

Appendix (Abbreviations)

This appendix gives a collection of i) abbreviations frequently used in the text and ii) abbreviations for organic metals and one-dimensional solids containing transition-metal atoms.

Abbreviations

AO	atomic orbital
APW	augmented plane wave
BOAW	bond-order alternation wave
CDW	charge density wave
CI	configuration interaction
CO	crystal orbital
CORR	correlation
DA	donor-acceptor
DOS	density of states
EPR	electron paramagnetic resonance
EXAFS	extended X-ray absorption fine structure
GC	grand canonical
HF	Hartree-Fock
INDO	intermediate neglect of differential overlap
IP	ionization potential
LA	local approach
LCAO	linear combination of atomic orbitals
LDA	local density approximation
LR	long-range
MM	metal-metal (interaction)
MLM	metal-ligand-metal (interaction)
MO	molecular orbital
MPREL	pair-relaxation (energy)
MPREM	pair-removal (energy)
MREL	relaxation (energy)
NSI	neighbor strand interaction
OM	organic metal
OPW	orthogonalized plane wave
QP	quasi-particle
SA	symmetry-adapted
SB	symmetry-broken
SCEF	self-consistent-electrostatic-field
SCF	self-consistent-field

SECH	screened-exchange-plus-Coulomb-hole
SR	short range
STO	Slater type orbital
TDSHF	time-dependent screened Hartree-Fock
TM	transition-metal
VB	valence bond
VEH	valence effective Hamiltonian
WH	Wolfsberg-Helmholtz
ZDO	zero differential overlap

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional

Low-Dimensional Systems

Organic Metals

HMTSeF	hexamethylenetetraselenofulvalene
PA	polyacetylene
TCNQ	tetracyanoquinodimethane
TTF	tetrathiofulvalene
TTT	tetrathiotetracene

Systems containing transition-metal atoms

Co(pc)	(phthalocyaninato)Co(II)
Co(tp)	(tetrazaporphyrinato)Co(II)
Fe(gly) ₂ (py)	(bisglyoximato-pyrazine)Fe(II)
Ni(gly) ₂	(bisglyoximato)Ni(II)
Ni(bqd) ₂	(bis-1,2-benzoquinonedioximato)Ni(II)
Ni(p)	(porphyrinato)Ni(II)
Ni(omtbp)	1,4,5,8,9,12,13,16-(octamethyltetrabenzporphyrinato)Ni(II)
Ni(tbp)	(tetrabenzporphyrinato)Ni(II)
Ni(tmp)	5,10,15,20-(tetramethylporphyrinato)Ni(II)
TCP	tetracyanoplatinate
TTSqNi	(tetrathiosquarato)Ni(II)