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Interbilayer repulsion forces between tension-free lipid bilayers from simulation: Supporting Information

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Structure factor

The scattering functions of alkyl chains obtained from experiments and simulations shown in Figure 1. The experimental scattering data are for the full (RH=98%) and intermediate hydration (RH=75%). The simulation data are for the full (d_w = 3.8 nm), intermediate (d_w = 1.6 nm), and low hydration (d_w = 1.0 nm). The experimental scattering intensity is in Photon counts, but a chamber background has been subtracted. The square root of the intensity is an approximation for the statistical error. The data (after chamber background subtraction) shows the chain-correlation

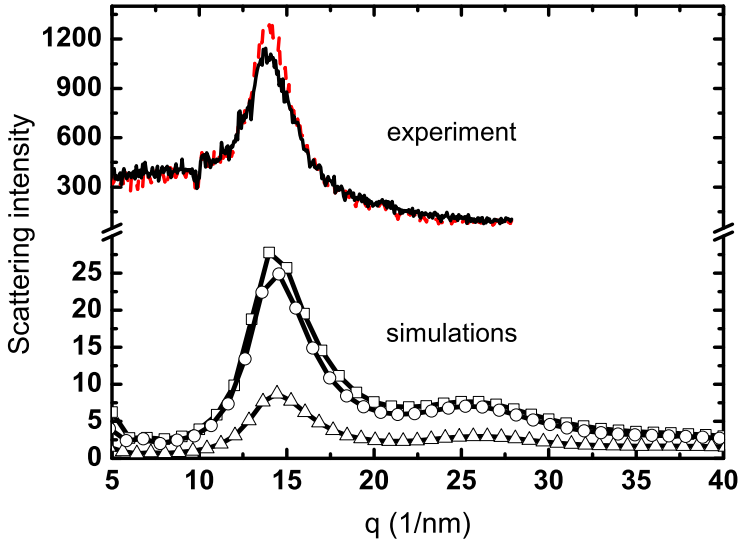

Figure 1: Scattering intensity for experimental (full line (RH=98%) and dashed line (RH=75%)) and simulation (squares ($d_w = 1.0\,\mathrm{nm}$), circles ($d_w = 1.6\,\mathrm{nm}$), and triangles ($d_w = 3.8\,\mathrm{nm}$)) data.

peak on a lipid sample related background, q-values are in reciprocal manometers and are very precise. The simulation scattering intensity was calculated using the formula

$$S(\mathbf{q}) = 1 + \frac{1}{N\langle f\rangle^2}\sum_{i\neq j} f_j^* f_i \exp(i\mathbf{q}\mathbf{r}_{ij}), \tag{1}$$

where f_i is the scattering factor of a coarse grained bead i (for chain beads scattering factors were calculated like for carbon atoms, using Cromer-Mann fit). The sum goes over all pairs of beads (excluding the self-term) in the periodic cubic cell of size L and is evaluated at $q_{lmn} = \frac{2\pi}{L}\sqrt{l^2+m^2+n^2}$ for a system with periodic boundary conditions. Only x and y components of the distance $\mathbf{r}_{ij}$ are used. The step size along q is defined by the system size L. Both experimental and simulation scattering functions show the chain-correlation peak at about $14\,\mathrm{nm}^{-1}$, though the

second peak at ~25 nm^{-1} is only present in simulation data. The scattering intensity increases with dehydration for experiments and simulations in similar fashion, indicating a tendency of lipids to order.

Bilayer thickness change upon dehydration

Here we present data points related to Figure 5.

d_{com}/nm	d_w/nm	d_{hh}/nm
7.40	3.35	3.99 ± 0.01
7.05	3.05	4.02 ± 0.04
6.70	2.75	4.11 ± 0.07
6.36	2.32	3.94 ± 0.01
6.01	2.04	3.96 ± 0.01
5.67	1.73	3.91 ± 0.02
5.34	1.48	3.91 ± 0.01
5.01	1.27	3.85 ± 0.03
4.79	1.11	3.74 ± 0.02

Table 1: The bilayers center-of-mass distance, d_{com}, the water, d_w, and the bilayer, d_{hh}, thickness are given for the umbrella sampling system. Only some data points are given.

N_w/N_{lip}	d_w(small)/nm	d_{hh}(small)/nm	d_w(large)/nm	d_{hh}(large)/nm
37.5	3.82	3.96 ± 0.03	3.78	4.02 ± 0.02
28.1	2.97	3.94 ± 0.01	2.89	4.02 ± 0.02
25.0	2.65	3.98 ± 0.04	2.63	4.05 ± 0.01
21.9	2.41	3.93 ± 0.06	2.35	4.02 ± 0.02
20.3	2.22	3.99 ± 0.01	2.19	4.00 ± 0.01
18.8	2.14	3.93 ± 0.04	2.08	4.04 ± 0.01
17.2	1.99	3.96 ± 0.05	1.94	4.01 ± 0.01
15.6	1.83	3.99 ± 0.02	1.81	4.05 ± 0.01
14.1	1.71	4.00 ± 0.02	1.67	4.04 ± 0.02
12.5	1.61	3.98 ± 0.04	1.55	4.05 ± 0.02
10.9	1.49	4.00 ± 0.01	1.43	4.07 ± 0.02
9.4	1.32	4.05 ± 0.03	1.31	4.08 ± 0.01
7.8	1.25	4.09 ± 0.04	1.22	4.13 ± 0.01
6.3	1.19	4.11 ± 0.02	1.16	4.14 ± 0.01
5.0	1.02	4.21 ± 0.03	1.03	4.20 ± 0.01

Table 2: The number of water molecules per lipid, N_w/N_{lip}, the water, d_w, and the bilayer, d_{hh}, thickness are given for the small (one bilayer) and large (two bilayers) system.

P_{osm}/bar	d/Å	d_{hh}/Å	d_w/Å
58 ± 20	53.48 ± 0.13	38.63	14.85
102 ± 20	52.59 ± 0.13	39.34	13.26
137 ± 20	52.37 ± 0.08	39.82	12.55
176 ± 21	52.24 ± 0.10	40.22	12.02
215 ± 21	52.14 ± 0.13	40.56	11.58
255 ± 21	52.13 ± 0.12	40.93	11.20
295 ± 21	52.14 ± 0.13	41.27	10.87
338 ± 22	52.14 ± 0.13	41.57	10.58
429 ± 23	52.20 ± 0.08	42.13	10.07
523 ± 23	52.32 ± 0.05	42.63	9.69
627 ± 24	52.38 ± 0.09	43.04	9.35
737 ± 26	52.48 ± 0.06	43.39	9.09
860 ± 27	52.60 ± 0.12	43.74	8.86

Table 3: Experimental data for the osmotic pressure, P_{osm}, the lamellar spacing, d, the bilayer, d_{hh}, and the water, d_w, thickness.