

List of Symbols

C_p	Specific head capacity
κ_T	Isothermal compressibility
α_P	Coefficient of thermal expansion
δ^-	Partial negative charge
δ^+	Partial positive charge
m_i	Mass of i^{th} particle
$\partial^2 r_i$	Second order derivative of displacement
F_i	Force on i^{th} particle
∂V	Potential on i^{th} particle
Δt	Time step
K	Kinetic energy
N_f	Number of degrees of freedom
τ_T	Time constant associated with temperature coupling
P_0	Reference pressure
P	Pressure generated during simulation
τ_P	Time constant associated with pressure coupling
S_{CD}	Deuterium order parameter
θ	Angle between C-D vector and bilayer normal
$S(t)$	Survival probability
$\sum_{i=1}^N$	Summation over N molecules
$\prod_{t_k=t_0}^{t_0+t}$	Product of probabilities of water molecule residing in a specific region
$P_i^{dt}(k)$	Probability of water molecules residing in a layer d for time t_k
$\langle \rangle$	Averaging over time origins
ρ_N	Particle density

D_{trans}	Translational diffusion coefficient
α	Anomalous diffusion exponent
D_L	Lateral diffusion coefficient
$C_v(t)$	Velocity auto correlation function
$v_i(t)$	Velocity of i^{th} particle at time t
$v_i(t_0)$	Velocity of i^{th} particle at initial time t_0
D_A	Diffusion coefficient obtained using Green Kubo relation
$\alpha_2(t)$	Non gaussian parameter
$\Delta r(t)$	Displacement of the molecule
$C_{vl}(t)$	Reorientational auto correlation function
P_l	Legendre polynomial of l^{th} order
$e_i^v(t)$	Bond vector at time t
$C_{HB}(t)$	Hydrogen bonding auto correlation function
τ_{HB}	Hydrogen bond lifetime
τ_α	α -relaxation time
τ_i	Intermediate time relaxation
τ_l	Long time relaxation
τ_s	Short time relaxation
k	Forward rate constant
ΔG^\ddagger	Gibbs energy of hydrogen bond activation
K_B	Boltzmann constant
h	Planck's constant
T	Temperature
δ	Dirac-delta function