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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

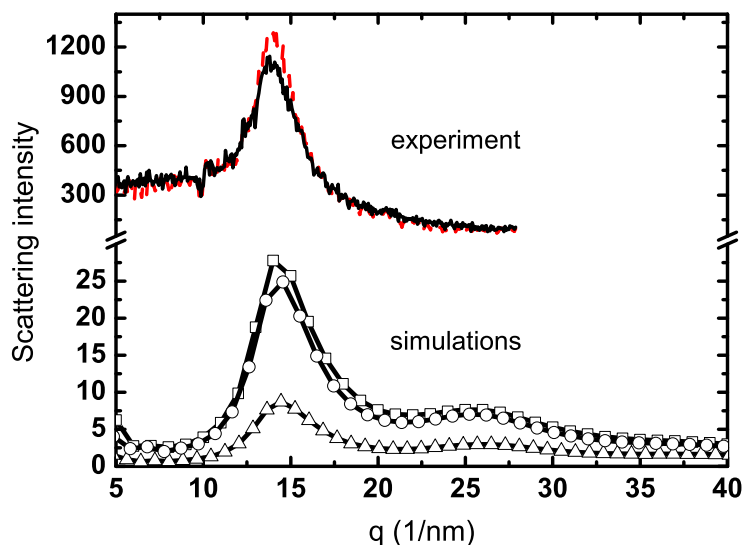


Figure 1: Scattering intensity for experimental (full line (RH=98%) and dashed line (RH=75%)) and simulation (squares ( $d_w = 1.0$  nm), circles ( $d_w = 1.6$  nm), and triangles ( $d_w = 3.8$  nm)) data.

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

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

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  $14 \text{ nm}^{-1}$ , though the

second peak at  $\sim 25 \text{ nm}^{-1}$  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.

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

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

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

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.

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

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