RESULTS

Structural parameters

Table 3 – Structural properties of bilayers calculated via molecular dynamics simulation using GAFFlipid and comparison to experiment and, where available, simulations using standard GAFF parameters, for three system sizes of six different phospholipid types.

Lipid system	Area per lipid A_L (Å^2)	Volume per lipid V_L (Å^3)	Isothermal area compressibility modulus K_A (mNm^{-1})	Peak distance D_{HH} (Å)
DLPC				
72	59.97±0.0007	1008.79±0.14	291±64	31.6
288	60.45±0.059	1009.98±0.17	336±7	30.6
2x288	62.4±0.42	1007.78±0.4	422±297	31.5±0.85
Experiment	63.2[36]	991[36]	-	30.8[36]
DMPC				
72	59.95±0.15	1117.83±0.51	299±75	33.6±1
288	60.38±0.0039	1115.81±0.31	368±74	34.6
2x288	61.05±0.72	1105.11±0.36	150±150	37±1
GAFF	55.8[23]	1097.4[23]	-	35.2[23]
Experiment	60.6[39]	1101[1, 36]	234[40]	35.3[39]
DPPC				
72	61.24±0.4	1265.46±0.8	274±22	37.6±0.72
288	61.77±0.21	1264.51±0.63	243±21	37.6
2x288	61.75±0.012	1267.24±0.29	713±143	39
Experiment	63[41]	1232[1]	231[1]	38.3[1]
DOPC				
72	66.79±0.069	1327.41±0.38	314±39	37.6±0.14
288	67.4±0.03	1328.9±0.11	392±87	37.6
2x288	67.17±0.061	1326.35±0.11	1317±359	38
GAFF	65[23],62[22]	1333.8[23]	-	38.4[23],40[22]
Experiment	67.4,[41] 72.5[1]	1303[1]	254,[42] 265[40]	35.3[43]
POPC				
72	63.74±0.22	1277.31±0.16	391±81	37.6
288	63.91±0.059	1279.97±0.15	259±276	37.6±0.71
2x288	64±0.058	1276.91±0.29	1147±23	37.5±0.5
GAFF	50.5[21]	-	-	-
Experiment	64.3,[44] 68.3[37]	1256[37]	180-330[45]	37[37]
POPE				
72	55.64±0.19	1185.21±0.68	484±34	43.4±0.28
288	55.33±0.11	1175.3±0.25	282±116	43.6±0.41
2x288	56.15±0.19	1185.58	847±244	43
Experiment	59-60[46]	1180[46]	-	39.5[46]