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

Y.G. Smirnova[1,*], S. Aeffner[2], H.J. Risselada[3], T. Salditt[2], S.J. Marrink[4], M. Müller[1] and V. Knecht[5,6]

[1]Georg August University, Institute for Theoretical Physics, 37077 Göttingen, Germany

[2]Georg August University, Institute for X-Ray Physics, 37077 Göttingen, Germany

[3]Max-Planck Institute for Biophysical Chemistry, 37077 Göttingen, Germany

[4]Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

[5]Max-Planck Institute of Colloids and Interfaces, Department of Theory and Bio-Systems, Research Campus Golm, 14424 Potsdam, Germany

[6]Albert Ludwigs University, Institute of Physics, 79104 Freiburg, Germany

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

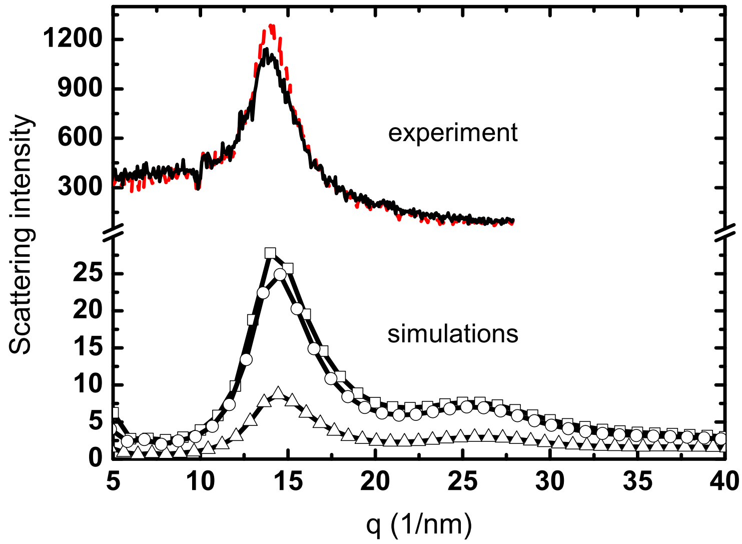

Figure 1: Scattering intensity for experimental (full line (RH=98%) and dashed line (RH=75%)) and simulation (squares (d_w = 1.0 nm), circles (d_w = 1.6 nm), and triangles (d_w = 3.8 nm)) data.

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 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.