

List of Tables

<i>Table</i>	<i>Title</i>	<i>Page</i>
2.1	Parameters for SPC, TIP3P and TIP4P/2005 water models.	18
2.2	Categorization of hydrated systems based on force fields and water models.	20
2.3	Area per head-group (a_h), bilayer thickness (d), deuterium order parameter ($ S_{CD} $), lateral diffusivity (D_L) and surface tension (γ_s) of the DMPC bilayer from our simulations and previously performed experiments at 308 K.	23
2.4	Residence time scales for water computed over 1 ns time window with sampling frequency of 1 ps. Correlation coefficient is >0.99	26
2.5	Diffusion constants (D_{trans}) (in 10^9 D, m^2s^{-1}) calculated from VACF and MSD of BW for both models.	28
3.1	Values of α and diffusion coefficient (D_{trans}) for translational MSD fitted with function At^α . Correlation coefficients for all classes are >0.99	39
3.2	Reorientational relaxation time scales for \hat{n} for all classes of water. Correlation coefficients are >0.99 . Slow relaxation time scale (τ_s) for second order rotational auto-correlation function for \hat{n} of the IW and the BW are compared with experimental and simulation data showing the applicability of Berger force fields in combination with TIP4P/2005 water model.	42
3.3	Reorientational relaxation time scales for \vec{OH} for all classes of water. Correlation coefficients are >0.99 .	43
3.4	Reorientational relaxation time scales for \vec{HH} for all classes of water. Correlation coefficients are >0.99 .	44
3.5	Reorientational relaxation time scales for $\vec{\mu}$ for all classes of water. Correlation coefficients are >0.99 .	45
3.6	Hydrogen bond lifetime and Gibbs energy of activation for interface and bulk waters. Hydrogen bond lifetime (τ_{HB}) of the IW and the BW are compared with the previous simulation and experimental data to show the suitability of the Berger force fields in combination with TIP4P/2005 water model.	48
4.1	Relaxation time scales (τ_{α_2}) for all classes of IW and BW corresponding to peak of NGP.	59
4.2	Fitting parameters of SISFs for all classes of IW and BW. Correlation coefficients are >0.99 . The relaxation times of IW (τ_l) and BW (τ_α) are compared with literature showing the suitability of Berger force fields in combination with TIP4P/2005 water model.	63
4.3	Reorientational correlation relaxation time scales for lipid head, tail and IW. All correlation coefficients were >0.99 .	64
5.1	Time of entrance to the sub-diffusive regime for different classes of IW^{HB} as obtained from 10 sets of MSD_{XY} .	80
5.2	Time of entrance to the sub-diffusive regime of DMPC beads as obtained from average of 10 sets of MSD_{XY} .	83
5.3	Fitted parameters of SISF of different moieties of DMPC molecule for $\lambda = 0.60$ nm along the chain. All correlation coefficients are >0.99 .	84
5.4	Fitted parameters of SISF of all classes of IW^{HB} for $\lambda = 0.60$ nm. Correlation coefficients are >0.99 .	84

