

Abbreviations

AO	Atomic orbital
BZ	Brillouin zone
CI	Configuration interaction
CPA	Coherent potential approximation
CEPA	Coupled electron pair approximation
CNDO	Complete neglect of differential overlap
CO	Crystal orbital
CT	Charge transfer
DEMBPT	Double excitation many-body perturbation theory
DODS	Different orbitals for different spins
EA	Electron affinity
EHF	Extended Hartree-Fock
HF	Hartree-Fock
HFS	Hartree-Fock-Slater
IP	Ionization potential
LCAO	Linear combination of atomic orbitals
LCMTO	Linear combination of muffin tin orbitals
MCSCF	Multi-configuration self-consistent field
MINDO	Modified intermediate neglect of differential overlap
MNDO	Modified neglect of differential overlap
NDDO	Neglect of diatomic differential overlap
PDA	Polydiacetylenes
PPP	Pariser-Parr-Pople
SP	Sugar phosphate
TF	Thomas-Fermi
TFD	Thomas-Fermi-Dirac
UHF	Unrestricted Hartree-Fock