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APPENDIX

C

GLOSSARY

A

ADEX
Atomic Decomposition of Exchange

ADFT
Analytic Density Functional Theory

ADLD
Atomic Decomposition of London Dispersion

ALPB
Analytical Linearized Poisson-Boltzmann

B

BB
Boys-Bernardi

BSSE
Basis Set Superposition Error

BUPO
Bubblepoles

C

CC
Coupled-Cluster

cc-pVXZ
Dunning's Corrleation Consistent Polarized Valence Basis Set Family of x-tuple Zeta Quality

CCSD
Coupled-Cluster with Singles and Doubles

CCSD(T)
Coupled-Cluster with Singles, Doubles and Perturbative Triples

CI
Configuration Interaction

CNDO
Complete Neglect of Differential Overlap

CP-SCF
Coupled Perturbed Self Consisten Field

CPCM
Conductor-like Continuum Polarization Model

CSF
Configuration State Function

D

DFT
Density Functional Theory

DIIS
Direct Inversion in Iterative Subspace

DLPNO
Domain-Based Local Pair Natural Orbital

DMRG
Density Matrix Renormalization Group

E

ECP
Effective Core Potential

EPR
Electron Paramagnetic Resonance

F

FB
Foster Boys Orbital Localization

FCI
Full Configuration Interaction

G

gCP
Geometrical Counterpoise

GGA
Generalized Gradient Approximation

GS-ROCIS
General-spin Restricted Open-Shell Configuration Interaction Singles

GVPT2
Generalized Vibrational Perturbation Theory of Second Order

H

HF
Hartree-Fock

HOMO
Highest Occupied Molecular Orbital

I

ICE
Iterative Configuration Expansion

INDO
Intermediate Neglect of Differential Overlap

K

KDIIS
Kolmar's DIIS

L

LED
Local Energy Decomposition

LMO
Localized Molecular Orbital

LUMO
Lowest Unoccupied Molecular Orbital

M

MNDO
Modified Neglect of Diatomic Overlap

MO
Molecular Orbital

MP2
M\oller-Plesset Perturbation Theory of Second Order

N

NBO
Natural Bond Orbitals

NCS
Natural Chemical Shielding Analysis

NDDO
Neglect of Diatomic Differential Overlap

NDO
Neglect of Differential Overlap

NMR
Nuclear Magnetic Resonance

O

OO
Orbital-optimized

OPI
ORCA Python Interface

P

PCM
Polarizable Continuum Model

PM
Pipek Mezey Orbital Localization

PNO
Pair Natural Orbital

PP
Pseudopotential

Q

QRO
Quasi-restricted Orbitals

R

RHF
Restricted Hartree Fock

RI
Resolution of the Identity

RIXS
Resonant Inelastic X-ray Scattering

ROCIS
Restricted Open-Shell Configuration Interaction Singles

ROHF
Restricted Open-Shell Hartree Fock

RPA
Random Phase Approximation

S

SCF
Self-consistent Field

SOC
Spin-orbit Coupling

SSC
Spin-spin Coupling

T

TDA
Tamm-Dancoff Approximation

TRAH
Trust-Region Augmented Hessian

U

UCO
Unrestricted Corresponding Orbital

UHF
Unrestricted Hartree-Fock

UKS
Unrestricted Kohn-Sham

UNO
Unrestricted Natural Orbital

V

VCD
Vibrational Circular Dichroism

VPT2
Second-order Vibrational Perturbation Theory

W

WBO
Wiberg Bond Order

WFT
Wave Function Theory

X

X2C
Exact Two-Component

XAS
X-ray Absorption Spectroscopy

XES
X-ray Emission Spectroscopy

XMCD
X-ray Magnetic Circular Dichroism

XPS
X-ray Photoelectron Spectroscopy

Z

ZORA
: Zeroth-Order Regular Approximation

ZPE
: Zero-Point Energy