List of Abbreviations

CWA: Chemical warfare agents
AO: Atomic orbital
SE: Surface energy
COSMO: Conductor-like screening model
OP: Organophosphorus
DFT: Density functional theory
GGA: Generalized gradient approximation
GTO: Gaussian type orbital
UFF: Universal force field
LDA: Local density approximation
MESP: Molecular electrostatic potential
MD: Molecular dynamics
PWC: Perdew-Wang correlational
PCM: Polarized continuum model
PBC: Periodic bond chain
IEF-PCM: Integral equation formalism polarizable continuum model
B3LYP: Becke3 Lee Yang Parr method
SEM: Scanning electron microscopy
SCF: Self-Consistent field
IE: Interaction energy
ZPVE: Zero-point vibrational energy
MP2: Second-order Møller-Plesset theory
BCP: Bond critical point