

List of Abbreviations

AA	All-atom
APS	Area per surfactant
ATB	Automated Topology Builder
B3LYP	Becke, 3-parameter, Lee-Yang-Parr
BTMAC	Behenyl trimethylammonium chloride
CG	Coarse-grained
C_n TAB	Alkyl trimethyl ammonium bromide
COM	Centre of Mass
CPK	Corey Pauling Koltun
DFTB	Density functional tight binding
DFT	Density functional theory
DLS	Dynamic Light Scattering
DNA	Deoxyribonucleic Acid
DSC	Differential Scanning Calorimetry
EPR	Electron Paramagnetic Resonance
fs	Femtosecond
GROMACS	Groningen Machine for Chemical Simulation
LH	Left Handed
LJ	Lennard Jones
MD	Molecular Dynamics
μ s	Microsecond
nm	Nanometer
NMR	Nuclear Magnetic Resonance
NPT	Constant number of particles, pressure and temperature
ns	Nanosecond
NVT	Constant number of particles, volume and temperature
P-1	Peptide-perylenediimide molecule (Phe-Phe motif and PDI core)
PBC	Periodic Boundary Conditions
PDI	Perylenediimide

phe	Phenyl
PME	Particle Mesh Ewald
PMF	Potential of mean force
ps	Picosecond
RDF	Radial Distribution Function
RH	Right Handed
SASA	Solvent Accessible Surface Area
SA	Stearyl alcohol
SAXS	Small-angle X-ray Scattering
SCC	Self-Consistent Charges
SDS	Sodium dodecyl sulphate
SPC/E	Simple Point Charge/Extended
SPC	Simple Point Charge
THF	Tetrahydrofuran
UV-vis	Ultraviolet visible spectroscopy
VDW	van der Waals
VMD	Visual Molecular Dynamics
VOTCA	Versatile Object-Oriented Toolkit for Coarse-Graining Applications
VPS	Volume per surfactant
V-Rescale	Velocity rescale