List of Symbols

v_0	Critical chain volume
a_h	Optimal head-group area
l_c	Critical chain length
$\vec{E}$	Electric field
μ	Dipole moment
q	Charge
α	Polarizability
V	Potential energy
k	Force constant
σ	Distance of closest approach
ϵ	Interaction strength
ϵ_0	Permittivity of free space
F	Force
m	Mass
a	Acceleration
∇	Gradient
d	Bilayer thickness
I	Interdigitation
$g(r)$	Radial distribution function
N	Total number of particles
ρ	Mean particle density
R_g	Radius of gyration
R_h	Hydrodynamic radius
I_{min}, I_{avg}	Minimum of moment of inertia and average of moment of inertia
e	Eccentricity
β	Angle between C-D bond vector and bilayer normal
S_{CD}	Deuterium order parameter
$P(q,T)$	Bonded distribution
$U(q,T)$	Coarse-grained bonded potential energy

K_B	Boltzmann constant
λ	Asymmetry
$O_{overlap}$	Extent of interdigitation
L_a	Average chain length
$S_{conf}^{per-chain}$	Per chain configurational entropy
T	Temperature
M	3N-dimensional diagonal matrix
C	Covariance matrix
$\vec{r}_{th}$	Head to tail vector
θ_{tilt}	Tilt angle
P_2	Second rank order parameter
S_0	Residual entropy
R	Universal gas constant
T_s	Kinetic energy
E	Kohn Sham energy
$E_{ME}, E_{DE}, \Delta E_{BE}$	Monomer, dimer and binding energy
$U^b(r), U^u(r)$	Biased and unbiased potential energy
ξ	Reaction co-ordinate
$u_i(\xi)$	Biased potential
$P_i^b(\xi), P_i^u(\xi)$	Biased and unbiased distribution
$F_i(\xi)$	Unbiased free energy
U_{rot}	Potential due to rotation restraint
ω	Rotation matrix
$\hat{V}$	Unit vector parallel to the axis of rotation
$\sigma_{PMF}(\xi)$	Standard deviation in bootstrapped PMF
$r^2(t)$	Mean square displacement
t, t_0	Time and time origin
D	Diffusion co-efficient
$C_{HB}(t)$	Hydrogen bond auto correlation function
τ	Relaxation time
$G_{break}^{\ddagger}$	Free energy for hydrogen bond breaking
h	Planck's constant
$<>$	Time averaging