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LIST OF ABBREVIATIONS

Å	=	Ångström
ADF	=	Angular distribution function
au	=	Atomic unit
B3LYP	=	Becke three-parameter hybrid functional combined with Lee-Yang-Parr correlation function
BJH	=	Flexible water model developed by Bopp, Jancsó and Heinzinger
BSSE	=	Basis set superposition error
PH ₄ ⁺	=	Phosphonium ion
CF2	=	Central force model version 2
cm ⁻¹	=	Wavenumber
CN	=	Coordination number
CPMD	=	Car-Parrinello molecular dynamics
CPU	=	Central processing unit
DFT	=	Density functional theory
def2-SVP	=	Split valence with polarization functions on heavy and light atoms

LIST OF ABBREVIATIONS (Continued)

e	=	Electron charge
E_{tot}	=	Total interaction energy
E_{MM}	=	Interactions within MM region
E_{QM-MM}	=	Interactions between QM and MM regions
$E^{ONIOM-XS}$	=	The potential energy of the entire system for ONIOM-XS
ECP	=	Effective core potential
<i>etc</i>	=	et cetera
F_i	=	Force acting on each particle
F_{MM}	=	MM force
F_{QM}	=	QM force
fs	=	Femtosecond
HF	=	Hartree-Fock
K	=	Kelvin
kcal/mol	=	Kilocalorie per mole
l	=	Number of particles in the switching layer
MC	=	Monte Carlo
MD	=	Molecular dynamics
MM	=	Molecular mechanics
MO	=	Molecular orbital
MP2	=	Second-order Møller-Plesset
MRT	=	Mean residence times

LIST OF ABBREVIATIONS (Continued)

m	=	Mass
m_e	=	Mass of electron
m_k	=	Mass of nucleus
n_1	=	Number of particles in the QM sphere
n_2	=	Number of particle in the MM region
N_{ex}	=	Number of exchange events
ONIOM	=	Own N-layered Integrated molecular Orbital and molecular Mechanics
ONIOM-XS	=	An extension of the ONIOM method for molecular simulation in condensed phase
PP	=	Pseudopotential
ps	=	Picosecond
QM	=	Quantum mechanics
QM/MM	=	Combined Quantum mechanics/molecular mechanics
RDF	=	Radial distribution function
RHF	=	Restricted Hartree-Fock
r_0	=	Distance characterizing the start of QM region
r_1	=	Distance characterizing the end of QM region
r_{min}	=	First minimum of RDF peak
r_{max}	=	First maximum of RDF peak
SCF	=	Self-consistent field
SPC/E	=	Simple point charge effective pair water model

LIST OF ABBREVIATIONS (Continued)

$S_m(r)$	=	Smoothing function
VACF	=	Velocity autocorrelation functions
μ	=	Chemical potential
h	=	Planck's constant
$^{\circ}$	=	Degree
τ_{H_2O}	=	MRT of water molecules
λ	=	Wavelength
t^*	=	Time for observing the number of exchange water
t_{sim}	=	Simulation time