECP	(1) effective core potential approxn.(in electronic structure calcn.) (2) exchange core polarization (3) exponential corrugated potential
ECP-CPP	effective core potential (augmented by)-core polarization potential
ECPMET	extended coupled pair many electron theory
ECPSSR	energy-loss Coulomb-repulsion perturbed-stationary-state relativistic
ECRR	energy-corrected rigid-rotor approximation
ECS	energy-corrected sudden (scaling theory in molecular collisions)
ECS-EP	energy-corrected sudden-exponential polynomial (scaling law)
ECS-P	energy-corrected sudden-polynomial (scaling law)
ECT	ergodic collision theory (for collisional energy transfer) - S. Nordholm, B.C. Freasier, and D.L. Jolly, *Chem. Phys.*, **25**, 433 (1977); B.C. Freasier, D.L. Jolly, and S. Nordholm, *Chem. Phys.*, **32**, 161 (1978)
ECTFP	empty-core Thomas-Fermi pseudopotential
EDC	electronic dynamic coordinates
EDEC	equal distances equal charges model
EDF	energy density functional (theory in electronic-property calcn.)
EDW	(1) exchange distorted-wave (2) exponential distorted wave approximation
EDWA	exponential distorted-wave approxn. (atom-ion electron-exchange calcns.)
EDWBA	exponential distorted wave Born approximation
EEM	electronegativity equalization method
EESOP	electronegativity equalization with s-orbital participation
EFA	envelope function (i.e.,plane-wave) approxn. (in band-structure calcn.)
EFG GTO	electric field gradient gaussian-type orbital
EFH	extended Fenske-Hall (LCAO MO method)
EFP	effective fragment potential method
EFV	electric-field-variant function (in CI method)
EFVAO	electric-field variant atomic orbital
EFV GTO	electric-field-variant gaussian-type orbital
EFV STO	electric-field-variant Slater-type orbital
EGCI	exponentially generated configuration interaction
EGL	exponential gap law (in rotational energy transfer) - J.C. Polanyi and K.B. Woodall, *J. Chem. Phys.*, **56**, 1563 (1972)
EGM	electron gas model
EGO	ellipsoidal gaussian orbital
EHB	extended Hubbard (hamiltonian)
EHCO	extended Hückel crystal orbital
EHF	extended Hartree-Fock
EHM	extended Hubbard model (hamiltonian)
EHMO	extended Hückel molecular orbital
EHP	electron-hole potential method
EHT	extended Hückel theory
EIA	Eikonal impulse approxn. (in ion-atom inelatic collisions)
EICVOM	equivalent ionic core virtual orbital model
EIMP	energy independent model pseudopotential
EINP	energy-independent nonlocal pseudopotential

EIP	eigenvalue-independent partitioning (in coupled-cluster calcns.)
EIS	Eikonal initial state (in scattering calcns.)
EJS-TST	an angular-momentum-conserving variation of EMS-TST - T. D. Sewell, H. W. Schranz, D. L. Thompson, and L. M. Raff, *J. Chem. Phys.* **95**, 8089 (1991)
EJZ-TST	EJS-TST restricted to ensembles with J=0.
EK	extended Koopmans (method in ionization potential calcns.)
EKB	Einstein-Brillouin-Keller (quantization method)
EKT	extended Koopmans theorem
ELEPS	extended London-Eyring-Polyani-Sato (potential energy surface)
ELF	electron localization function
ELMO	energy-localized molecular orbital
ELO	(1) edge localized orbital (2) equivalent localized orbitals
EMA	(1) effective mass approxn. (for impurity energy levels) (2) effective medium approximation
EMAP	energy-modified adiabatic phase (matrix method)
EMM	effective mass model (used in explaining quantum confinement effects in clusters)
EMOA	extended maximum overlap approximation
EMP	(1) electrostatic molecular potential (for electronic-structure) (2) empirical pseudopotential method
EMS	efficient microcanonical sampling method - E. S. Severin, B. C. Freasier, N. D. Hamer, D. L. Jolly, and S. Nordholm, *Chem Phys. Lett.* **57**, 117 (1978)
EMS-TST	efficient microcanonical sampling transition state theory - H.W. Schranz, L.M. Raff, and D.L. Thompson, *J. Chem. Phys.*, **94**, 4219 (1991)
EMT	(1) effective mass theory (in electronic wave functions calcn.) (2) effective-medium theory (of bonding in metallic systems)
EMTO	extended muffin-tin orbital method
EMZDO	exchange modified zero differential overlap
ENC	effective nuclear charge (model for molecular property calcns.)
EO	equivalent orbital
EOM	equations of motion method
EOM-CC	equation of motion-coupled cluster
EP	(1) effective core potential (2) effective potential (approximation) see also UEFF [N. Markovic and S. Nordholm *Chem. Phys.* **135** 109 (1989)]
EPA	(1) electron population analysis (2) environment potential approach (in electronic-structure calcn.) (3) extended pair approxn. (in electronic conductivity calcn.)
EPCE	effective pair correlation energy method
EPCE-F2(SIGMA)	effective pair correlation energy method with the factor-two (F2) approximation for sigma-electron systems
EPEN	empirical potential (based on interaction of) electrons (and) nuclei
EPM	empirical pseudopotential method

EPT	exponential perturbation theory
EPV	exclusion-principle violating
ER	exchange repulsion (energy)
ERM	electron redistribution model
ERMM	effective r-matrix model (in reactive electron-molecule scattering)
ERPA	extended random phase approximation
ERT	effective-range theory (in molecular calcns.)
ES	(1) energy sudden (approxn. in scattering calcns.) (2) elastic scattering
ESA	energy sudden approxn. (in calcns. on reactive scattering)
ESE	exact static-exchange (approxn. in scattering calcns.)
ESEDD	excited state electron density differential method
ESE MO	essential-structure-elements molecular orbital
ESEP	exact static exchange (plus) polarization (potential)
ESF	electrostatic force (theory for molecular calcns.)
ESMO	excited-state molecular orbital
ESMSV	exponential-spline Morse-spline van der Waals (interatomic potential)
ESPT	electron spin polarization transfer
ETB	extended tight-binding (method for electronic-structure calcns.)
ETBM	empirical tight-binding method (in electronic structure calcn.)
ETEAO	even-tempered exponential atomic orbital
ETF	(1) exponential-type function (an atomic orbital) (2) extended Thomas-Fermi (model)
ETGAO	even-tempered gaussian atomic orbital
ETO	(1) elliptical-type orbital (2) exponential-type orbital
EVB	effective valence bond (hamiltonian)
EWBA	Eikonal wave Born approximation
EWIA	Eikonal (distorted) wave impulse approxn. (f0r scattering)
EWMO	energy weighted maximum overlap method
EXGEM	extended geminal (model correlated wave function)
EXGF(1)	extended group function(1) (model wave function accounting
EXPL	exchange polarization

F

FAAO	free-atom atomic orbital
FAKE	fast accurate kinetic-energy (mo method)
FAO	(1) floating atomic orbital (2) frozen atomic orbital
FARM	fixed-angle reaction model (in quantum calcns. on reactive scattering)
FBA	first Born approximation
FBR	finite basis representation (in wave function calcn. for nuclear motion on potential energy surface)
FC	(1) frozen core (approxn. for electron-atom scattering calcns.) (2) Franck-Condon (principle or factor)
FCA	frozen-core appproximation
FCHF	frozen-core Hartree-Fock
FCI	full configuration interaction
FCM	finite-cluster model (for calcns. on electromigration)

FCP	function counterpoise (method for eliminating basis set superposition error) - S.F. Boys and F. Bernardi, *Mol. Phys.*, **19**, 553 (1970).
FCSA	frequency-corrected sudden approxn. (in mol. collision calcns.)
FDBVM	finite difference boundary value method
FEGE	free electron gas exchange approximation
FEGO	floating ellipsoidal gaussian orbital
FEM	(1) finite element method (in at.. Hartree-Fock calcns.) (2) free electron model
FEMO	free-electron molecular orbital
FEMP	free of empirical parameters (e.g., SINDO/FEMP)
FEN	free electron network
FEOE	full equalization of orbital electronegativity
FFM	finite field method (in molecular polarizabilities calcns.)
FF-MBPT	finite-field many-body perturbation theory
FFT	fast Fourier transform - A.H. Press, B.P. Flannery, S.A. Teukolsky, and W.T. Vetterling, *Numerical Recipes (Fortran Version)* (Cambridge University Press, New York, 1989)
FG	FG (matrix method in normal mode analysis: F = force-constant matrix; G = mass matrix) - E.B. Wilson Jnr, J.C. Decius, and P.C. Cross, *Molecular Vibrations. The theory of infrared and raman vibrational spectra* (McGraw Hill, New York, 1955 (reprinted in 1980 by Dover Books))
FGH	Fourier-grid hamiltonian
FHBS	finite Hilbert basis set
FHMO	Fenske-Hall molecular orbital
FHNC	Fermi hypernetted chain method (in quantum statistics)
FID	free induction decay function (a distribution function of quantum spins in a crystal)
FIM	forced impulse method (in atom ion-impact ionization)
FIP	full intra-pair (spin-coupling) (wave function)
FISCI	final ionic state configuration interaction
FLAPW	full-potential linearized augmented plane wave
FLCAO	factorized LCAO
FLMTO	film linearized muffin-tin orbital (for surface electronic structure calcns.)
FLO	face localized orbital
FMAP	Fano-Macek alignment parameter (in electron-impact excitation of ions)
FMF	frozen molecular fragment (method in calcn. of intermolecular potentials and charge distributions)
FMO	(1) floating molecular orbital (2) frontier molecular orbital
FMTBA	fitted modified tight-binding approxn.
FNO	frozen natural orbital
FOA	frozen orbital approximation
FOCI	first-order configuration interaction
FOCO	first-order correlation orbital
FO-CPHF	first-order coupled perturbed Hartree-Fock theory
FOE	first-order exchange (in electron-atom scattering calcn.)
FOEA	first-order Eikonal approximation
FO-ECP	frozen orbital-effective core potential
FOGO	floating orbital geometry optimization
FOJT	first-order Jahn-Teller
FOM	(1) forced oscillator model- H.K. Shin, in *Dynamics of Molecular Collisions,* edited by W.H. Miller, (Plenum Press,

	New York, 1976), Vol. A, p. 131 (2) frozen orientation model
FOMBT	first-order many-body theory
FO-NACME	first-order nonadiabatic coupling matrix elements
FONDA	first order non-degenerate adiabatic (approximation)
FOND PT	finite-order nondegenerate perturbation theory
FOPIM	first order perturbation iteration method
FOPPA	first-order polarization propagator approxn.
FORS	full optimized reaction space
FOS	first-order sudden
FOTO	forced oscillation of tightening oscillator
FOTOS	first-order theory of oscillator strength
FOURPI	Fourier path integral
FP	finite perturbation
FPC	fractional parentage coefficient (in group-theory calcns.)
FPI	Fourier path integral
FP-LMTO	full-potential linear combination of muffin-tin orbitals
FP-MC	finite perturbation-multiconfigurational method
FPP	finite perturbation and polarization
FP-SCF-INDO	finite perturbation-SCF-INDO
FPT	finite field perturbation theory
FQO	forced quantum oscillator method – the following discusses aspects of FQO, although the acronym is not used - H.K. Shin, in *Dynamics of Molecular Collisions,* edited by W.H. Miller, (Plenum Press, New York, 1976), Vol. A, p. 131
FRC	frozen core approxn.
FRSW	finite range scattering wave function
FSGO	floating spherical gaussian orbital - A. A. Frost, *J. Chem. Phys.* **47**, 3707 (1967)
FSMRCC	Fock space multireference coupled cluster
FSMRCCSD	Fock space multireference coupled cluster (with) single (and) double excitations
FTHF	finite-temperature Hartree-Fock
FTHFB	finite-temperature Hartree-Fock-Bogolyubov
FTOTF	finite temperature optimized Thomas-Fermi theory.
FTST	flexible transition state theory - D.M. Wardlaw and R.A. Marcus, *J. Chem. Phys.*, **83**, 3462 (1985)
FV-CAS-SCF	full valence-complete active space-SCF
FVEH	fragment valence effective hamiltonian (in electronic-structure calcns. on mol. fragments)
FV-MC-SCF	full valence multiconfiguration self-consistent field
FVRCI	full valence Rydberg configuration interaction
FVVM	finite volume variational method (for molecular calcns.)
FWE	Faddeev-Watson expansion (for t-operator in atomic collisions)

G

G1	gaussian-one (theory for calculating molecular energies)
G2	gaussian-two (an ab initio MO theory for molecular energies calcn.)
GA	Glauber approximation (in electron-atom scattering)
GAEP	generalized atomic effective potential
GAGP	generalized antisymmetrized geminal power (wave function)

GAMESS	a computer program for solving the electronic Schrödinger equation - M.F. Guest, Daresbury Laboratory, Warrington, U.K. (1989)
GAPT	generalized atomic polar tensors
GAUSSIAN-n	a computer program for solving the electronic Schrödinger equation - J.A. Pople and co-workers, Gaussian Inc., Pittsburgh, PA, U.S.A.
GBA	generalized Born approxn.
GBS	generalized Bohr-Sommerfeld (quantization method)
GBT	generalized Brillouin theorem
GC	grand canonical (ensemble) (in statistical mechanics)
GCA	generator coordinate approxn.
GCHF	generator coordinate Hartree-Fock
GCLDA	gradient-corrected local density approximation
GCLSDA	gradient-corrected local spin density approximation
GCM	generator-coordinate method
GCMC	grand canonical Monte-Carlo - M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids* (Oxford Science Publications, Oxford, 1990), Chapter 4
GCO	general coupling operator (in calcns. of vector coupling for atoms and ions)
GDF	generalized density-functional (theory)
GDIM	generalized diatomics-in-molecules (theory)
GDO	generalized diatomic orbital
GDT	generalized dilatation transformation (method in study of stationarity principle for atomic and molecular resonance states)
GDWB	generalized distorted-wave Born (approxn. or theory)
GEA	gradient-expansion approxn. (in exchange-energy calcns.)
GEASIC	gradient-expansion approxn. self-interaction correction (functional, in total-energy calcns. for atoms)
GEH	generalized effective hamiltonian
GEKT	generalized extended Koopmans theorem
GFEMO	generalized free electron molecular orbital
GFF	Green function formalism
GFHF	Galitskii-Feynman-Hartree-Fock
GFMC	Green function Monte-Carlo (quantum method)
GFMT	Green function muffin tin (method in electronic structure study)
GFPE	generalized Fokker-Planck equation D.A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976)
GFQMC	Green function quantum Monte-Carlo
GGA	generalized gradient approxn.
GGC	generalized gradient-corrected (density-functional)
GGWD	generalized gaussian wave-packet dynamics
GGWPD	generalized gaussian wave-packet dynamics
GHF	(1) generalized Hartree-Fock method (2) generalized Hellmann-Feynman (theorem)
GHL	generalized Heitler-London
GHO	generalized hybrid orbital (AO)
GHW-HF	Griffin-Hill-Wheeler-Hartree-Fock
GI	many electron wave functions that are simultaneously eigen-functions of the total spin projection operators and satisfy the Pauli principle
GIAO	(1) gauge independent atomic orbitals - R. Ditchfield, *Molec. Phys.*, **27**, 789 (1974)

	(2) gauge-including atomic orbital (3) gauge invariant atomic orbital
GIOS	generalized infinite order sudden
GIPM	ground state inversion potential method (in photoionization cross sections calcn.)
GIPM/D	ground state inversion potential method including diffraction
GIPQ	gauge-invariant periodic quantization
GKS	Gaspar-Kohn-Sham (potential for exchange and correlation in band structure calcns.)
GLAO	generalized localized AO
GLE	generalized Langevin equation - D.A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976)
GLF	gaussian lobe function
GLJ	generalized Lennard-Jones (potential)
GLO	gaussian lobe orbital
GMC	Gibbs Monte-Carlo (method for direct simulation of fliud phase equilbria) - A.Z.S. Panagiotopoulos A.J. and M. Alderton, *Mol. Phys.*, **61**, 813 (1987)
GMD	grand canonical molecular dynamics.
GME	generalized master equation (in quantum statistical mechanics)
GMO	(1) generalized molecular orbital (2) group molecular orbital
GMP	generalized Møller-Plesset (perturbation theory)
GMP2	generalized Møller-Plesset second-order (perturbation theory)
GNLSE	generalized nonlinear Schrödinger equation
GNMP	generalized nonlocal model potential
GNO	geminal natural orbital
GNVP	generalized Newton variational principle
GO	(1) gaussian overlap (approxn. in molecular calcns.) (2) generalized overlap
GOCE	gaussian overlap potential with constant well depth
GOE	gaussian orthogonal ensemble (of random matrices in quantum chaoticity study in atomic and nuclear energy levels)
GOPW	gaussian orthogonalized plane wave
GOS	generalized oscillator strength
GO-SCF	gaussian orbital self-consistent field
GPEF	generalized potential energy function
GPF	gaussian polarization function
GPM	generalized perturbation method (in electronic theory of phase stability of alloys)
GPS	generalized phase shift formalism
GPT	generalized pseudopotential theory
GPUCHF	geometric perturbed uncoupled Hartree-Fock method
GQDPT	generalized quasidegenerate perturbation theory
GRHF	generalized restricted Hartree-Fock
GRINDOL	ghost (and) Rydberg INDO
GROMOS	a computer program for simulation of macromolecules - W.F. van Gunsteren, H.J.C. Berensden, Univerisity of Groningen, The Netherlands.
GRPA	generalized random-phase approximation
GRVB	generalized resonating valence bond
GRWA	generalized rotating-wave approxn. (in energy level calcns.)

GS	Gelius-Siegbahn (MO approxn.)
GSA	(1) generalized sudden approximation (2) generator-state approach (in many-body quantum theory)
GSAC	generalized symmetry adapted cluster (theory)
GSBE	generalized semiconductor Bloch equations - J. R. Kuklinski and S. Mukamel, *Phys. Rev. B* **44**, 11,253
GSCF	generalized self-consistent field
GSCRF	generalized self-consistent reaction field
GSLO	group symmetric localized orbital.
GSMO	ground-state molecular orbital
GSNO	ground-state natural orbital
GSO	general spin orbital
GSZ	Green-Sellin-Zachor model potential (for atoms)
GT	(1) general term of the interaction potential (2) Gelfand-Tsetlin basis function
GTDA	generalized Tamm-Dancoff approximation
GTF	gaussian-type (wave) function
GTG	gaussian-type geminal
GTO	gaussian-type orbital - W. J. Hehre, L. Radom, P. v. R. Schleyer and J. A. Pople, *Ab Initio Molecular Orbital Theory* (Wiley-Interscience, 1986), p. 18
GTST	generalised transition state theory B.C. Garrett and D.G. Truhlar, *J. Phys. Chem.*, **83**, 1052 (1979)
GUE	gaussian unitary ensemble (of random matrixes in quantum-transport studies)
GUGA	graphical unitary group approach
GVB	generalized valence bond - W. J. Hunt, P. J. Hay, and W. A. Goddard, *J. Chem. Phys.* **57**, 738 (1972)
GVB-CI	generalized valence bond-configuration interaction (wave function)
GVB-MDSA	generalized valence bond-molecular dynamics simulated annealing
GVB-PP	generalized valence bond-perfect pairing (wave function)
GVDW	generalized van der waals (a free-energy density-functional theory)
GVFF	generalized valence force field
GVV	generalised Van Vleck nearly degenerate perturbation theory
GVVPT	generalised Van Vleck nearly degenerate perturbation theory
GW	one-particle Green function(g)-screened Coulomb interaction(w)
GWB	Gopinathan-Whitehead-Bogdanovic (Fermi-hole parameters)
GWD	gaussian wave packet dynamics
GWF	generalized Wannier function
GWHF	Griffin-Wheeler-Hartree-Fock
GWP	gaussian wave packet
GW-PG	gaussian-weighted planar grid (method in calcns. of electron-momentum distributions)
GWPM	gaussian wave-packet method
GX	generalized exchange

H

HA	harmonic approximation
HAAMP	Heine-Abarenkov-Animalu (type) model potential
HAM	hydrogenic atoms in molecules
HAM/N	hydrogenic atoms in molecules, n = 2, 3, ...
HAO	(1) hybrid atomic orbital (2) hydrogenic atomic orbital
HAOM	hybrid atomic orbital model
HB	Hartree-Bogolyubov
HBJ	Hougen-Bunker-Johns (hamiltonian for molecular calcns.)
HBV	Hartree-Bogolyubov-Valatin (theory in calcn. of wave functions)
HCDW	hydrogenic continuum distorted wave (a wave function in calcns. on atomic and molecular collisions)
H-CI	Hylleraas- configuration interaction
HCPA	homomorphic cluster coherent potential approximation
HCPT	hard-core perturbation theory
HCWP	hard corrugated wall potential
HDVV	Heisenberg-Dirac-Van Vleck (hamiltonian or exchange parameter)
HE	half-electron method for open shell systems using a closed shell wavefunction - M. J. S. Dewar, J. R. Hashmall, C. G. Venier, *J. Am. Chem. Soc.*, **90**, 1953 (1968)
HF	Hartree-Fock
H-F	Hellmann-Feynman
HF MO LCAO	Hartree-Fock MO LCAO
HFB	Hartree Fock Bogolyubov
HFB SCF RPA	Hartree Fock Bogolyubov SCF random phase approximation
HFD	Hartree-Fock-dispersion (type of intermolecular potential)
HFD-B	Hartree-Fock dispersion-b (potential, where b = adjustable parameter that modifies the HFD potential)
HFD-C	Hartree-Fock-dispersion with repulsive SCF component (intermolecular potential)
HFDR	Hartree-Fock-Dirac-Roothaan
HFEGE	Hara free-electron-gas exchange (potential)
HFF	Hellmann-Feynman force approximation
HFFC	Hartree-Fock frozen core
HFG	Hartree-Fock-Gopinathan (quantum theory or wave function)
HFJ	Hartree-Fock-Jucys (in electron-correlation corrections calcn.)
HFKS	Hartree-Fock-Kohn-Sham method (density-functional theory) - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989)
HFMD	Hellmann-Feynman mol.-dynamics (method in electronic structure and geometry calcns.)
HFO	Hartree-Fock orbital
HFP	(1) Hartree-Fock (plus) Pauli (terms) (2) Hartree-Fock perturbation
HFPD	Hartree-Fock with proper dissociation (wave function)
HFPP	Hartree-Fock pseudopotential
HFPT	Hartree-Fock perturbation theory
HFR	Hartree-Fock-Roothaan
HFRSPT	Hartree-Fock Rayleigh-Schrödinger perturbation theory
HFS	Hartree Fock Slater
HFWS	Hartree-Fock-Wigner-Seitz
HG	Hermite-gaussian (functions)

HGF	Hermite gaussian function
HGTF	Hermite gaussian-type function
HHH	Henon-Heiles hamiltonian used for the study of chaotic motion, effect of anharmonic coupling in intramolecular energy redistribution (IVR) and other phenonmena - K.G. Kay and B. Ramachandran, *J. Chem. Phys.*, **88**, 5688 (1988)
HHOB	high-energy higher-order Born (approxn. for scattering calcns.)
HKS	(1) Hartree-Kohn-Sham (quantum theory) (2) Hohenberg-Kohn-Sham (quantum theory)
HLAO	high-lying antibonding orbital
HLG	Hedin-Lundqvist-Gunnarsson (spin density functional)
HLH	heavy-light-heavy (triatomic reaction system where a light atom is transfered: HL + H -> H + LH)
HLSP	Heitler-London-Slater-Pauling
HLVB	Heitler-London valence bond
HMC	hybrid Monte-Carlo
HMC SCF	hybrid multiconfiguration self-consistent field
HMI	Hornbeck-Molnar ionization (homonuclear associative ionization in atomic collisions)
HMM	half molecule model (for electron scattering by molecules)
HMO	Hückel molecular orbital
HMSA	hybrid mean spherical approximation
HNFETB	hybridization of nearly free elctrons with tightly bound states (for band-structure calcns.)
HOCO	highest occupied crystal orbital
HOCS	harmonic-oscillator coherent states
HOEF	harmonic oscillator with external field model (in collisions)
HOFF	hybrid orbital force field
HOMBA	higher-order modified Born approxn. (in potential scattering)
HOMO	highest occupied molecular orbital
HONDO	a computer program for solving the electronic Schrödinger equation - M. Dupuis, J. Rys, and H. F. King, *QCPE Program* 336
HPHF	half-projected Hartree-Fock model
HPM	(1) hole-potential model (in calcn. of mol. excited states) (2) hypervirial-perturbative method
HPPM	hole-particle potential model (in mol. excited states calcns.)
HQE	hemiquantal equations
HQM	hemiquantal mechanics (in molecular calcns.)
HRPA	higher random phase approximation
HS	hard sphere (approximation in statistical mechanics, liquid-structure, and gas-kinetic theories)
HSA	hyperspherical adiabatic (for resonances in electron-atom scattering. energy levels, and wave functions)
HSBOW	helical spin bond-order wave
HSC	hyperspherical coordinate (representation in calcns. on electron-atom scattering)
HSD	hyperspherical diabatic (wave functions)
HSF	Hiller-Sucher-Feinberg (equation for calcn. of spin densities and charge densities in molecules)
HSK	Hylleraas Scherr Knight (variational perturbation procedure)
HS-MR-CCSD	Hilbert space-multireference-coupled cluster (with) single (and) double (excitations)

HSOS-CCSD	high-spin open-shell-CCSD
HT	Herzberg-Teller (wave functions)
HTD	Hancock-Truhlar-Dykstra (potential energy surface)
HVT	hypervirial theory
HY-CI	Hylleraas-configuration interaction
HY-CIVB	Hylleraas-configuration interaction valence bond

I

IA	impulse approximation
IAM	(1) independent atom model (2) internal axis method (in calcns. of rotational excitation in atom-molecule collisions)
IAPA	independent asymptotic pair approxn. (in electronic structure)
IBC	independent binary collision (theory)
IBMOL	a computer program for solving the electronic Schrödinger equation - A. Veillard, IBM, San Jose, California.
IBS	incomplete basis set
IC-ACPF	internally contracted (multireference) averaged coupled pair functional
ICBA	improved (final-state) Coulomb Born approximation
ICC	intraatomic correlation correction
ICDW	incommensurate charge density wave
ICF-CI	interacting correlated fragment-CI (wave function) (see also SA-MCSCF)
ICSCF	internally consistent self-consistent field
ICT	impulsive collision theory: see IECT
ICVT	improved canonical variational theory
IDAF	interacting distributed approximating function (propagator, in study of wave-packet propagation)
IDI	ion dipole induced (potential term in potential energy surfaces) see also LEPS-IDI
IECT	impulsive ergodic collision theory
IECT	impulsive ergodic collision theory (for collisional energy transfer), orgininally called "impulsive collision theory" (ICT) - H.W. Schranz and S. Nordholm, *Int. J. Chem. Kinet.*, **13**, 1051 (1981)
IEH	intermediate effective hamiltonian
IEHMO	iterative extended Hückel MO
IEHT	iterative extended Hückel theory
IEM	independent electron model (for ionization in ion-atom collisions)
IEM	interstitial electron model
IEPA	independent electron pair approximation - W. Kutzelnigg in *Modern Theoretical Chemistry*, Vol. **3**, H. F. Schaefer, ed. (Plenum, New York) 1977
IERM	intermediate energy r-matrix (theory in scattering calcns.)
IEV	independent event (model in ion-atom collisions)
IF DRM	inversion-free direct recursion method (for surface electronic structure)
IFOT	invariant Fock operator technique
IFPM	independent Fermi particle model (in atom-ion impact ionization)

IGAIM	individual gauges (for) atoms in molecules
IGF	irreducible Green function
IGLO	individual gauge for localized orbitals - M. Schindler and W. Kutzelnigg, *J. Chem. Phys.*, **76**, 1919 (1982)
IHF	inhomogeneous Hartree-Fock
IIP	isotropic part of the intermolecular potential
IISCI	initial ionic state comfiguration interaction
IMBPT	interaction many-body perturbation theory
IMC	interacting monomers and clusters model
IME	Intermolecular energy
IMO	intermolecular mol. orbital
IMOA	iterative maximum overlap approximation
IMOM	iterative method of maximum overlap
IMP	Intermolecular potential energy surface
IMPPT	(1) interaction Møller-Plesset perturbation theory (2) intermolecular Møller-Plesset perturbation theory
IMPT	intermolecular perturbation theory
IMS	incomplete model space (in many-body calcns.)
INDO	intermediate neglect of differential overlap - J. N. Murrell & A. J. Harget, *Semi-empirical Self-consistent-field Molecular Orbital Theory of Molecules*, Wiley-Interscience, 1972
INDO/2-AHP	INDO/2-average hole potential
INDO/2-HP	INDO/2-hole potential
INDO/C	INDO/conformation
INDO/CS	INDO/conformation spectra
INDO/RZ	intermediate neglect of differential overlap/Ridley-Zerner
INDO/S	(1) INDO/spectroscopic approxn. (2) intermediate neglect of differential overlap screened approxn.
INDO/SP	intermediate neglect of differential overlap/spin polarization
INO	iterative natural orbital
IOC-OMEGA	inclusion of overlap charges in omega technique
IODS	identical orbitals for different spins
IOS	infinite order sudden approximation (method for reactive scattering) - G.C. Schatz, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 1
IOSA	infinite order sudden approxn. (for mol. scattering calcns.) (see IOS) - G.C. Schatz, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 1
IOS-BS	infinite order sudden-breathing sphere
IOS-1'-SAIP	infinite-order sudden approximation for strongly anisotropic interactions with $l=l'=1$final
IOS-1-SAIP	infinite-order sudden approximation for strongly anisotropic interactions with $l=1$initial
IOS-PSI	infinite-order sudden approximation for point-contact-like interactions
IOS-SAIP	infinite-order sudden approximation for strongly anisotropic interaction
IOSRR	infinite order sudden rigid-rotor approximation
IOSVR	infinite order sudden vib-rotor approximation
IP	(1) impact parameter approximation - D.R. Bates, *Atomic and Molecular Collision Processes* (Academic Press, 1962)
IPA	(1) independent-pair approximation (2) independent-particle approximation (in quantum calcns.

	on solids) (3) inverted perturbation approach (in mol. potential-energy curves calcn.)
IPM	(1) independent particle model (2) impact parameter method for separating translational from the internal motions - D.R. Bates, *Atomic and Molecular Collision Processes* (Academic Press, 1962)
IPNO	independent-pair natural orbital
IPNSO	independent-pair natural spin orbital
IPPA	independent pair-potential approximation
IPPP	inner projections (of the) polarization propagator (in calcns. on nuclear spin coupling)
IPPP	iterative Pariser-Parr-Pople method
IPWO	interface plane wave orbitals
IQG	independent quasigeminals
IR	(1) isolated resonance (2) irreducible representation (in symmetry or group theory) (3) infrared
IRC	intrinsic reaction coordinate (calcn. method) - B.C. Garrett, M.J. Redmon, R. Steckler, D.G. Truhlar, K. Baldridge, D. Bartol, M.W. Schmidt, and M.S. Gordon, *J. Phys. Chem.*, **92**, 1476 (1988)
IRC(S)	intrinsic reaction coordinate (on separatrix)
IRDO	intermediate retention of differential overlap
ISCI	initial-state configuration interaction
ISC-PEM-MO	iterative self-consistent partition of energy method and MO formalism
ISCRF	inhomogeneous self-consistent reaction field theory
ISE	iterative secular equation (method for solving the Schrödinger equation)
ISM	(1) interaction site model (in statistical mechanics of fluids) (2) intersecting spheres model (for electronic-structure calcns.) (3) inverse scattering method
ITDHO	improved time-dependent harmonic oscillator
ITFITS	improvement to forced oscillator, impulsive transfer semiclassical
ITFW	improved Thomas-Fermi-Weizaecker (model)
ITP	inner turning point (a criterion for determining between direct collisions and complex-forming collisions in classical molecular dynamics simulations)
ITPOT	improved two-parameter omega technique
IUAM	independent united atom model (in positron scattering by mols.)
IUCHF	improved uncoupled Hartree Fock
IVAP	intimate valence alternation pairs (bonding model in electronic structure calcns.)
IVM	internal vibronic mechanism (for intermolecular energy transfer)
IVO	improved virtual orbital
IWOP	integration within (an ordered product of) operators
IVR	intramolecular vibrational relaxation
IVTST	interpolated variational transitional state theory - A. Gonzalez-Lafont, T.N. Truong, and D.G. Truhlar, *J. Chem. Phys.*, **95**, 8875 (1991)

J

J(Z)CCS	(1) J(z) conserving centrifugal sudden approximation (in molecular collisions, J(z) = total angular momentum along z axis) (2) J(z)-conserving coupled states method (for rotationally inelastic atom-molecule collisions, J(z) = rotor angular momentum along z axis)
JTE	Jahn-Teller effect
JWF	Jastrow wave function
JWKB	(1) Jeffreys-Wentzel-Kramers-Brillouin (scattering potential) (2) the Jeffreys-Wentzel-Kramers-Brillouin (approximation in scattering theory) - M.S. Child, in R.B. Bernstein, ed., *Atom-Molecule Collision theory: A guide for the experimentalist* (Plenum Press, New York, 1979), p 427

K

KAM	Kolmogorov-Arnold-Moser (theorem in quantum stochasticity)
KCS	k-matrix centrifugal sudden (in mol.-scattering theory)
KDV	Korteweg-de Vries (equation for solitons)
KEDF	kinetic-energy density functional
KKR	Korringa-Kohn-Rostoker (in band structure calcn.)
KKRASA	Korringa-Kohn-Rostoker atomic-sphere approxn. (in band structure)
KKRZ	Korringa-Kohn-Rostoker-Ziman (in energy-band calcns.)
KR	Kuharski and Rossky potential - R. A. Kuharski and P. J. Rossky, *J. Am. Chem. Soc.* **106**, 5786 (1984)
KRHF	Kramers restricted Hartree-Fock
KRMC	Kinetic referenced modified Cayley method - R. S. Judson, D. B. McGarrah, O. A. Sharafeddin, D. J. Kouri, and D. K. Hoffman, *J. Chem. Phys.* **94**, 3577 (1991)
KRMP2	Kramers restricted Møller-Plesset second-order (perturbation theory)
KRSSO	kinetic referenced symmetric split operator method.
KS	Kohn-Sham method - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989)
KSA	Kirkwood superposition approximation
KS-LDA	Kohn-Sham local density approximation - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989)
KT	Koopmans' theorem - T. A. Koopmans, *Physica* , **1**, 104 (1933)
KVP	Kohn variational principle

L

L^2	square integrable (in mathematics: a class of functions which could be infinite, but whose squared values have finite integrals), (commonly applied to wave functions in electron-atom or -mol. collisions) - H.L. Royden, *Real Analysis*, 2nd Ed. (MacMillan, New York, 1968)
LACO	linearized atomic cell orbital (in energy-band calcn.)
LA(G)	least action ground
LAM	large amplitude motion

LAOM	localized atomic orbital method (in electronic structure calcn.)
LAPW	linearized augmented plane wave (for band-structure calcns.)
LASTO	linear augmented Slater-type orbital (for electronic structure)
LBF	local basis function method (for solid state band structure)
LBO	localized Born-Oppenheimer
LBW	Lennard-Jones-Brillouin-Wigner
LAM	large amplitude motion
LC	large curvature (tunnelling approximation)
LCAO	linear combination of atomic orbitals
LCAO CO	linear combination of atomic orbitals crystal orbital
LCAO LSD	linear combination of atomic orbitals-local spin density
LCAS MS	linear combination of atomic spinors-molecular spinors
LCBO	(1) linear combination of Bloch orbitals (2) linear combination of bonding orbitals
LCCA	linearized coupled-cluster approach
LCCD	linear coupled-cluster (method with) double (excitations)
LCCM	linearized coupled cluster method
LCCO	linear combination of cellular orbitals
LCCSD	linearized coupled-cluster (theory with) single (and) double (excitations) (in molecular potential calcns.)
LCCW	linear combination of configurational wave functions
LCDA MO	linear combination of donor-acceptor molecular orbital theory
LCDAO	linear combination of distorted atomic orbitals
LCDO	linear combination of diatomic orbitals
LCFC	linear combination of fragment configuration
LCFFUA	linear combination of floating functions of united atom
LCG	large curvature ground state
LCGDO	linear combination of generalized diatomic orbitals
LCGO	(1) linear combination of gaussian orbitals (2) linear combination of group orbitals
LCGTO	linear combination of gaussian type orbitals
LCGTO-DF	linear combination of gaussian type orbitals-density functional
LCGTO-LDF	linear combination of gaussian-type orbitals-local density functional
LCGTO-LSD-VWN	linear combination of gaussian type orbitals-local spin density-Vosko-Wilk-Nusair
LCGTO-MCP-LSD	linear combination of gaussian-type orbitals-model core potential-local spin density
LCHAO	linear combination of hybrid atomic orbitals
LCHOP	linear combination (of) harmonic oscillator products
LCI-CNDO	limited configuration interaction-complete neglect of differential overlap
LCI-SCSCFMO	limited configuration interaction single-configuration SCF MO
LCIF	linear combination of interacting forces
LCLO	linear combination of localized orbitals
LCM	lines of centers model (where only the relative kinetic energy directed along the line of centres is considered important for reaction *i.e.*, orbital angular momentum is factored out)
LCMBPT	linked cluster many body perturbation theory
LCMO	linear combination of molecular orbitals

LCMTO	linear combination of muffin-tin orbitals
LCMVAO	linear combination of modified valence atomic orbital
LCOAO	linear combination of orthogonal atomic orbitals
LCOPW	linear combination of orthogonalized plane waves
LCP	local complex potential (in electron-atom scattering)
LCPA	local coherent potential approximation
LCPH	localized chemical pseudopotential hamiltonian
L-CPMET	linearized coupled-pair many-electron theory
LCRA	linear combination of Rydberg orbitals
LCSPM	inear combination of symmetry-adopted products of Morse wave functions
LCSPM-HO	linear combination of symmetry-adapted products of Morse harmonic oscillator (wave functions)
LCTAO	linear combination of travelling atomic orbitals
LCVO	linear combination of valence orbitals
LDA	local density approximation (in electron-configuration calcns.) - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989)
LDF	local density functional
LDGUGA	loop-driven graphical unitary-group approach (in MC-SCF calcns.)
LDO	locked dipole approximation (in calculations of ion-molecule collision rates) - T. Su and M.T. Bowers, in *Gas Phase Ion Chemistry,* edited by M.T. Bowers, (Academic Press, New York, 1979), Vol. 1, p. 83
LDOS	local density of states
LDPO	linearly driven parametric oscillator (model in energy transfer calcns. in mol. collisions)
LDQ	Linnett double quartet (equivalent to nonpairing spatial orbital theory)
LEDO	limited expansion of diatomic overlap
LEES	local excess-electron state (a molecular-crystal wave function)
LEMAO	least energy minimal atomic orbital
LEMO	lowest empty molecular orbital (equivalent to LUMO)
LEP	local electron pair (model for intra- & intermolecular interactions)
LEPS	London, Eyring, Polanyi and Sato (potential-energy surface) (originally for $H + H_2$) - S. Sato, *J. Chem. Phys.*, **23**, 592, 2465 (1965)
LEPS+IDI	London-Eyring-Polanyi-Sato + ion dipole induced [potential]
LFCC	laboratory-frame close-coupling (for electron-molecule scattering)
LFER	linear free energy relationships
LFHO	linearly forced harmonic oscillator
LFMO	ligand field method combined with linear combination of atomic orbitals-molecular orbital method
LGM	linearized Green-function method (for electronic-structure)
LHL	light-heavy-light (triatomic reaction system where a heavy atom is transfered: $LH + L \rightarrow L + HL$)
LHM	Longuet-Higgins-Murrell approximation
LHP-RHF	Longuet-Higgins-Pople restricted Hartree-Fock method
LHSF	local hyperspherical surface functions (in quantum calcns. on reactive scattering)
LI	localization index

LJ	Lennard-Jones (potential) $V = Ar^{-n} + Br^{-m}$
LKKR	layer Korringa-Kohn-Rostoker (in interface electronic structures)
LMO	(1) localized molecular orbital (2) localized molecular spin orbital
LMTO	linear combination of muffin-tin orbitals (see also LCMTO which is the preferred acronym)
LNDO	local neglect of differential overlap
LNO	(1) localized natural orbital (2) localized natural spin orbital
LO	localized orbital
LOCADB	line-of-centers angle - dependent - barrier model
LOCV	lowest-order constrained variation
LOGMO	lowest occupied gaussian molecular orbital
LOMO	lowest occupied molecular orbital
LOPT	large-order perturbation theory
LORG	localized orbital/local origin - A. E. Hansen andT. D. Bouman, *J. Chem. Phys.*, **82**, 5035 (1985)
LOVA	lowest-order variational approxn. (for electron-phonon interactions in metals)
LPA	(1) linearized propagator approximation (2) local plasma approxn. (in calcns. of stopping powers for ions by films) (3) Löwdin population analysis
LPD	large phonon displacement (state) - Ning Lu and S. Mukamel, *J. Chem. Phys.* **95**, 1588 (1991)
LPUMP	l-fold (spin) projected unrestricted Møller-Plesset
LRCI	low-rank configuration interaction
LR-SCF	low-rank SCF
LSA	(1) linear superposition approximation (2) local space approximation
LSD(A)	local spin density (approxn.) (in electronic structure calcn.) - V. von Barth and L. Hedin, *J. Phys. C*, **5**, 1629 (1972)
LSDC	local spin density correlation (functional)
LSDF	local spin density functional
LSD-GX	local spin density functional-generalized exchange
LSD-GX-CSEP	LSD-GX-with correction of statistical exchange potential
LSD-GX-SIC	LSD-GX-with generalized exchange-self-interaction corrected
LSDSIC	local-spin-density self-interaction-correction approxn. (in total energy calcns. for atoms)
LSDX	local-spin-density (with exact) exchange
LSDXC	local-spin-density-exchange-correlation (for molecular property)
LSDXS	local-spin-density (with) screened exchange
LSDXS-SIC	local-spin-density (with) screened exchange (and) self-interaction correction
LSTH	Liu-Siegbahn-Truhlar-Horowitz (potential-energy surface)
LSW	localized spherical wave (in electronic structure calcns.)
LT	(1) Landau-Teller (form or plot for temperature dependence of rate constants) (2) Landau-Teller (model for vibrational energy transfer) - J.T. Yardley, *Introduction to Molecular Energy Transfer* (Academic Press, London, 1980) (3) Landau-Teller (potential for atom+diatom collisions)
LTH	linearized time-dependent Hartree (approxn., in calcn. of electronic properties of solids)

LTO	Laguerre-type orbital (an AO)
LUC	large unit cell semiempirical approxn. (for band structure)
LUCO	lowest unoccupied crystal orbital
LUMO	lowest unoccupied molecular orbital
LVM-ST	least-squares variational method (involving only) square-integrable (test functions) (for wave functions in scattering)
LZ	Landau-Zener (model for probability of hopping from one electronic surface to another at an avoided crossing) - *eg,* H. Eyring, J. Walter and E.W. Kimball, *Quantum Chemistry* (Wiley, New York, 1944) pp. 326–330

M

MAB	molecular Aharonov-Bohm (electronic-structure effect)
MACS	modified atomic charge superposition (in calcns. on atom-surface scattering potentials)
MAGW	momentum-averaged gaussian-weighted (method in calcns. of electron-momentum distributions)
MAM	modified atoms (in) molecules
MAMO	multiparameter alternant molecular orbital
MAO	modified atomic orbital
MAPW	modified augmented plane wave
MASP-HMO	mutual additive substituent parameter-Hückel molecular orbital
MB-SAPT	many-body symmetry-adapted perturbation theory
MBBSIS	mixed-basis band-structure interpolation scheme
MBDOS	many-body density of states
MBE	many-body expansion (in molecular potential energy surface calcn.)
MBESHO	maximum bond-energy symmetry hybrid orbital
MBGF	many-body Green function
MBP	mixed basis pseudopotential (method for electronic-structure)
MBPT	many-body perturbation theory
MBPTn	many-body perturbation theory of order n. (= MPPTn = MPn) - H. P. Kelly, *Phys. Rev.* **131**, 684 (1963)
MBPV	mixed-basis potential variation (for electronic-structure calcn.)
MBRSPT	many-body Rayleigh-Schrödinger perturbation theory
MBS	minimum basis set wave function
MBSP	molecular basis set for parameterization (of a semiempirical model).
MBSCI	minimum basis set configuration interaction
MBT	many-body theory
MC	(1) McLean-Chandler basis set (2) Monte-Carlo method - J.M. Hammersley and D.C. Handscomb, *Monte-Carlo Methods* (Metheun, London, 1964); Y.A. Shrieder, *The Monte-Carlo Method: the Method of Statistical Trials* (Pergamon Press, Oxford, 1966)
MCBS	monomer centred basis set (in quantum calculations of dimers)
MCC	(1) molecular coupled-cluster (method) (2) multiple curve crossing
MCCHF	multiconfiguration coupled Hartree-Fock
MC CI	multiconfigurational configuration interaction
MC CMO	multiconfigurational complex molecular orbital
MCDF	multiconfiguration Dirac-Fock

MCDF-EAL	multiconfiguration Dirac-Fock-extended average level (for energy levels and wave functions calcn. for atoms)
MCDF-OL	multiconfiguration Dirac-Fock optimum level
MCDW	matrix continuum distorted wave
MC-DWBA	multichannel distorted wave Born approxn.
MCE	multichannel Eikonal (method for scattering calcns.)
MCEB	multiconfiguration energy bound
MCEB-NEV	multiconfigurational energy bound-natural eigenvalue method
MCEP	multiconfigurational electron propagator (in ionization potential calcns.)
MCF	mutually consistent field method (in calcns. on intermolecular interactions)
MCGR	Monte-Carlo renormalization group (see MCRG below)
MCHF	multiconfiguration Hartree-Fock
MCHF-BP	multiconfiguration Hartree-Fock Breit-Pauli
MC-INDO	molecular cluster-intermediate neglect of differential overlap
MCLR	multiconfigurational linear response (an MC-SCF method)
MCM	multiconfigurational (variation of) moments (for MO correlation diagrams calcn.)
MC-MBPT	multiconfiguration many-body perturbation theory
MCMP	modified corrugated Morse potential
MCNDO	modified complete neglect of differential overlap
MCOPM	multiconfiguration optimized potential model
MCP	(1) Marcus - Coltrin path (2) model core potential
MCP2P	multiconfigurational particle-particle propagator
MCPA	molecular coherent-potential approximation
MCPF	self-consistent field modified coupled-pair functional (method in CI calcns.)
MCPF+R	modified coupled-pair functional (method with) relativistic (correction)
MCPI	Monte-Carlo path integration
MCPN	matrix coherent potential approximation
MCPSAG	Marcus-Coltrin-path semiclassical adiabatic ground-state (transmission coeffs.)
MCQDA	multichannel quantum defect analysis
MCQDT	multichannel quantum defect theory
MCRG	Monte-Carlo renormalization group
MCRHF	multiconfigurational relativistic Hartree-Fock
MCRPA	multiconfigurational random phase approxn.
MCRRPA	multiconfiguration relativistic random phase approxn.
MCSCF	multi-configuration self-consistent field theory.
MC-SCF	(1) Monte-Carlo self-consistent-field (2) multiconfiguration self-consistent field method for solution of the electronic Schrödinger equation, involving simulataneous optimization of molecular orbitals and linear combinations of configurations
MCSCO	multiconfiguration self-consistent orbital
MCSCRF	multiconfiguration self-consistent reaction field
MC-SEA	multichannel static-exchange approximation
MCSTEP	multiconfigurational spin-tensor electron propagator
MCSX	multiconfiguration single excitation
MCTDH	multiconfigurational time-dependent Hartree (theory)
MCTDHF	multiconfiguration time-dependent Hartree-Fock
MC-TD-SCF	multiconfiguration-time dependent-self-consistent field

MCTI	multiconfiguration thermodynamic integration - T.P. Straatsma & J.A. McCammon, *J. Chem. Phys.*, **95**, 1175 (1991)
MCWF	Monte-Carlo wave function (method in study of dissipative processes in quantum optics)
MCY	Matsuoka-Clementi-Yoshimine (potential function) - G.C. Lie, E. Clementi, and M. Yoshimine, *J. Chem. Phys.*, **64**, 2314 (1976)
MCZDO	many center zero differential overlap
MD	molecular dynamics - M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids* (Oxford Science Publications, Oxford, 1990); D.M. Hirst, *A Computational Approach to Chemistry* (Blackwells Scientific, Oxford, 1990)
MDC	molecular dynamic coordinates
MDI	modified dipole interaction(model for mol.-polarizability calcn.)
MD/MC-CEM	molecular dynamics/Monte-Carlo-corrected effective medium
MDS	matrix-diagonalization sudden approximation (for atom surface scattering calcns.)
MDW	(1) mixed density wave (2) multichannel distorted wave (Born approxn.)
MEAN	multipole-extracted adiabatic-nuclei (for electron-molecule collisions)
MECI	(1) monoexcited configuration interaction (2) multielectron configuration interaction
MECOP	modified electron correlation polarization (potential)
MEDO	multipole expansion of diatomic overlap approximation
MEDOC	multipole expansion defined (on) one center (a wave function in calcns. on atomic and molecular collisions)
MEG	(1) mixed exponentially generated (wave function) (2) modified electron gas (quantum calcn. method)
MEG4	multiexponentially generated 4 (wave functions)
MEHT	modified extended Hückel theory
MEMPT	many-electron many-photon theory (in dynamic-polarizability calcns. for atoms and ions)
MEMTB	many-electron molecule tight-binding (for electronic structures)
MEP	(1) matrix effective potential (for scattering calcns.) (2) molecular electrostatic potential (3) minimum energy path (usually taken to be the "intrinsic reaction path") - eg., S. Glasstone, K.J. Laidler, and H. Eyring, *The Theory of Rate Processes* (McGraw-Hill, New York, 1941)
MERP	minimum energy reaction path - see MEP (3)
MERT	modified effective-range theory (for electron-mol. scattering)
MESQUAC-MO	mixed electrostatic quantum chemical calculation-mo
MET	(1) many electron theory (for singlet ground state) (2) multichannel Eikonal theory (in atom electron-impact excitation)
MEUG	minimum energy uncertainty gaussian (wave packets)
MF	muffin tin (potential energy function)
MFA	(1) molecular-field approximation (2) mean field approximation

MFC	multiconfigurational frozen core (approxn. for electron-atom scattering calcns.)
MFE	modulated free electron orbital method
MFP	magnetic field perturbative (method)
MGA	modified Glauber approxn. (in atom-particle scattering)
MG-FSGO	multiple gaussian-floating spherical gaussian orbital method
MGVB	modified generalized valence bond
MHA	Mott-Hubbard-Anderson (model in band-structure calcns.)
MHW MO	Mulliken-Helmholz-Wolfsberg molecular orbital
MIA	multiplicative integral approxn. (in 2-electron integral calcn.)
MIAM	modified independent-atom model (for electron-molecule scattering)
MIDI*	split valence plus polarization function (basis set)
MIDI-N	split-type contracted GTO basis set (n = 1,2,3, or 4)
MIEHM	modified iterative extended Hückel method
MIES	maximum ionicity excited state (model in energy calcn. of mols.)
MIH	method of intermediate hamiltonians
MIM	(1) molecules in molecules (2) multipole-induced-multipole model
MINDO	modified intermediate neglect of differential overlap - T. Clark, *A Handbook of Computational Chemistry: A Practical Guide to Chemical Structure and Energy Calculations* (Wiley, New York, 1985)
MINDO/3	modified intermediate neglect of differential overlap, version3 - a method for solving the electronic Schrödinger equation semiempirically - M. J. S. Dewar, R. C. Bingham, & D. H. Lo, *J. Am. Chem. Soc.* **97**, 1285 (1975) QCPE program 506, QCPE Bull., **6** (1986)
MINDO/3L	modified intermediate neglect of differential overlap, version3, for limited electrons
MINDO/SR	MINDO s=overlap integral r=internuclear distance
MINI-N	minimal-type contracted GTO basis set (n= 1,2,3, or 4)
MIOSA	modified (rotational) infinite order sudden approxn.
MITFITS	modified ITFITS
MLCT	metal-to-ligand charge-transfer (state)
MM	molecular mechanics - M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids* (Oxford Science Publications, Oxford, 1990); D.M. Hirst, *A Computational Approach to Chemistry* (Blackwells Scientific, Oxford, 1990)
MM2	a computer program using molecular mechanics - N. L. Allinger, *J. Am. Chem. Soc.* **99**, 3279 (1977)
MMC	molecular mechanics for clusters model - C.E. Dykstra, *J. Am. Chem. Soc.*, **111**, 6168 (1989)
MMCDF	multichannel multiconfiguration Dirac-Fock method
MMSV	Morse-Morse-spline-Van der Waals (potential function)
MNDO	modified neglect of diatomic overlap - a method for solving the electronic Schrödinger equation semiempirically , which implements a version of the NDDO (neglect of diatomic differential overlap) scheme - M. J. S. Dewar and W. Thiel, *J. Am. Chem. Soc.* **99**, 4907 (1977)
MNDOC	modified neglect of diatomic overlap with a perturbative treatment of electron correlation, a computer program for obtaining a semiempirical solution to the electronic

	Schrödinger equation - W. Thiel, *J. Am Chem. Soc.* **103**, 1413 (1981)
MNDOD	modified neglect of diatomic overlap with d atomic orbitals - W. Thiel, A. A. Voityuk, *Theoret. chim. Acta*, **81**, 391 (1992)
MNDO/H	MNDO for H-bonded systems
MNDO-HE	modified neglect of differential diatomic overlap-half electron
MNDO/M	modified MNDO
MNDO-PM3	modified neglect of diatomic overlap-parameterization method 3 - J. J. P. Stewart, *J. Comput. Chem.*, **10**, 209 (1989)
MO	molecular orbital
MOA	maximum overlap approximation
MOAG	MINDO optimized adjusted geometries
MOBI	MO bond index
MOBK	modified Oppenheimer-Brinkman-Kramers (approxn. in calcns. on atomic and molecular collisions with ions)
MOCD	molecular orbital correlation diagram
MOCED	molecular orbital constrained electron diffraction method
MOCETGAO	molecule-optimized contracted even-tempered gaussian atomic orbital
MOCIC	MO constraint of interaction coordinates
MOEXP	Morse oscillator exponential repulsion potential
MOLCAS	a computer program for solving the electronic Schrödinger equation - G. Karlstrom, P.-A. Malmquist, B. O. Roos, A. J. Sadlej, and P. O. Widmark, MOLCAS-1 (University of Lund and Lund Institute of Technology, Sweden, 1990)
MOLECULE	a computer program for solving the electronic Schrödinger equation.
MOLVIB	a computer program for normal coordinate treatment of molecular vibrations - T. Sundius, *J. Mol. Struct.* **218**, 321 (1990)
MOM	(1) maximum overlap method (2) modified operator method (for energy-level calcns.)
MOMM	a hybrid method combining molecular orbital and molecular mechanics techniques - J. Kao and N. L. Allinger, *J. Am. Chem. Soc.*, **99**, 975 (1977)
MOMO	maximum overlap molecular orbital
MONSTERGAUSS	a computer program for solving the electronic Schrödinger equation (later developed as MUNGAUSS) - M. R. Peterson and R. A. Poirier, Chemistry Department, Memorial University of Newfoundland, St. John's, Newfoundland, Canada
MOPAC	a computer program for obtaining a semiempirical solution to the electronic Schrödinger equation - J. J. P. Stewart, *QCPE*, Program 455 (1983)
MOPW	modified orthogonalized plane wave
MORBID	Morse oscillator-rigid bender internal dynamics (hamiltonian in rotational-vibrational energy levels calcn.)
MORT	molecular orbital resonance theory
MOSHO	maximum overlap symmetry hybrid orbital
MOSMO	maximum overlap symmetry molecular orbital
MOSO	maximum overlap symmetry orbital (MO for mols.)
MOT	multistate orbital treatment
MOVB	MO-valence bond
MOVBET	molecular orbital (into) valence bond exponential transformation

MOVFF	modified orbital valence force field
MOVS	molecular orbital valence state
MP	Markovian process
MP2	Møller-Plesset second-order perturbation theory
MP2(FU)	MP2(full) inner-core electrons are included in the approxn.
MP2(FC)	MP2(frozen core) only (outer) valence electrons included in the approximation
MP3	Møller-Plesset third-order perturbation theory
MP4(DQ)	Møller-Plesset perturbation treatment to fourth order in the space of double and quadruple substitutions
MP4(SDTQ)	Møller-Plesset (perturbation theory to) 4th order with single, double, triple and quadruple (excitations)
MPA	Mulliken population analysis
M-PCILO	modified PCILO
MPDS	moment-polarized Dirac-Slater
MPHF	maximally paired Hartree Fock
MPI	(1) modified perturbation iteration (2) many-particle interaction
MPn	Moller-Plesset perturbation theory of order n for electron correlation - C. Moller and M. S. Plesset, *RevPhys.* . **46**, 618 (1934)
MPNO	molecular pair natural orbital
MPnSD	Moller-Plesset perturbation theory of order n including single and double excitations
MPnSDQ	Moller-Plesset perturbation theory of order n including single, double, and quadruple excitations
MPnSDQT	Moller-Plesset perturbation theory of order n including single, double, quadruple, and triple excitations
MPO	modified polarized orbital
MPOBK	model potential Oppenheimer-Brinkman-Kramers
MPPA	most probable path approach
MPPT	Møller-Plesset perturbation theory
MPPTn	Moller-Plesset perturbation theory of order n
MP-QMC	model potential-quantum Monte-Carlo
MPT	(1) matrix perturbation theory (2) mean passage time (theory) - G. Weiss, *Adv. Chem. Phys.*, **13**, 1 (1967)
MPW	multiple plane wave (in electronic-property for metals)
MQDT	multichannel quantum defect theory
MQW	multi(quantum well) (electronic structure as in superlattices of semiconductor films)
MR-ACPF	multireference-averaged coupled pair functional
MRBW	multireference Brillouin-Wigner
MRCC	multireference coupled cluster
MR-CCI	multireference contracted configuration interaction
MR-CCSD	multireference-CCSD
MRCEPA	multireference coupled-electron-pair approxn.
MR-CEPM	multireference-coupled electron pair method
MR-CI	multireference-CI
MR-CI-PS	multireference-CI-perturbatively selected
MRD-CI	(1) multireference determinant configuration interaction (2) multireference double-excitation configuration interaction
MRINDO	modified Rydberg intermediate neglect of differential overlap
MRINDO/S	modified Rydberg intermediate neglect of differential overlap/spectral(or screening)

MRLCC	multireference linearized coupled cluster
MR-L-CEPM	multireference-linearized-coupled electron pair method
MR-MBPT	multireference-many-body perturbation theory
MR-MP	multireference Møller-Plesset (perturbation theory)
MR-MP2	multireference Møller-Plesset for two-configuration wave function
MR-RWA	many resonance-rotating wave approxn.
MR-SAC	multireference symmetry-adapted-cluster (quantum theory or wave function for molecular calcns.)
MRSD-CI	multireference single and double excitation CI
MRSD-CI+D	MRSD-CI (with) Davidson correction
MRSD-CI+P	MRSD-CI (with) Pople correction
MRSPT	modified Rayleigh-Schrödinger perturbation theory
MS	(1) molecular spinor (2) multiple scattering
MS X(ALPHA)	multiple-scattering X(alpha) exchange method
MSA	(1) many-trajectory semiclassical approxn. (in at.-collision theory) (2) mean spherical approximation.
MSAE	multistate atomic expansion (method for at. collisions)
MSC	molecular simulated crystal method (in Compton profile calcns.)
MSCE	modified semiclassical exchange (aproxn. in scattering calcns.)
MSM	(1) multiple-scattering model (2) multishell method
MSMA	Murrell-Shaw-Musher-Amos exchange perturbation theory
MSMO	multiple scattering molecular orbital method (also known as X(alpha) scattered-wave)
MSO	(1) maximum similarity (spin) orbital (2) modified Slater orbital (3) molecular spin orbital
MSPO	method of successive partial orthogonalizations
MS-RC(XI)	multiple scattering relativistic correlated (calcn. method)
MS-RHFR	momentum-space restricted Hartree-Fock-Roothaan
MST	multiple scattering theory
MSV	Morse-spline-Van der Waals (interatomic potential)
MSW-X(ALPHA)	multiple scattered wave-SCF-X(alpha)
MT	muffin-tin (potential)
MTA	(1) momentum translation approximation (2) muffin-tin approxn. (of potentials in quantum calcns.) (3) many trajectories approach (4) mean trajectory approximation - S. Sawada, A. Nitzan, and H. Metiu, *Phys. Rev. B*: Condens. Matter **32**, 851 (1985)
MTBA	modified tight-binding approxn.
MTGF	muffin-tin Green function
MTGLE	molecular time scale generalized Langevin equation (in statistical-mech. calcns. on reactions)
MT-MSX(ALPHA)	muffin tin-multiple scattering statistical exchange
MTO	muffin-tin orbital
MTX(ALPHA)	muffin-tin X(alpha) statistical exchange
MUBFF	modified Urey Bradley force field
MUCA	molecular unit cell approxn.
MUCS	minimum-uncertainty coherent states (wave functions)

MULAP	Mulliken approximation
MUNGAUSS	a computer program for solving the electronic Schrödinger equation - R. A. Poirier, M. R. Peterson, and A. Yadav, Chemistry Department, Memorial University of Newfoundland, St. John's, Newfoundland, Canada
MUSIC	multiple signal classification method
MVFF	modified valence force field
MVO	modified virtual orbital
MVT	molecular virial theorem - K. V. Darvesh and R. J. Boyd, *J. Chem. Phys.* **87**, 5329 (1987)
mVTST	microcanonical variational transitional state theory - (eg., R.G. Gilbert and S.C. Smith, *Theory of Unimolecular and Recombination Reactions* (Blackwells Scientific, Oxford, 1990)
MWDA	modified weighted density approximation - A. R. Denton and N. W. Ashcroft, *Phys. Rev. A* , **39**, 4701 (1989)
MWH	Mulliken-Wolfsberg-Helmholz (molecular orbital method)
MWP	moving wave packet (model for molecular scattering)
MZDO	modified zero differential overlap

N

NAO	natural atomic orbital
NAP	nearest approach point
NAPA	numerical analytical propagator algorithm - M. Tuckerman, G. Martyne, and B. J. Berne, *J. Chem. Phys.* **93**, 1287 (1990)
NBMO	nonbonded molecular orbital
NBO	natural bond orbital
NCC	natural collision coordinates - R.A. Marcus, *J. Chem. Phys.*, **45**, 4500 (1966)
NCMET	nonclosed shell many electron theory
ND	nonlinear dynamics
NDC	nuclear dynamic coordinates
NDDO	neglect of diatomic differential overlap (approximation used for solution of the electronic Schrödinger equation) - J. N. Murrell & A. J. Harget, *Semi-empirical Self-consistent-field Molecular Orbital Theory of Molecules*, Wiley-Interscience, 1972
NDLM	nondiagonal Lagrange multiplier
NDO	neglect of differential overlap
NDOL(ND0-l)	neglect of differential overlap-azimutal quantum number (of valence AO's)
NDWBA	normalized distorted-wave Born approximation
NEBD	nonequilibrium Brownian dynamics
NEMD	nonequilibrium molecular dynamics - (eg) M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids* (Oxford Science Publications, Oxford, 1990), Chapter 8
NEMO	nonempirical molecular orbital
NEVE	nonempirical valence electron method
NFE-TB	nearly-free-electron tight-bonding (for electronic structure)
NHF	(1) nonrelativistic numerical Hartree-Fock (2) numerical Hartree-Fock
NHF(FC)	nonrelativistic numerical Hartree-Fock (frozen-core potential)
NHFPT	nonorthogonal Hartree-Fock perturbation theory

NHO	natural hybrid orbital
NHOMO	next highest occupied molecular orbital
NI	nonadiabatic interaction
NIEM	noniterative integral equation method
NISTO	non-integer Slater-type orbital
NITM	normalized irreducible tensorial matrix
NLDA	nonlocal density approxn.
NLDF	nonlocal density functional
NLMO	(1) natural localized molecular orbital (2) nonorthogonal localized molecular orbital
NLRT	non linear relaxation time
NLS	nonlinear Schrödinger equation
NL-SCF	nonlocal (density functional)-self-consistent field
NLSD	nonlocal spin density (functional theory)
NLSLE	nonlinear Schrödinger-Langevin equation
NLXC	nonlocal exchange correlation (potential)
NMCSCF	numerical multiconfiguration self-consistent field
NMO	natural magnetic orbital
NMPIMC	normal mode path integral Monte-Carlo
NNBI	neglect of nonbonded interactions
NNDO	neglect of nonbonded differential overlap
NO	natural orbital
NOEL	number of overlapping electrons
NOLMOs	nonorthogonal (strictly) local molecular orbitals
NOONS	natural orbitals occupation numbers
NPA	natural population analysis (for electron configuration of molecules)
NPSO	nonpaired spatial orbital
NPSSMO	nonpaired spin spatial molecular orbital
NRCT	near-resonance charge transfer
NRHF	numerical restricted Hartree-Fock
NRIOSA	nonreactive infinite-order sudden approxn.
NRO	natural reaction orbital
NRRW	nonreversible random walk
NSCF	non-self-consistent field
NSE	nonlinear Schrödinger equation
NSH	normalized spherical harmonic (hamiltonian)
NSO	natural spin orbitals
NTB	nonorthogonal tight-binding
NTO	natural transition orbital method (for excited states)
NVP	Newton variational principle
NZRPA	normalized zero-range potential approxn.

O

OAO	orthogonalized atomic orbital
OBE	optical Bloch equations (combining the Schrödinger and Maxwell equations for the interaction of a molecule with a radiation field - J Akerhalt and B. Shore, *Phys. Rev.*, **A16**, 277 (1977)
OBK	Oppenheimer-Brinkman-Kramers (approxn. in atom-ion electron-exchange calcns.)
OBK2	second-order Oppenheimer-Brinkman-Kramers
OBK3	third-order Oppenheimer-Brinkman-Kramers
OBS-MCSC	optimized basis set-multiconfiguration spin coupled
OCAMS	orbital correspondence analysis in maximum symmetry
OCBSE	orthogonality constrained basis set expansion prodedure

OCCSD	open-shell coupled-cluster (with) single (and) double (excitations)
OCD	overlapping charge density (model in electronic structure)
OCE	one-center expansion (SCF MO method)
OCE-DF	one-center expansion Dirac-Fock
OCEE	overlap corrected electronegativity equalization
OCH	Ochkur (approxn. in electron-atom scattering calcns.)
OCOS	orbital charge-ordering state
OCSC	orbital-charge-self-consistent (in electronic state calcn.)
OCT	optimized cluster theory
ODC	optimized double configuration
ODCPA	off-diagonal (disorder) coherent-potential approxn.
ODFS	optimized Dirac-Fock-Slater
ODLRO	off-diagonal long-range order
ODP	optical deformation potential
OEAO	overlap enhanced atomic orbital
OEDM	one-electron diatomic molecule method
OEH	one-electron Hamiltonian (quantum method)
OEMO	one electron molecular orbital
OEMTB	one-electron molecular tight-binding (for electronic structure)
OEO	overlap-enhanced orbital
OEP	optimized effective-potential (quantum method)
OEP-SIC	optimized effective potential self-interaction correction
OFPT	operator form (of) perturbation theory
OHAO	orthogonalized hybrid atomic orbital
OHCE	one-and-a-half-centered expansion (method for calcns. on charge transfer in ion-atom scattering)
OHFS	optimized Hartree-Fock-Slater
OIP	optimized inner projection (method for molecular property calcns.)
OLCAO	orthogonalized linear combination of atomic orbitals
OLDRO	off-diagonal long-range order
OLPA	orbital local plasma approxn. (in stopping power calcn. for ions by films)
OMEGA	method in molecular orbital calculations
OMO	(1) orthogonalized magnetic orbital (2) orthonormal molecular orbital
OMP	optimized model potential
OMPW	orthogonalized modulated plane wave (wave function)
OMTP	overlap-multipole-expansion procedure
ONCV	orthonormality constrained variation (quantum method)
OODR	optical-optical double resonance
OP	overlap population
OPCI	optimum path for intrinsic coordinate
OPCI	optimum path for intrinsic coordinate
OPGF	one-particle Green function
OPHF	orbital-polarized Hartree-Fock
OPLS	optimized potentials for liquid simulations - W.L. Jorgensen and J. Tirado-Ries, *J. Am. Chem. Soc.*, **110**, 1657 (1988)
OPM	optimized potential model
OPT	open-shell perturbation theory
OPW	orthogonalized plane wave
OREM	off-ridge eigenvector minimization
OREMWA	off-ridge eigenvector minimization with annealing
ORPA	optimized random phase approximation
ORPP	optimized relativistic pseudopotential

ORSTB	overlap-reduced semiempirical tight-binding
OS	overlapping spheres (method)
OSCCM	open-shell coupled-cluster method (in electronic property calcn.)
OSM	overlapping sphere model
OSMSX(ALPHA)	overlapping-sphere multiple-scattering X(alpha)
OSRHF	open-shell restricted-Hartree-Fock
OSRSCF	open-shell restricted SCF
OTA	optimal trajectory approach
OTF	optimized Thomas-Fermi theory
OVB	orthogonalized valence bond method
OVC	optimized valence configuration
OVFF	orbital valence force field
OVGF	outer valence Green function method (for ionization-energy calcns.) - L. S. Cederbaum, *Theor. Chim. Acta* , **31**, 139 (1973); *J. Phys. B,* **8**, 290 (1975)
OVMO	occupied valence-type mol. orbital
OVOS	optimized virtual orbital space approximation (for correlated calcns.)
OWVP	outgoing wave variational principle

P

PAM	periodic Anderson model
PAO	(1) polarized atomic orbital (2) pseudo-atomic orbital
PB	polarized Born
PBO	polarized Born-Oppenheimer
PC	phase conjugator
PC-TD-SCF	perturbation-corrected time-dependent SCF
PCA	principal-component analysis (for determining which variables are most important in complex systems. Used in analysis of statistical data, complex kinetic systems, *etc*)
PCCS	phase-corrected coupled-states (approxn. for scattering calcns.)
PCDW	Pluvinage continuum distorted wave (a wave function in calcns. on atomic and molecular collisions)
PCDW	projectile continuum distorted wave (in atom collision calcns.)
PCEM	point-charge electrostatic model
PCGVB	pairwise correlated generalized valence bond method
PCI	perturbative configuration interaction
PCID	point-charge-induced-dipole (model, in crystal-field-splitting)
PCILO	perturbative configuration interaction using localized orbitals
PCILOCC	PCILO for crystal calculations
PCMO	precanonical molecular orbital
PCO	perturbational crystal orbital
PCOP	positron correlation polarization (potential)
PDDO	projection of diatomic differential overlap
PDF	pair distribution function (mainly in statistical mechanics of fluids) - *eg,* D.A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976)
PDI	point dipole interaction (model for mol.-polarizability calcns.)

PE	(1) potential energy (2) promotion energy
PEDM	perturbation expansion (of the) density matrix
PEMA	pseudoeffective mass approxn. (for impurity energy levels in semiconductors)
PEMC	pair-excitation multiconfiguration (type of wave function)
PEOE	partial equalization of orbital electronegativity (model)
PEP	Pauli exclusion principle.
PERTCI	perturbational configuration interaction
PES	potential energy surface
PFC	polarized frozen core approximation
PFEO	perimeter free electron orbital
PFOE	polarized first-order exchange
PGF	pseudo Green function
PGL	(statistical) power-gap law (in rotational energy transfer: also called SPL) - T.A. Brunner, N. Smith, A.W. Karp, and D.E. Pritchard, *J. Chem. Phys.*, **74**, 3324 (1981)
PGO	phantom group orbital
PHBTD	(number)projected-Hartree-Bogolyubov Tamm-Dancoff(quantum method)
PHD	p-helicity decoupling scheme (p=momentum)
PHF	(1) periodic Hartree-Fock (2) perturbative Hartree-Fock (3) projected Hartree Fock
PHF-OCE	perturbative Hartree-Fock one-center expansion
PHFS	perturbative Hartree-Fock-Slater
PHO	pseudoharmonic oscillator
PIA	peaking impulse approxn. (for electron-exchange collisions)
PIB	potential induced breathing (model in electronic-structure studies in superconductors)
PIHMC	path integral hybrid Monte-Carlo
PIMC	path-integral Monte-Carlo
PIMD	path integral molecular dynamics
PIMS	photoionization mass spectrometer
PIVCDW	phase integral variational continuum distorted wave
PLO	partially localized orbital
PM3	modified intermediate neglect of differential overlap - parameterization method 3 - a computer program for obtaining semiempirical solutions to the electronic Schrödinger equation - J. J. P. Stewart, *J. Comput. Chem.* **10**, 209 (1989)
PMC-SCF	pair multiconfiguration-SCF (with electron pair optimization)
PMF	potential of mean force (in statistical mechanics of liquids) - *eg* D.A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976)
PMHB	pumped-mode-heat bath model
PMO	(1) perturbation molecular orbital theory - M. J. S. Dewar and R. C. Dougherty, *The PMO Theory of Organic Chemistry*, Plenum Press, New York, 1975 (2) perturbed Morse oscillator (model potential)
PMP2	(spin)projected Møller-Plesset second-order (perturbation theory)
PMP4	(spin) projected Møller-Plesset fourth-order (perturbation theory)
PMPO	perturbed Morse Pekeris oscillator (model potential)

PNDDO	partial neglect of diatomic differential overlap
PNDO	partial neglect of differential overlap
PNO	(1) pair natural orbital (2) pseudonatural orbital
PNO-CE	pseudonatural orbital-configuration expansion
PNO-CEPA	pseudonatural orbital-coupled electron pair approximation
PNO-CI	pseudonatural orbital-configuration interaction
PO	(1) polarization orbital (2) projection operator (3) pseudo-orbital
PO-DVR	potential optimized-discrete variable representation
PO-DVR-REV	potential optimized-discrete variable representation-ray eigenvector
PO-MO	pars orbital-MO
POA	Peierls-Onsager approxn. (in electronic structure calcns.)
POAV	π-orbital axis vector analysis (electronic-structure model)
POCH	polarized Ochkur
POCI	parent orbital configuration interaction
POCV	pair orthogonality constrained variation method
PODS	periodic orbit dividing surface (which separates reactive and non-reactive trajectories) - E. Pollak, M.S. Child, and P. Pechukas, *J. Chem. Phys.*, **72**, 1669 (1980)
POL-CI	polarization configuration interaction
POLYATOM	a computer program for obtaining solutions to the electronic Schrödinger equation - D. B. Newmann, H. Basch, R. L. Korregay, L. C. Snyder, J. Moskowitz, C. Hornback, and P. Liebman, *QCPE* Program 199
POLYRATE	a computer program for calculating rate coefficients by D.G. Truhlar et al. Version 5 is described in Quantum chemistry program exchange Bulletin, **13**, 28-29 (1993)
POM	projection-operator method
POPW	partially orthogonalized plane wave
POS	points-on-a-sphere (repulsion potential model, a variant of the valence-shell-electron pair-repulsion theory)
PP	(1) Pariser Parr (2) polarization propagator
PP-MRD-CI	pseudopotential-multireference double excitation-CI
PPBA	plane-wave plane-wave Born approximation
PPGVB	perfect pairing generalized valence bond (wave function)
PPM	pair population method
PPMSVX	pseudopotential multiple-scattering valence-exchange
PPP	(1) Pariser-Parr-Pople method for obtaining semiempirical solutions to the electronic Schrödinger equation - R. G. Parr, *The Quantum Theory of Molecular Electronic Structure* Benjamin, New York, 1963 (2) positron polarization potential
PPPM	particle-particle and particle-mesh (method for fluid simulation of ionic systems) - J.W. Eastwood, R.W. Hockney and D Lawrence, *Comput. Phys. Comm.*, **19**, 215 (1980)
PPT-MCF	pseudo-polarization tensor-mutually consistent field (for molecular interactions)
PRDDO	partial retention of diatomic differential overlap
PRMM	propagative r-matrix method (reactive electron-molecule scattering)
PRMO	partially restricted molecular orbital
PRS	perturbed rotational state (method for ion-molecule collisions)

PS	pseudospectral (method in quantum scattering) - S.A. Orszag, *Studies Applied Math.*, **51**, 253 (1972); D. Gooylieb and S.A. Orszag, *Numerical Analysis of Spectral Mehods, Theory and Application* (SIAM, Philadelphia, 1977)
PSA-CCSD	partially spin adapted-CCSD
PSCA	periodic small-cluster approach (a many-body technique in electronic-structure calcns.)
PSCC	pseudostate close coupling
PSCI	(1) partitioned (orbital hessian) super-configuration interaction (2) pseudo configuration interaction
PSEP	polyhedral skeletal electron pair (for metal clusters)
PSHF	pseudospectral Hartree-Fock
PSMO	pseudo MO
PSNO	pseudonatural orbital
PSOM	pseudostate optical model
PSRG	position-space renormalization group (for density-of-states calcns.)
PSS	perturbed stationary state
PSSCF	pseudo SCF
PSSR	perturbed stationary state with relativistic effects
PST	phase space theory
PT	perturbation theory
PT2D	second-order perturbation theory (with) diagonal (part of Fock matrix)
PT2F	second-order perturbation theory (with) Fock (matrix)
PTGF	perturbative-type Green function
PTM	perturbation trajectory method (in gas-surface collision dynamics)
PTNO	perturbation theory natural orbital
PTSPGF	perturbative-type single-particle Green function
PUCHF	perturbed uncoupled Hartree-Fock
PUHF	(spin)-projected unrestricted Hartree-Fock
PUHFS	projected unrestricted-Hartree-Fock-Slater
PUMP	(1) projected unrestricted Møller-Plesset (2) pure (alpha-spin-state) unrestricted Møller-Plesset nth-order (wave function)
PV-RR	perturbational-variational-Rayleigh-Ritz (matrix method in mol. calcns.)
PVB	projected valence bond
PVB-CSF	projected valence bond-configuration state function
PVO	pseudovalence orbital
PW-TDSE	plane wave-time dependent Schrödinger equation
PWBA	plane wave Born approximation
PWBA-BCPR	PWBA with binding-energy, Coulomb-deflection, polarization, and relativistic effects
PWBA-C	Coulomb corrected plane wave Born approxn.
PWBA-C-EX	Coulomb corrected plane wave Born approxn. (with) exchange
PWBA-EX	plane wave Born approxn. (with) exchange
PWBA-R	plane wave Born approxn. with relativistic effects
PWBE	plane-wave Born approxn. with exchange
PWEM	partial-wave-expansion method (in electron scattering calcns.)
PWETF	plane-wave electronic translational factor (ion-atom collisions)

PWFB	plane-wave first Born
PWG SCF	plane-wave gaussian self-consistent field method
PWHF	plane-wave Hartree-Fock
PWIA	plane-wave impulse approximation
PWMC	plane wave based momentum cutoff procedure - N. Makri, *Chem. Phys. Lett.*, **159**, 489 (1989)
PWO	plane wave orbital
PWSB	plane-wave second Born
PWSCF	partial-wave self-consistent field
PWTF	plane-wave translation factors (in atom-ion inelastic collisions)
PWTM	plane-wave t-matrix (for electron-atom scattering)

Q

Q-DAS	quenched decay associated spectrum
QAFM	quantum antiferromagnetic Heisenberg model
QAPW	quadratic augmented plane wave (in band-structure calcn.)
QBCF	quasiband crystal field (ab initio SCF method for defects and impurity levels in solids)
QBM	quantal Brownian motion (model)
QBO	quantitative basis orbital (an MO or AO)
QC	quasi continuum , a dense manifold of (rovibrational) quantum states
QC-SCF	quadratically convergent SCF (for closed-shell systems)
QCA	(1) quasichemical approxn. (in calcns. on semiconductors) (2) quasicrystalline approximation
QCCA	quasiclassical close-coupling approximation
QCD	quantum chromodynamics
QCE	quantum confinement effects (in clusters)
QCFF/PI	quantum mechanical consistent force field method for pi-electron systems
QCI	quadratic configuration interaction
QCISD	quadratic configuration interaction (with) single (and) double (excitations)
QCISD(T)	quadratic configuration interaction technique including single and double excitations and correction for triple excitations - J. A. Pople, M. Head-Gordon, and K. Raghavachari, *J. Chem. Phys.*, **87**, 5968 (1987)
QCPE	Quantum Chemistry Program Exchange - Creative Arts Building 181, 840 Highway 46 Bypass, Indiana University Bloomington, IN 47405, USA
QCT	quasiclassical trajectory (method for molecular dynamics) D.M. Hirst, *A Computational Approach to Chemistry* (Blackwells Scientific, Oxford, 1990); M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids* (Oxford Science Publications, Oxford, 1990)
QCT-IEQMT	quasiclassical trajectory-internal energy quantum mechanical threshold
QD-MBPT	quasi-degenerate many-body perturbation theory
QDM	quadrature discretization method (in electron transport properties calcns.)
QDM	quantum defect method
QDO	quantum-defect orbital (theory)
QDPT	quasi-degenerate perturbation theory
QDT	quantum-defect theory
QDVPT	quasidegenerate variational perturbation theory

QDWT	quantum density-wave theory (in theory of freezing of quantum systems)
QEEC	quasimol. extended elementary cell (for electronic structure calcns. of crystals)
QET	quasiequilibrium theory for the calculation of reaction rate coefficients, a variant of transition state theory (TST)
QFD	quantum fluid dynamics
QFDFT	quantum-fluid density-functional theory
QFE	quasifree electron model
QFT	quantum field theory
QG	quasigeminals
QGLE	quantum generalized Langevin equation
QHA	quasi-harmonic approxn. (in intramol. vibrational relaxation)
QIOS	quantum infinite-order sudden (method for collisions): see IOSA
QISM	quantum inverse scattering method
QKM	quadratic Kohn method (variational method for scattering)
QLCPMET	quasilinearized coupled-pair-many-electron theory
QLDA	quasilocal density functional approxn.
QLGM	quantum lattice gas model (in helium superfluid transition temperature in zeolite pores)
QLSM	quadratic least-squares method (variational for scattering)
QLUC	quasimolecular large unit cell (model for electronic-structure calcns. on solids)
QMC	quantum Monte-Carlo (theory for many-electron atoms and mols.) - *eg.* P.J. Reynolds, D.M. Ceperley, B.J. Adler and W.A. Lester, *J. Chem. Phys.*, **77**, 5593 (1982)
QMCRG	quantum Monte-Carlo renormalization group (for quantum phase transitions)
QMD	quantum molecular dynamics (for calcns. on the dynamics of a quantum particle coupled to a classical many-body system)
QMM	quasimolecular mechanism (for intermolecular energy transfer).
QMO	quaternionic molecular orbital method
QPEN	quantum-mechanical potential (based on interactios of) electrons (and) nuclei
QPID	quadrupole induced dipole
QPLDA	quasiparticle local-density approxn.
QPM	quantum Poincare map
QPMDA	quasiparticle mean density approxn. (assocd. with local-density theory)
QR-MWH	quasi-relativistic Mulliken-Wolfsberg-Helmholz method
QRF	quadratic response function (a quantum propagator)
QRHF-CC	quasirestricted Hartree-Fock coupled cluster
QRIOSA	quantum reactive infinite order sudden approxn.
QRM	quadratic Rubinow method (variational method for scattering)
QSAR	quantitative structure-activity relationship
QSI	quantum statistical interference
QSM	(1) quantum shell model (2) quantum statistical mechanics (3) quantum-statistical model
QSSA	quasi-steady-state approximation in kinetics - *eg.* T. Turányi, A.S. Tomlin, and M.J. Pilling, *J. Phys. Chem.*, **97**, 163 (1993)

QSTLS	quantum Singwi-Tosi-Land-Sjolander (theory, see also STLS) (for electronic-property calcns. on electron-liquid models)
QTCS	quantum theorem of corresponding states
QTPT	quantum thermodynamic perturbation theory
QTST	quantum transition state theory
QUAPI	quasiadiabatic propagator path integral method
QUE	quantized universal enveloping (algebras in mol. vibrational spectra calcns.)
QUPID	quantum path integral (molecular) dynamics (method in molecular calcns.)
QVB	quasiempirical valence bond (method)
QVE	quasivibrational energy (formalism in multiphoton dissocn.)
R	
R	(1) reactance (matrix method in scattering calculations) - J.C. Light and R.B. Walker, *J. Chem. Phys.*, **65**, 4272 (1976) (2) rotational (energy, often used in the context of energy transfer or in RRKM calculations)
R-CNDO/1X	relativistic complete neglect of differential overlap (method)
R-GVB	resonating-generalized valence bond (wave function)
R-MR-CI	restricted-multireference-CI
R-R	rotational-to-rotational (energy transfer)
R-T	rotational-to-translational (energy transfer)
R-V	rotational-to-vibrational (energy transfer)
RAA	rigid-atom approxn. (in electronic structure calcns.)
RADW	rotationally-adiabatic-distorted-wave (approximation for reactive scattering calculations) - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
RAM	(1) reference-system average Mayer-function (in perturbation theory) (2) renormalized atom model (for electronic-structure calcns.)
RAPW	relativistic augmented plane wave
RAS	restricted active space (wave function)
RASW	relativistic augmented spherical wave method
RATM	renormalized average t-matrix (for density-of-states calcns.)
RATTLE	"velocity" version of the SHAKE algorithm for molecular dynamics calculations - H.C. Andersen, *J. Comput. Phys.*, **72**, 2384 (1980)
RB	renormalized band (method in electronic-structure calcns.)
RBA	refined Born approximation (for atom-molecule collisions)
RBM	rigid band model
RC	(1) radical-complex (mechanism) (2) reaction coordinate
RC(XI)	(fully) correlated relativistic local-density
RCHF	relaxed-core Hartree-Fock (approxn. in calcns. on molecular K-shell excitation spectra)
RCI	(1) relativistic configuration interaction (2) restricted configuration interaction
RCIOSA	reactive classical-infinite-order-sudden approxn.
RCISD	restricted CI (with) single (and) double (excitations)
RCM	rotated-coordinate method
RCNDO	Rydberg CNDO

RCNDO/S	Rydberg CNDO/screened
RCS	recoupled centrifugal sudden (approxn., in molecular scattering)
RCSF	reference configuration-state function
RDEQ	reduced dimensionality exact quantum (method for reactive scattering) - G.C. Schatz, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 1
RDF	(1) restricted Dirac-Fock (quantum calcn. method) (2) radial distribution function (mainly in neutron and X-ray scattering, and in the statistical mechanics of fluids)- *eg,* D.A. McQuarrie, *Statistical Mechanics* (Harper and Row, New York, 1976)
RDGTO	(back-)rotated distributed gaussian-type orbital
RDO	reduced density operator
RDQ	reduced-dimensionality quantum (calcn. method)
RDW	relativistic distorted wave
RE	(1) recoupled states (in orbiting resonances calcns. in atom-mol. inelastic scattering) - K. McLenithan and D. Secrest, J. *Chem. Phys.*, **80**, 2480 (1984) (2) relativistic Eikonal
RECA	regional energy convergence approxn. (in total energies calcns.)
RECP	relativistic effective core potential
RECP-CVC	relativistic effective-core potential with core-valence correlation
REMPI	resonantly enhanced multiphoton ionisation
REOM	reduced equations of motion (method in molecular-scattering calcns.)
REP	relativistic effective potential
REPE	resonance energy per pi electron
RESPA	reference system propagator algorithm - M. Tuckerman, B. J. Berne, and A. Rossi, *J. Chem. Phys.* **94**, 1465 (1991)
REV	ray eigenvector (a wave function)
REX	relativistically parametrized extended Hückel
RFA	renormalized free atom (model, in band-structure calcns.)
RFBCM	random-field Blume-Capel model (hamiltonian for magnetic system)
RHF	(1) relativistic-Hartree-Fock (2) (spin)-restricted Hartree-Fock method for the SCF calculation for open-shell molecules- C. C. J. Roothaan, *Rev. Mod. Phys.*, **32**, 179 (1960) (3) Roothaan-Hartree-Fock
RHF-HE	half-electron method for open shell systems using a closed shell wavefunction - M. J. S. Dewar, J. R. Hashmall, C. G. Venier, *J. Am. Chem. Soc.*, **90**, 1953 (1968)
RHF SP	restricted Hartree Fock spin polarization
RHFDZ	restricted Hartree-Fock calculation with a double zeta basis set
RHFO	relativistic Hartree-Fock one-channel (for scattering)
RHFR	(1) relativistic Hartree-Fock-Roothaan (2) restricted Hartree-Fock-Roothaan
RHFS	(1) relativistic Hartree-Fock-Slater (2) restricted Hartree-Fock-Slater
RHFT	relativistic Hartree-Fock two-channel (for scattering)
RHO	reduced hamiltonian orbital method
RHT	restricted Hückel method

RINDO	Rydberg intermediate neglect of differential overlap
RIOS	reactive infinite-order sudden (approximation for reactive scattering) (see RIOSA)
RIOSA	(1) reactive infinite-order sudden approximation (method for reactive scattering) - M. Baer and D.J. Kouri, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 167 (2) rotational infinite order sudden approxn.
RISM	reference interaction site model (for mol. fluids)
RKB	restricted kinetic balance (method in calcns. of wave functions and energies)
RKKR-GF	relativistic Koringa-Kohn-Rostoker Green function
RKKY	Ruderman-Kittel-Kasuya-Yoshida (indirect electron exchange mechanism)
RKR	Rydberg-Klein-Rees method for determining potential energy curves - J.T. Vanderslice, E.A. Mason, W.G. Maisch, and E.R. Lippincott, *J. Mol. Spectrosc.*, **3**, 17 (1959)
RKRV	Rydberg-Klein-Rees-Vanderslice
RKRVL	Rydberg-Klein-Rees-Vanderslice-Lakshman (for potential energy)
RLF	radially localized (wave) function
RLM	rotating linear model (for reactive scattering) - R. E. Wyatt, *J. Chem. Phys* ., **51**, 3489 (1969)
RLMTO	relativistic linear muffin-tin orbital
RMBPT	relativistic many-body perturbation theory
RMC	relativistic multiconfiguration
RMCS	rotated Morse curve spline - R. T. Wall and R. N. Porter, *J. Chem. Phys.*, **36**, 3256 (1962)
RMCSTEP	repartitioned multiconfigurational spin-tensor electron propagator
RME	reduced matrix equations
RMF	rotating Morse function (in potential-surface calcn.)
RMO	rotated Morse oscillator (function for potential surface)
RMOS	rotated Morse oscillator spline (function for potential surface calcn.)
RMP	(1) relativistic model potential (2) resonant model potential (3) restricted Møller-Plesset
RMP2	restricted Møller-Plesset second-order (perturbation theory)
RMP4	restricted Møller-Plesset fourth-order (perturbation theory)
RMPM	renormalized multicenter potential model (for scattering)
RMT	random matrix theory
RMTA	rigid muffin-tin approxn.
RMTO	relativistic muffin-tin orbital
RNO	reaction natural orbital
ROA	relaxed orbital approximation
ROBK1	relativistic first-order Oppenheimer-Brinkman-Kramers
ROBK2	relativistic second-order Oppenheimer-Brinkman-Kramers (in ion-scattering calcns.)
ROBO	rotating bond order (model in potential surface calcns.)
ROHF	restricted open-shell Hartree-Fock
ROMP	restricted open-shell Møller-Plesset
ROS	restricted (or Roothaan) open-shell (hamiltonian)
ROVP	reactance operator variational principle
RPA	random phase approximation
RPAE	random phase approximation with exchange

RPC	reduced potential curve (method for analysis of potential functions and spectra of diatomic molecules)
RPD	retarding potential difference
RPE	renormalized perturbation expansion
RPEHMO	relativistically parametrized extended Hückel MO
RPM	(1) radical pair mechanism (2) restricted primative model (potential for ion-ion interactions) - *eg,* M.P. Allen and D.J. Tildesley, *Computer Simulations of Liquids* (Oxford Science Publications, Oxford, 1990), p. 298
RPO	resonant periodic orbit (on potential energy surface in atom or molecule scattering)
RPWBA	relativistic plane-wave Born approximation
RPWBA-BC	relativistic plane-wave Born approximation with corrections for increased binding energy and Coulomb deflection
RQDO	relativistic quantum defect orbital (method in calcns. of oscillator strengths)
RR	resonance Raman
RRGM	recursive residue generation method - R.E. Wyatt, *Adv. Chem. Phys.* **73**, 231 (1989)
RRHO	rigid rotor-harmonic oscillator (model in which rotations are approximated as rigid rotors, vibrations as harmonic oscillators, and rovibrational coupling is ignored)
RRK	early microcanonical version of transition state theory due to Rice, Ramsperger, and Kassel - (eg) W. Forst, *Theory of Unimolecular Reactions* (Academic Press, New York, 1973)
RRKM	microcanonical version of transition state theory due to Rice, Ramsperger, Kassel, and Marcus - (eg) R.G. Gilbert and S.C. Smith, *Theory of Unimolecular and Recombination Reactions* (Blackwells Scientific, Oxford, 1990)
RRM	(1) Rayleigh-Ritz method (for quantum calculations) (2) rotating rod model
RRPA	(1) relativistic random phase approximation (2) renormalized random-phase approxn.
RS	(1) Rayleigh Schrödinger (perturbation theory) (2) Roos-Siegbahn
RS-HFPT	Rayleigh-Schrödinger Hartree-Fock perturbation theory
RSCA	relativistic semiclassical approximation (for atomic scattering)
RSCF	relativistic self-consistent field
RSCPA	reduced (second order) self-consistent phonon approxn. (a Green-function calcn. method)
RSE	relativistic symmetric Eikonal
RSK	Rajagopal-Singhal-Kimball (local-spin-density potential for electronic structure calcns.)
RSM	reduction symmetry method (in crystal field theory)
RSMP	Rayleigh-Schrödinger-Møller-Plesset perturbation
RSMST	real-space multiple-scattering theory (in electronic structure)
RSPE	Rayleigh Schrödinger perturbation expansion
RSPT	Rayleigh-Schrödinger perturbation theory
RSRG	real-space renormalization group (method in calcn. of Green functions for electrons in crystals)
RSSC-CPA	real-space-scattering cluster coherent potential approxn.
RT	Renner-Teller (effect), (the splitting of the potential-energy function when bending a linear molecule)

RTCDW	relativistic target continuum distorted wave (approxn. for electron capture in ion-atom collisions)
RTFDW	relativistic Thomas-Fermi-Dirac-Weizsaecker (electron-density theory)
RTPM	radical-triplet pair mechanism
RVB	resonating valence bond (theory of high-T_c superconductors)
RVCM	renormalized virtual-crystal method (for electronic structure)
RVS-SCF	reduced variational space-self-consistent field (in quantum calcns. on hydrogen bonding)
RWA	rotating wave approximation
RWKB	relativistic Wentzel-Kramers-Brillouin

S

S-MPPT	supermolecular Møller-Plesset perturbation theory
SA	(1) sudden approximation (2) statistical approximation
SA-CAS-SCF	state-averaged-complete active space-SCF
SA-LCAO	symmetry-adapted linear combination of atomic orbitals
SA-MCSCF	state averaged multiconfiguration self-consistent field (wave function) (see also ICF-CI)
SAAO	symmetry-adapted atomic orbital
SAAP	spin adapted antisymmetrized product (in MC-SCF theory)
SAC	symmetry-adapted cluster (expansion method for calcg. wave functions) - H. Nakatsuji and K. Hirao, *J. Chem. Phys.*, **68**, 2035 (1978)
SAC-CI	symmetry-adapted cluster configuration interaction (theory for wave-function expansion) - H. Nakatsuji, *Chem. Phys. Lett.* **59**, 362 (1978); **67**, 329 (1979); **67**, 334 (1979)
SACF	symmetry-adapted configuration function
SACM	statistical adiabatic channel model - J. Troe, *J. Chem. Phys.*, **79**, 6017 (1983)
SADPT	symmetry-adapted double perturbation theory
SADVR	symmetry-adapted discrete variable representation (in molecular wave function calcn. for nuclear motion on a given PES)
SAF	symmetry adapted function (in CI calcns.)
SAG	semiclassical adiabatic ground
SAI	(1) simplified *ab initio* method (2) spline-fitted *ab initio* (potential energy surface) (3) strongly anisotropic interaction
SAIM	scaled atoms-in-molecules
SALCCSD	spin-adapted linear coupled-cluster (with) single and double (excitations)
SAM1	semi-empirical *ab initio* method - version 1 - M. J. S. Dewar, C. Jie, G. Yu, *Tetrahedron*, **23**, 5003 (1993)
SAMO	simulated *ab initio* molecular orbital
SANO	symmetry-adapted natural orbital
SAO	symmetric atomic orbital
SAPS	spherical average pseudopotential
SAPT	symmetry adapted perturbation theory – *eg.* I.G. Kaplan, *Intermolecular Interactions,* (Elsevier, Amsterdam, 1987)
SAPW	symmetrized augmented plane wave
SAR	(1) sequential adiabatic reduction (2) structure-activity relationship

SAW	self-avoiding walk - *eg.* D.M. Hirst, *A Computational Approach to Chemistry* (Blackwells Scientific, Oxford, 1990), p. 419
SBA	second Born approximation
SBCPA	single-bond coherent potential approximation
SBE	semiconductor Bloch equations - H. Haug and S. W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, Worls Scientific, Singapore, 1990
SBMF	slave-boson mean field (in electronic-structure calcns.)
SBMO	subjacent molecular orbital
SC	strong collision (assumption in unimolecular reaction rate theory)
SC-FLAPW	self-consistent full-potential linearized-augmented-plane-wave
SC-GCM	self-consistent generator coordinate method
SC-MBPT	single-configuration many-body perturbation theory
SC-MEH-MO	self-consistent-modified extended Hückel-mo
SC-RPA	single-channel random phase approximation
SC-SCF	semiclassical self-consistent field
SC-SEA	single-channel static-exchange approximation
SC-SI	semiclassical state interaction (method for solving Schrödinger equation)
SC-VB	spin-coupled valence bond
SCA	(1) screened Coulomb approximation (in correlation-energy calcns. for autoionizing energy levels of two-electron systems) (2) self-consistent approximation (3) semiclassical approximation (4) semiclassical Coulomb approximation
SCA-QD-MBPT	self-consistently adapted (core reference state) quasidegenerate many-body perturbation theory
SCAF	self-consistent anisotropic field
SCAP	self-consistent average phonon (theory)
SCASA	semiclassical approxn. separated atom
SCAUA	semiclassical approxn. united atom
SCBA	self-consistent Born approximation
SCBC	self-consistent basis and configuration
SCBF	semiclassical approximation with body-fixed molecular orientation
SCBSA	self-consistent boundary-site approxn. (for density-of-states)
SCC	(1) self-consistent charge method (2) self-consistent collective coordinate (in reactive collisions) (3) semiclassical coupled-channel (4) superposition of correlated configurations (variational method)
SCC-DVM	self-consistent-charge-discrete-variational method
SCCC	self-consistent charge and configuration method
SCCEH	self-consistent charge extended Hückel method
SCCF	(1) self-consistent continued fraction (2) self-consistent crystal field (method for calcns. on molecular crystals) (3) spin-correlated crystal field
SCCM	self-consistent cell model
SCCP	strong-coupling correspondence principle

SCCR	self-consistent current relaxation (in electronic dynamic structure factor calcns.)
SCCSA	self-consistent central-site approxn. (for density-of-states)
SCCT	semiclassical complex trajectory
SCDM	self-consistent diagrammatic method (in calcn. on electronic excitation transfer)
SCE	(1) self-consistent energy (method in atomic and molecular calcns. with an einsteinian relativistic theory (2) semiclassical exchange approximation
SCEKT	single configurational extended Koopmans theorem
SCEM	self-consistent Eikonal method (in electronic transition calcn.)
SCEP	self-consistent electron-pair theory
SCEPM	self-consistent empirical pseudopotential method
SCF	(1) self consistent field (2) self-consistent field theory - C. C. J. Roothaan, *Rev. Mod. Phys.*, **23**, 69 (1951)
SCF MO	self-consistent field molecular orbital
SCF-X(ALPHA)-SW	self-consistent field (X-alpha) scattered-wave
SCF-X(ALPHA)-SWCMO	self-consistent field-(X-alpha)-scattered wave cluster MO
SCFX-CI	excited-state self-consistent field configuration interaction
SCGF	self-consistent group function
SCHA	self-consistent harmonic approxn.
SCI	(1) single excitation configuration interaction (2) super configuration interaction - F. Grein and T.C. Chang, *Chem. Phys. Lett.*, **12**, 44 (1971)
SCIA	(1) semiclassical impact approxn. (in ionizing atomic and molecular collision calcns.) (2) semiclassical impulse approxn.
SCIBM	semiclassical infinite-barrier model
SCLO	self-consistent local orbital
SCLR	single configuration linear response (theory)
SCM	(1) self-consistent multipolar (method in metal cluster calcns.) (2) spherical cellular model
SCMP	self-consistent madelung potential
SCMPs	spin-corrected Møller-Plesset nth-order
SCO	self-consistent orbital
SCOP	spherical complex optical potential (in quantum calcn. on molecular scattering)
SCOPW	self-consistent orthogonalized plane wave
SCP-IOS	semiclassical perturbation-infinite order sudden (model for reaction dynamics) - W.H. Miller and S.-H. Shi, *J. Chem. Phys.*, **75**, 2258 (1981)
SCPA	**(1)** self-consistent phonon approximation (for lattice dynamics of quantum crystals) **(2)** single-site coherent-potential approximation (for electronic structure calcns.)
SCPF	(1) self-consistent perturbation field (2) self-consistent polarization field method
SCPHP	self-consistent particle-hole propagator
SCPP	self-consistent polarization propagator
SCPT	self-consistent-perturbation theory
SCPW	symmetrized combination of plane waves
SCRF MO	self-consistent reaction field
SCRF	self-consistent reaction field - O. Tapia and G. Johannin, *J. Chem. Phys.*, **75**, 3624 (1981)

SCROPW	self-consistent relativistic orthogonalized-plane-wave
SCRPA	self-consistent random phase approximation
SCS	semiclassical coupled-states
SCSA	small-curvature semiclassical adiabatic (approxn. for molecular energy levels)
SCSF	semiclassical approximation with space-fixed molecular orientation
SCSOPW	self-consistent symmetrized orthogonalized-plane-wave
SCT	small curvature tunnelling (approximation)
SCTB	self-consistent tight-binding (in electronic structure)
SD-MBPT	single (and) double (substituted states) many-body perturbation theory
SD-POE	sigma-dependent pi-orbital electronegativity model
SDCI	single and double excitation configuration interaction model
SDCPA	site-dependent coherent potential approxn.
SDECI	singly and doubly excited configuration interaction
SDF	spin(-unrestricted) density functional
SDGUGA	shape-driven graphical unitary group approach
SDIM	scaled diatomics-in-molecules
SDO	shielded diatomic orbital
SDQ-MBPT	single (and) double (and) quadruple (substituted states) many-body perturbation theory
SDQ-MBPT	single-double-quadruple excitation many-body perturbation theory
SDSR-CI	single and double excitations from single reference state function-CI method
SDTQ-MBPT	single-double-triple-quadruple excitation (contribution) MBPT
SDW	spin density wave
SE	symmetric Eikonal (approxn. in calcns. on ion scattering)
SEAMO	single-excitations-adapted molecular orbital
SEC	scaled external correlation (extrapolation method in CI calcn.)
SECH	screened exchange plus Coulomb hole method
SECI	single excitation configuration interaction
SEE	static exact exchange (approxn. in electron-molecule scattering)
SEHF	spin-extended Hartree-Fock
SEMPI	singly excited modified perturbation theory
SEPT	secular equation (with) perturbation theory
SERHF	symmetry-equivalenced restricted Hartree-Fock
SESAO	semiempirical scaled atomic orbital
SESMO	semiempirical scaled molecular orbital
SETB	semiempirical tight binding
SETM	statistical electron transfer model (for electron-exchange collisions)
SEVB	semiempirical valence bond
SEW	site electron-density wave
SF CC	space-fixed close-coupled (equation, for quantum calculations)
SF-PNM	step function perturbative numerical method
SFCCCC	space-fixed complex-coordinate coupled-channel method
SGA	symmetric group approach
SGF	spherical gaussian function

SGFM	surface Green function matching (method in calcn. of electronic and phonon properties of crystal surfaces and interfaces)
SGGA	symmetric group graphical approach (in CI calcns.)
SGO	spherical gaussian orbital
SGTF	spherical gaussian-type function
SGVFF	simplified general valence force field
SHAKE	an algorithm for adjusting atomic positions to satisfy constraint conditions in molecular dynamics - J.P. Ryckaert, G. Ciccotti, and H.J.C. Berendsen, *J. Comput. Phys.*, **23**, 327 (1977)
SHC	symmetrized hyperspherical coordinates (in quantum calcns. on reactive scattering)
SHM	screened hydrogenic model (for electronic structure in plasmas)
SHT	surface hopping trajectory (model for molecular scattering)
SI	(1) state interaction method (2) Stieltje imaging (method for calcg. wave functions) (3) spherical interaction approximation
SIAM	single-impurity Anderson model
SIBFA	sum (of) interactions between fragments (computed) ab initio
SIC LDF	self-interaction corrected local density functional
SIC	self-interaction correction (in exchange-energy calcns.) - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989)
SIC-GX-LSD	self-interaction corrected generalized exchange local spin density
SIC-LSD	self-interaction correction-local spin density
SIFDT	selected ion flow-drift tube
SIFT	selected ion flow tube
SIMS	secondary ion mass spectroscopy
SINDO	(1) scaled intermediate neglect of differential overlap (2) symmetrically orthogonalized intermediate neglect of differential overlap - D. N. Nanda, K. Jug, *Theoret. chim. Acta*, **57**, 95 (1980)
SINDO/F	SINDO free of empirical parameters
SIOS	semiclassical infinite-order sudden (in rotationally-inelastic scattering calcns.)
SKS	Slater-Kohn-Sham
SLAPW	(1) superlinearized augmented plane wave (2) surface linearized augmented plane wave
SLBO	strictly localized bond orbital
SLE	stochastic liouville equation (in quantum statistical mechanics)
SLF	Slater-Laguerre (hydrogenic-type wave) function
SLG	strictly localized geminal - P. R. Surjan, *Phys. Rev. A*, **30**, 43 (1984)
SLMO	(1) strictly localized molecular orbital (2) symmetry-adapted localized orbital (3) symmetry-adapted semilocalized molecular orbital
SLMTO	surface linear (combination) of muffin-tin orbitals
SLO	strictly localized orbital
SMC	Schwinger multichannel (for electron-molecule scattering)
SME	static model exchange (approxn. in electron-molmolecule scattering)
SMM	spin matrix mapping

SMMO	strictly monomer molecular orbital
SMSA	soft-core mean spherical approxn.
SMSO	spinor molecular symmetry orbital
SNO	spin natural orbital
SNVE	smallest non-vanishing eigenvalue (method)
SO	(1) Stieltjes orbitals (for mol. photoionization continua) (2) second order (3) spin-orbit(al)
SO SCF	spin-optimized self-consistent field
SO-LAPW	spin-orbit (coupling) linearized augmented plane wave
SOBO	spin-orbit (coupled) bond orbital
SOC	superposition of configurations (wave functions)
SOCI	(1) second-order configuration interaction (2) spin-orbit configuration interaction
SOCO	second-order correlation orbital
SODW	second-order distorted wave (in electron-atom scattering)
SOEH	scaled one-electron hamiltonian (in SCF calcns. on molecules)
SOGVB	(1) spin optimized generalized valence bond method (2) strongly-orthogonal generalized valence-bond (wave function)
SOLO	second-order correlated localized orbital-local origin (method)
SOMBT	(1) second-order many-body theory (2) spin-orbital many-body theory
SOMO	(1) semioccupied molecular orbital (2) singly occupied molecular orbital
SOP	(1) second-order potential (method for positron-atom scattering) (2) semiclassical optical potential
SOPHF	spin and orbital polarized Hartree-Fock
SOPPA	second-order polarization propagator approxn. (2) surfaces of section method (semiclassical calcn. of eigenvalues)
SP-RPAE	spin polarized-random phase approxn. (with) exchange
SPA	(1) self-consistent phonon approximation (2) separated pair approxn. (wave function) (3) shielded-potential approxn. (in electronic structure)
SPB	strong-potential Born (approxn. for atomic collision calcns.)
SPC	simple point charge (potential function) - H.J.C. Berendsen *et al.*, in B. Pullman, ed., *Intermolecular Forces* (D. Reidel, Dordrecht, 1981)
SPC/E	extended simple point charge (potential function) - H.J.C. Berendsen, J.R. Grigera, and T.P. Straatsma, *J. Phys. Chem.*, **91**, 6269 (1987)
SPD	small phonon displacement (state) - Ning Lu and S. Mukamel, *J. Chem. Phys.*, **95**, 1588 (1991)
SPDM	single-particle density matrix
SPEMC-SCF	selected paired excitational expansion multiconfiguration-SCF
SPF	Simons-Parr-Finlan (potential) - G. Simons, R. G. Parr, and J. M. Finlan, *J. Chem. Phys.*, **59**, 3229 (1973)
SPFD	Simons-Parr-Finlan-Dunham (interatomic potential)
SPG	sequential product (of) geminals
SPHF	spin-polarized Hartree-Fock
SPINDO	spectroscopic potentials adjusted intermediate neglect of differential overlap

SPL	statistical power-gap law (in rotational energy transfer: also called PGL) - T.A. Brunner, N. Smith, A.W. Karp, and D.E. Pritchard, *J. Chem. Phys.*, **74**, 3324 (1981)
SPMC	stationary phase Monte-Carlo
SPPA	self-consistent polarization propagator approximation
SPUMPn	single-annihilation procedure unrestricted Møller-Plesset nth-order
SPW	symmetrized plane wave
SQCC	semiclassical quantization (by) circuit counting
SQF	second-quantized formulation (in many-body quantum theory)
SQM	scaled quantum mechanical (vibrational force field) (in ab initio calcns.)
SQRD	square root Darwin term (correction to T and V operator)
SRA	sudden rotation approximation
SRAPW	scalar relativistic augmented plane wave
SRASE	symmetry restricted annihilation of single excitations
SRCC	single-reference coupled-cluster
SRCCSDT	single-reference coupled-cluster (with) single (and) double (and) triple (excitations)
SRCI	single reference configuration interaction
SRH	spin-adapted reduced hamiltonian
SRMCASE	symmetry-restricted multiconfiguration annihilation of single excitations method
SROS	spin-restricted open shell
SRS	symmetrized Rayleigh-Schrödinger (perturbation theory)
SS	split-shell (gaussian basis set)
SSA	(quasi-) steady-state approximation (in kinetics) - *eg.* T. Turányi, A.S. Tomlin, and M.J. Pilling, *J. Phys. Chem.*, **97**, 163 (1993)
SSB	semiclassical sudden Born (approxn. in ion-atom collisions)
SSCP	static screened Coulomb potential
SSCPA	single-site coherent-potential approximation
SSDW	static-static distorted-wave (approximation for reactive scattering calculations) - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
SSGF	self-consistent surface Green function
SSH	(1) Schwartz-Slawsky-Herzfeld (2) Su-Schieffer-Heeger (model hamiltonian for electronic-structure calcns.)
SSHF	spin-symmetrized Hartree-Fock (wave function)
SSM	semiclassical spectral method
SSQM	supersymmetric quantum mechanics
SSTL	Singwi Sjolander Tosi Land (interatomic potential)
ST	statistical theory (for calculation of reaction rate coefficients): see CVT, mVTST, RRKM, TST, VTST
ST4CCD	coupled cluster (with) double (substitutions and) single (and) triple (substitutions incorporated via) fourth-order (perturbation theory)
STA	single-transition approximation
STB	semiempirical tight binding
STBF	Slater-type basis function
STCA	simplified traveling-cluster approxn. (for electronic structure)
STF	Slater-type function
STHF	single-term Hartree-Fock
STIRAP	stimulated raman adiabatic passage
STLS	Singwi-Tosi-land-Sjolander (generalized random-phase approxn. for effective pair potentials of liq. metals)
STM	space-translation method (in atomic collision calcn.)

STMCTDHF	spin-tensor multiconfigurational time-dependent Hartree-Fock
STO	Slater type orbital - J. C. Slater, *Phys. Rev.*, **36**, 57 (1930).
STO(nG)	a combination of n Gaussian functions to approximate a Slater type orbital - W. J. Hehre, L. Radom, P. v. R. Schleyer, and J. A. Pople, *Ab Initio Molecular Orbital Theory* (Wiley-Interscience), 1986, Chapt. 4.
STODI	Slater-type orbital-point dipole interaction (in mol. polarizability calcns.)
STP	Slater-transform-preuss (wave functions)
STS	Slater transition state (for calcg. electronic transitions of atoms and molecules)
SUHF	spin-unrestricted-Hartree-Fock
SUMP	spin-constrained unrestricted Møller-Plesset
SUSYQM	supersymmetric quantum mechanics
SVD	single-valued decomposition
SVE	selected valence electron model
SVESS	selected valence-electron split-shell method (mo)
SVP	schwinger variational principle
SW X(ALPHA)	scattered wave (chi-alpha)
SWKB	supersymmetric wentzel-kramers-brillouin (quantum method)
SWM	statistical wave function model (for highly excited vibrational levels of mols.)
SWVP	scattered wave variational principle
SXNO	singly excited natural orbital

T

T	translational (energy, often used in the context of energy transfer)
T-J MODEL	heisenberg-hubbard model (hamiltonian)
TASO	terminal atom symmetry orbital
TBA	tight binding approximation
TBB	tight-binding bond (model in quantum calcns. on vacancies)
TBBA	tightly-bound-on-the-bond approxn. (band structure crystal)
TBEH	tight-binding extended Hückel (extended Hückel tight-binding)
TBM	tight binding model
TBMD	tight-binding molecular dynamics
TBNEM	tight-binding nearly free electron model
TBTE	tight-binding total-energy (calcn. method)
TC-GME	time-convolution generalize master equation (in quantum tunneling calcns.)
TCA	traveling-cluster approximation (a generalization of cpa for electronic-structure of alloys)
TCDE	two-center Dirac equation
TCDFT	two-component density functional theory
TCDW	target continuum distorted-wave (in at.-collision calcns.)
TCDW1	target continuum distorted-wave 1st-order (for at. collisions)
TCF	time correlation function
TCL-GME	time-convolutionless generalized master equation (in quantum tunneling calcns.)
TCSCF	two-configuration self-consistent field procedure
TD-CAC	time dependent-coupled arrangement channel (method for calcns. on reactive and dissociative collisions)
TDA	Tamm-Dancoff approximation - P. Jorgensen, *Ann. Rev. Phys. Chem.*, **26**, 359 (1975).
TDA-2PH	two-particle one hole tamm-dancoff approximation
TDCC	(1) time-dependent close-coupling (2) time-dependent coupled-cluster

TDCHF	time-dependent coupled Hartree-Fock
TDDFT	time-dependent density-functional theory
TDFGH	time-dependent Fourier grid hamiltonian (method)
TDFM	two-surface Dirac-Frenkel-Mclachlan (variational method)
TDGI	time-dependent gauge-invariant (quantum calcn. method)
TDH	time-dependent Hartree theory
TDHF	time-dependent Hartree-Fock approximation
TDHG	time-dependent Hartree grid (quantum method)
TDKS	time-dependent Kohn-Sham (d.-functional operator equation)
TDLDA	time-dependent local-density approximation
TDM	truncated diagonalization method
TDMCSCF	time-dependent mc-SCF
TDMF	time-dependent mean field
TDMO	time-dependent molecular orbital
TDO	truncated diatomic orbital (a mo)
TDPT	time-dependent perturbation theory
TDRH	time-dependent rotated Hartree (theory)
TDS	time-dependent sudden
TDSCF	time-dependent self-consistent field
TDSE	time-dependent Schrödinger equation
TDSF	time-dependent Spencer-Fano (in at. and mol. inelastic collisions)
TDSHF	time-dependent screened Hartree-Fock
TDT	temperature programmed desorption
TDTF	time-dependent Thomas-Fermi
TDVP	time-dependent variational principle (in scattering calcns.)
TDVPT	time-dependent variation-perturbation theory
TDWP	time dependent wavepacket (method for quantum scattering) - C. Leforestier, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 235.
TEC	teo electron counting method (for complexes, clusters)
TEMO	topological effects on mo
TEO	topological equivalent orbital
TESICO	threshold electron-secondary ion
TEXAS	a computer program for solving the electronic Schrödinger equation.
TFA	Thomas-Fermi-amaldi (equation)
TFDGW	Thomas-Fermi-Dirac-Gombas-Weizsaecker
TFDW	Thomas-Fermi-Dirac-von Weizsaecker (method for electronic structure calcns. on mols.)
TFW	Thomas-Fermi-Weizsaecker (electron-d. theory)
TGTF	trigonometric gaussian-type function
TGVBA	target generalized valence bond approximation
THFA	target Hartree-Fock approximation
THGF	trigonometric hermite gaussian function
THM	transcorrelated hamiltonian method
TICS	time reversal invariant closed shell (type of Hartree-Fock wave function)
TIPS	transferable intermol. potential functions
TISE	time independent Schrödinger equation
TLFPE	time-local Fokker-Planck equation
TLS	two-level system (with tunneling transitions between wells of double-well potential)
TLS	two-level system.
TMO	truncated molecular orbital
TNOA	target natural orbital approximation
TO	topological orbital (in graph theory of molecules)
TOM	transition operator method

TPM	two-potential model (in at. scattering calcns.)
TPMB	two-potential-modified Born (approxn. in inelastic collisions)
TPOT	two-parameter omega technique
TPW	transformed plane wave method
TS	transition state, a critical configuration that separates reactants from products - (eg) J.I. Steinfeld, J.S. Francisco, and W.L. Hase, *Chemical Kinetics and Dynamics* (Prentice Hall, Englewood Cliffs, 1989)
TSA	transition state approximation that any molecule(s) that pass the critical transition state configuration will form products irreversibly
TSAE	two-state atomic expansion (model for atom-ion collisions)
TSCW	torsional spin current wave (type of Hartree-Fock wave function)
TSDW	torsional spin density wave
TSH	(1) (classical) trajectory surface hopping - J.N. Murrell and S.D. Bosanac, *Introduction to the Theory of Atomic and Molecular Collisions* (John Wiley and Sons, Chichester, 1989), pp. 159–164 (2) tensor surface harmonic (method in bonding of metal clusters)
TSME	two-state molecular expansion (method in collisions calcn.)
TSS	transition state spectroscopy - R.B. Metz, S.E. Bradforth and D.M. Neumark, *Adv. Chem. Phys.*, 81, 1 (1991)
TST	transition state theory for the calculation of reaction rate coefficients - (eg) J.I. Steinfeld, J.S. Francisco, and W.L. Hase, *Chemical Kinetics and Dynamics* (Prentice Hall, Englewood Cliffs, 1989), Chapter 10
TSW	torsional spin wave (type of Hartree-Fock wave function)
TZ	triple zeta (basis set)
TZ2P	triple zeta plus two sets of polarization functions.
TZP	triple zeta plus a set of polarization functions.

U

UA	united atom
UAMO	unprojected alternant molecular orbital
UBA	unitarized Born approxn.
UBFF	Urey-Bradley force field - E.B. Wilson Jnr, J.C. Decius, and P.C. Cross, *Molecular Vibrations. The theory of infrared and raman vibrational spectra* (McGraw Hill, New York, 1955 (reprinted in 1980 by Dover Books)), p. 179
UCAS-SCF	unrestricted complete active space self-consistent field
UCC	unitary coupled-cluster
UCC(n)	unitary coupled-cluster [truncated to nth order]
UCCD	(spin)unrestricted coupled cluster (with) double (excitations)
UCDW	ultrarelativistic continuum distorted wave
UCEPA	unitary coupled electron pair approximation
UCHF	uncoupled Hartree-Fock
UCHFPT	uncoupled Hartree-Fock perturbation theory
UCID	unrestricted ci (with) single (and) double (excitations)
UDF	unrestricted Dirac-Fock
UDWA	unitarized distorted-wave approximation
UDWBA	unitarized disorted wave Born approxn. (for scattering)
UEBS	unitarized Eikonal Born series (in electron-atom scattering)
UEFF	effective potential (method for calculating association-reaction rates) - N. Markovic and S. Nordholm, *Chem. Phys.*, **135**, 109 (1989)
UGA	unitary-group approach (in quantum calcns.)

UGF	unitary-group formulation (in many-body quantum theory)
UHF	unrestricted open-shell Hartree-Fock method - A. Szabo & N. S. Ostlund, *Modern Quantum Chemistry* (Macmillan, New York, 1982)
UHF-AA	unrestricted Hartree-Fock (with spin) annihilation
UHF-CO	unrestricted Hartree-Fock crystal orbital
UHFQ	unrestricted Hartree-Fock with quartet annihilation
UHFS	unrestricted Hartree-Fock-Slater
UHV	ultrahigh vacuum.
UKB	unrestricted kinetic balance (in calcns. of wave functions and energies)
ULFM	unified ligand field model (for mol. electronic energies)
UMBPT(n)	unrestricted many-body perturbation theory of order n
UMINDO	spin-unrestricted modified intermediate neglect of differential overlap
UMNDO	spin-unrestricted modified neglect of diatomic overlap
UMO	unmodified molecular orbital
UMP	unrestricted Møller-Plesset
UMP2	unrestricted Møller-Plesset 2nd-order (perturbation theory)
UMP4SDTQ	unrestricted Møller-Plesset 4th-order (perturbation theory with) single, double, triple, and quadruple (excitations)
UNIMOL	the name given to several (and separate) computer programs for calculating unimolecular rate coefficients
UNO	unrestricted natural orbital
UNO-CAS	unrestricted natural orbital-complete active space
UOVMO	unoccupied valence-type mol. orbital
UPA	unitary-pole approximation
UPS	ultraviolet photoelectron spectroscopy.
UQ-NG	uniform-quality (basis set) constructed with a number (n) of gaussian (g) functions
UQCISD	unrestricted quadratic CI (with) single (and) double (excitations)
US	unified statistical
USPC	unoccupied-states potential correction
UTAO	undistorted traveling atomic orbital
UW-PG	uniformly weighted planar grid (method in calcns. of electron-momentum distributions)

V

V	vibrational (energy, often used in the context of energy transfer)
V-R	vibrational-to-rotational (energy transfer)
V-T	vibrational-to-translational (energy transfer)
V-V	vibrational-to-vibrational (energy transfer)
VADW	vibrationally-adiabatic-distorted-wave (approximation for reactive scattering calculations) - J.N.L. Connor, in *The Theory of Chemical Reaction Dynamics,* edited by D.C. Clary, (D. Reidel, Dordrecht, 1986), p. 247
VALMOP	valence (electron only) model potential
VAMO	variational alternant molecular orbital
VAP	valence alternation pair (bonding configuration model)
VB	valence bond
VBCI	valence bond configuration interaction
VBHL	valence bond Heitler-London (wave function)
VBM	valence-band model (in electronic structure calcns.)
VBR	variational basis representation (in quantum calcns.) - J. C. Light, I. P. Hamilton, and J. V. Lill, *J. Chem. Phys.*, **82**, 1400 (1985)
VBS	virtual bound state model
VBSCF	valence bond self-consistent field

VC-TSAE	variable-charge two-state atomic expansion (in collisions)
VCA	virtual crystal approximation
VCB-CPA	virtual crystal bandwidth-coherent potential approxn. (for electronic-structure calcns. on alloys)
VCC	(1) vibrational close-coupling technique (2) variable curvature coordinates (in calcns. on mol. vibrations)
VCC-IOS(A)	vibrational close-coupling-(rotational) infinite-order sudden (approximation) (for inelastic atom-molecule quantum scattering calculations) - D.C. Clary, *J. Chem. Phys.*, **75**, 209 (1981).
VCC-RIOS	vibrational close-coupled-rotational infinite order sudden (approximation for inelastic atom-molecule quantum scattering calculations) - D.C. Clary, *J. Chem. Phys.*, **75**, 209 (1981).
VCCPB	variable-charge Coulomb-projected Born (approxn. for electron-atom scattering)
VCD	vibrational circular dichroism
VCDW	vector charge-density wave
VCI	(1) valence configuration interaction (wave function) (2) variational configuration interaction (quantum calcn. method)
VCM	variational cellular method (for electronic structure calcns.)
VCP	virtuals-only counterpoise (method for eliminating basis set superposition error) - J.P. Daudey, P.Claverie, and J.P. Malrieu, Intern. *J. Quantum Chem.*, **8**, 1 (1974)
VCT	vibronic coupling theory
VD-RCC	vibrational diabatic-rotational close-coupled (method in mol. collision calcns.)
VD-RIOS	vibrational diabatic-rotational infinite order sudden
VDHF	variational Dirac-Hartree-Fock
VDW	van der Waals
VDW-RIOS	vibrational distorted wave-rotational infinite order sudden
VDZ	valence double-zeta basis set
VDZP	valence double-zeta plus polarization basis set
VE-PPP	variable electronegativity PPP
VEDW IOS	vibrational exponential-distorted-wave infinite-order-sudden (method for inelastic mol. collisions calcn.)
VEEH	variable electronegativity extended Hückel method
VEH	valence effective hamiltonian method (for electronic structure)
VENUS	a computer program for calculating quasiclassical trajectories and variational transition state theory rate coeffiecents - W.L. Hase, R.J. Duchovic, X. Hu, K.F. Lim, D.-H. Lu, G. Pesherbe, K.N. Swamy, S.R. Vande Linde, and R.J. Wolf, *QCPE* Program to be submitted.
VEO	valence electron only
VEOMP	valence-electron-only model potential (for mol. SCF calcns.)
VESCF	variable electronegativity self-consistent field
VF	valence force (model in bond properties calcns. in solids)
VFF	valence force field (in electronic-structure calcns.)
VFOT	variant Fock operator technique
VGAO	variable gauge atomic orbital
VIF	valency-point interaction formula (in graph theory with at. and mol. orbitals)
VIP	vibronic impact parameter (model for mol. scattering)

VIVAH	vibrational variational hyperspherical (for mol. calcns.)
VMC	variational Monte-Carlo (quantum calcn. method)
VMO	virtual molecular orbital
VO	(1) valence orbital (2) virtual orbital
VO/CI	virtual orbital/configuration interaction
VOFF	valence orbital force field
VOIE	valence orbital ionization energy
VOIP	valence orbital ionization potential
VP	vibrational predissociation
VPA	varied portions approach
VPAM	variable phase amplitude method (for electron-atom scattering)
VPD-CI	variational-perturbation approxn. to double excitation method in configuration interaction
VPM	variable phase method (for electron-atom scattering calcns.)
VPSA	Vainshtein-Presnyakov-Sobelman approxn. (for excitation in atom-ion collisions)
VPT	variational perturbation theory
VQMC	variational quantum Monte-Carlo
VQP	variable quadratic propagator (in quantum calcns.)
VR	vibrational relaxation
VRDDO	variable retention of diatomic differential overlap
VRIOSA	vibrational/rotational infinite-order sudden approximation
VRPA	variational random phase approxn.
VRRKM	variational RRKM: microcanonical variational transition state theory (see also mVTST, RRKM, and VTST) - R.G. Gilbert and S.C. Smith, *Theory of Unimolecular and Recombination Reactions* (Blackwells Scientific, Oxford, 1990)
VRT	vibration-rotation-tunneling (spectrum or transition)
VSEPR	valence shell electron pair repulsion (model)
VSIE	valence-state ionization energy
VSIP	valence-state ionization potential
VSM	variable screening model (for quasimols. and MO correlation diagrams)
VTST	variational transitional state theory - D.G. Truhlar and B.C. Garrett, *Acc. Chem. Res.*, **13**, 440 (1980); W.L. Hase, *Acc. Chem. Res.*, **16**, 258 (1983).
VU-CC	valence universal-coupled cluster
VU-CCSD/R	valence universal-coupled cluster (with) single (and) double (excitations) (r = radial components of the cluster amplitudes)
VU-LCC	valence-universal-linear coupled cluster
VUV	vacuum ultraviolet
VWN	Vosko-Wilk-Nusair (model potential in quantum calcns.)

W

WAO	Wannier atomic orbital
WBEPM	weakest bound electron potential model (theory in calcns. of ionization potentials)
WCA	Weeks-Chandler-Andersen (theory in liq.-structure calcns.)
WCUB	Wang Chang-Uhlenbeck-de Boer (quantum-mech. relation in rotational relaxation calcn.)
WDA	weighted density approximation (within d. functional formalism) - W. A. Curtin and N. W. Ashcroft, *Phys. Rev. A*, **32**, 2909 (1985)
WDF	Wigner distribution function (in study of quantum dynamics)
WHMO	Wolfsberg-Helmholz molecular orbital

WKB	Wentzel-Kramers-Brillouin (phase-shift formula for potential scattering), often called JWKB (Jeffreys-Wentzel-Kramers-Brillouin method - (eg) L.I. Schiff, *Quantum Mechanics*, 3rd Ed. (McGraw-Hill, Tokyo, 1968), p. 268
WLE	Wigner-Liouville equation (in study of quantum dynamics)
WMT	warped muffin-tin approximation
WPT	wave packet perturbation theory
WSOEA	Wallace second-order Eikonal approximation
WSTCM	Watson-sphere terminated cluster model (in electronic-structure calcns. on crystal defects)
	X
Xa	method of solving the Schrödinger equation - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989) **\X(greek "chi", not "X")**
X(ALPHA)	statistical exchange method **\X(greek "chi", not "X")** **see Xa??**
X(ALPHA)-MS	x(alpha)-multiple scattering **\X(greek "chi", not "X")**
XC	exchange-Coulomb potential
XCC	expectation-value coupled-cluster (in correlation energies and electronic properties of many-electron systems calcns.)
Xa	method of solving the Schrödinger equation - R. G. Parr & W. Yang, *Density-Functional Theory of Atoms and Molecules*, (OUP, 1989)
XPOLR	A.T. Brünger, J. Kuriyan & M. Karplus, *Science*, **235**, 458 (1987); distributed by Molecular Simulations, Burlington, MA01803-5297, USA
	Y
YBG	Yvon-Born-Green hierarchy of integral equations.
	Z
ZCC	zero core contribution (model for photodetachment calcns.)
ZCCSD	z-vector coupled cluster (with) single (and) double excitation
ZCT	**zero curvature tunnelling (approximation)** - **probably D.H. Truhlar *et al.***
ZDDO	zero diatomic differential overlap
ZDO	zero differential overlap - J. N. Murrell & A. J. Harget, *Semi-empirical Self-consistent-field Molecular Orbital Theory of Molecules*, Wiley-Interscience, 1972
ZFS	zero field splitting.
ZINDO	(set of programs developed by M. C. Zerner and coworkers) for SCF CIMO calcns.
ZOAO	zero overlap of atomic orbital approxn.
ZPC	zero-point (energy) corrections
ZPE	zero point energy
ZPV	zero point vibration
ZRPA	zero-radius potential approximation
ZRPA	zero-range potential approximation
ZTS	Z transition state [Z = nuclear charge] (method for calcg. isoelectronic energy differences and electrostatic potentials for atoms and molecules)
	2
2PH TDA	two-particle-hole Tamm-Dancoff approximation (for closed- shell