

List of Abbreviations

AIP	Adiabatic Ionization Potential
ANN	Artificial Neural Network
B3LYP	Combination of Becke exchange functional, three-parameter and Lee-Yang-Parr correlation functional
BCP	Bond Critical Point
BDE	Bond-Dissociation Energy
BE	Binding Energy
BO	Born-Oppenheimer
CC	Couple-Cluster
CFC	Chlorofluorocarbons
CI	Configuration Interaction
DFT	Density Functional Theory
DPF	Diesel Particulate Filter
ECP	Effective Core Potential
EHT	Extended Huckel theory
FES	Fluorinated Esters
GGA	Generalized Gradient Approximation
GTO	Gaussian Type Orbitals
GWP	Global Warming Potential
HCFC	Hydro Chlorofluorocarbons
HF	Hartree-Fock
HFC	Hydrofluorocarbons
HFE	Hydrofluoroethers
HOMO	Highest Occupied Molecular Orbital
IP	Ionization Potential
IRC	Intrinsic Reaction Coordinate
KS	Kohn-Sham
LANL2DZ	Los Alamos National Laboratory (LANL)

	ECP with Double Zeta valence basis set
LDA	Local Density Approximation
LH	Langmuir–Hinshelwood
LUMO	Lowest Unoccupied Molecular Orbital
MM	Molecular Mechanics
MO	Molecular Orbital
ODS	Ozone Depleting Substance
OLD	Ozone Layer Depletion
PBE	Perdew-Becke-Ernzerhof
PC	Product Complexes
PES	Potential Energy Surface
PW	Perdew and Wang
QTAIM	Quantum Theory of Atoms In Molecules
RC	Reactive Complexes
RCP	Ring Critical Point
SCF	Self-Consistent Field
SCR	Selective Catalytic Reduction
STO	Slater Type Orbitals
TFA	Trifluoroacetic Acid
TS	Transition States
TWCC	Three Way Catalytic Converter
TZPE	Thermal Zero Point Energy
UFF	Universal Force Field
VDZ	Valence Double Zeta
VEA	Vertical Electron Affinity
VIP	Vertical Ionization Potential
VOC	Volatile Organic Compounds
VTZ	Valence Triple Zeta
VWN	Vosko, Wilk and Nussair