List of abbreviations

Abbreviation	Meaning
1D, 2D, 3D	one, two, three dimensions (or -dimensional)
ACALDA	asymptotically corrected ALDA
ACFD	adiabatic-connection fluctuation–dissipation
ALDA	adiabatic local-density approximation
AOEP	adiabatic optimized effective potential
ATI	above-threshold ionization
BLYP	Becke–Lee–Yang–Parr
BO	Born–Oppenheimer
BSE	Bethe–Salpeter equation
BZ	Brillouin zone
CAS	complete active space
CASPT2	complete active space with second-order perturbation theory
CB	Coulomb blockade
CC	coupled-cluster method
CC2	iterative second-order coupled-cluster method
CC3	iterative third-order coupled-cluster method
CCSDR(3)	coupled-cluster singles and doubles with noniterative triples correction method
CDFT	current-density-functional theory
CI	configuration interaction
CIS	configuration interaction singles
DFT	density-functional theory
EELS	electron energy loss spectroscopy
FSSH	fewest-switching surface hopping
GEA	gradient expansion approximation
GGA	generalized gradient approximation
GK	Gross–Kohn
HF	Hartree–Fock
HHG	high-harmonic generation

HOMO	highest occupied molecular orbital
HWHM	half-width at half-maximum
IXSS	inelastic X-ray scattering spectroscopy
KLI	Krieger–Li–Iafrate
LDA	local-density approximation
LR	long-range
LSDA	local-spin-density approximation
LUMO	lowest unoccupied molecular orbital
m.a.e.	mean absolute error
MP2	second-order Møller–Plesset perturbation theory
NCT	Nifosì–Conti–Tosi
NEGF	nonequilibrium Green's function
OEP	optimized effective potential
PBE	Perdew–Burke–Ernzerhof
PGG	Petersilka–Gossmann–Gross
QV	Qian–Vignale
RPA	random-phase approximation
SDFT	spin-density-functional theory
SIC	self-interaction correction
SMA	small-matrix approximation
SPA	single-pole approximation
SR	short-range
TDA	Tamm–Dancoff approximation
TDCDFT	time-dependent current-density-functional theory
TDDFT	time-dependent density-functional theory
TDELF	time-dependent electron localization function
TDHF	time-dependent Hartree–Fock
TDKLI	time-dependent Krieger–Li–Iafrate
TDKS	time-dependent Kohn–Sham
TDOEP	time-dependent optimized effective potential
TDLDA	time-dependent local-density approximation
TDSDFT	time-dependent spin-density-functional theory
VK	Vignale–Kohn
xc	exchange–correlation