Asymmetric Nature of Lateral Pressure Profiles in Supported Lipid Membranes and Its Implications for Membrane Protein Functions-Supplementary Material

Chenyue Xing[1], O. H. Samuli Ollila[2], Ilpo Vattulainen[2,3,4], and Roland Faller[*,1]

[1]Department of Chemical Engineering and Materials Science, University of California, Davis, California, USA; [2]Department of Physics, Tampere University of Technology, Tampere, Finland; [3]MEMPHYS – Center forBiomembrane Physics, University of Southern Denmark; [4]Department of Applied Physics, Helsinki University of Technology, Finland

E-mail: rfaller@ucdavis.edu

Supporting Material

I. Visualization

The system is visualized in Figure S1.

II. The MARTINI coarse grain model

The MARTINI coarse grain model[1] is a semiquantitatively accurate model for amphiphilic molecules. Each coarse grained interaction site has an effective size of 0.47nm and a mass of 72 amu, representing 3-5 heavy atoms. The bonding and chain stiffness are described by harmonic potentials. Non-bonded interaction is described by Lennard-Jones potential and the electrostatic is treated by a Coulombic potential. Relative dielectric constant ε_0 is 20, for explicit screening. The model is systematically parameterized based on thermodynamic data, including experimental partitioning. It is shown to reproduce structural, elastic, dynamic and thermodynamic properties of a range of systems[2], including water, alkanes, lipids and cholesterols. It has also been used to study the phase behavior of the lipid systems[3-5].

We use a variant of the MARTINI model, which has a weakened water-water interaction[6]. The original water model in the MARTINI forcefield freezes too easily when a solid phase is present in the system. Although an anti-freeze particle type is introduced in the MARTINI model, we

have found it only working for systems at low temperature without a solid phase[7]. We found the compromised water-water interaction strength to accommodate our needs in studying the supported bilayer systems.

III. Comparison of CG and atomistic simulation models.

To illustrate the linkage, we need to compare the lateral pressure profiles of the bilayer systems using CG and atomistic simulation models. However, a simulation of a supported bilayer using an atomistic model is difficult to equilibrate because the equilibration of the water layer thickness between the bilayer and the substrate takes place on a microsecond scale even in a CG system.[7] It is thus more reasonable to compare the results of free-standing bilayers using different models. Figure S2 plots the two pressure profiles of free-standing DPPC bilayers, one atomistic and the other coarse-grained. In the atomistic case we used the same model described as in ref [8]. The pressure profile of the CG system is less pronounced than in the atomistic system, as expected due to coarse graining, but overall the qualitative agreement is good. Comparing the peak values obtained from the simulation models, a factor of about 4 is needed to map the CG to the atomistic model.

IV. Discussion of the slab size for density profile calculation:

For comparison, the influence of the choice of slab sizes on the density profiles is shown in Fig. S3. In the supported bilayer, larger slab size still reflects the strong ordering inflicted by the solid surface with a little smoothing effect. It reduced the possible artifacts introduced by using CG model which employs larger size interaction sites. In the free-standing bilayer, as no strong ordering exists in either leaflet, the CG model gives smooth density profile with both 0.1 nm and 0.2 nm slab sizes.

V. Lateral pressure profiles of CG supported bilayer with 512 DPPC lipids.

In the paper, we discussed the lateral pressure profile of supported bilayer with 128 DPPC lipids in both atomistic and CG models. As CG models allow simulations for larger systems, we here present the lateral pressure profile of a CG supported bilayer with 512 DPPC lipids (shown in

Fig. S4) to show that the heterogeneity of lateral pressure not only occurs in small system. The

simulation detail of the supported bilayer with 512 lipids was described in our previous

publication.[7]

From Fig. S4, we can still observe the local pressure peaks corresponding to the ordered proximal

water layer and proximal leaflet. While at distances larger than -1.5 nm, the peaks die out to

smooth curve, back to the situation of free standing bilayers. The lateral pressure profile of the

distal leaflet looks the same as that of the leaflets in free standing systems. In both sizes of

supported bilayers (with 128 lipids or 512 lipids), the proximal leaflets were suppressed by the

solid substrate which then led to strong tension at positions close to the substrate.

We also show the lateral pressure profile of a free standing DPPC bilayer of 512 lipids simulated
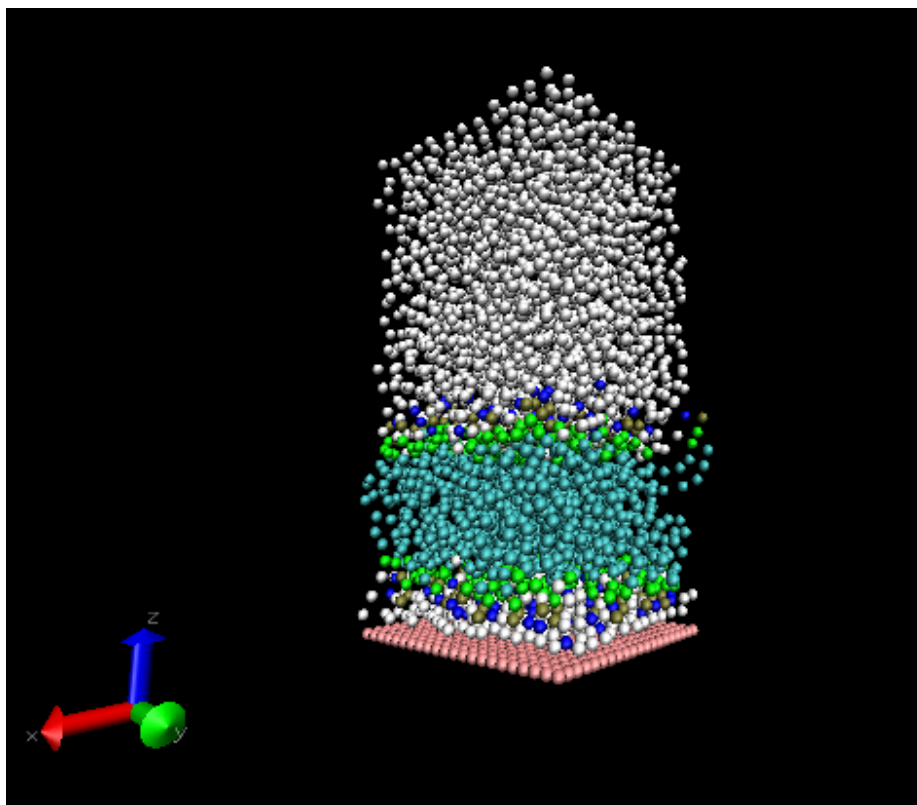
by CG model (Fig. S5).

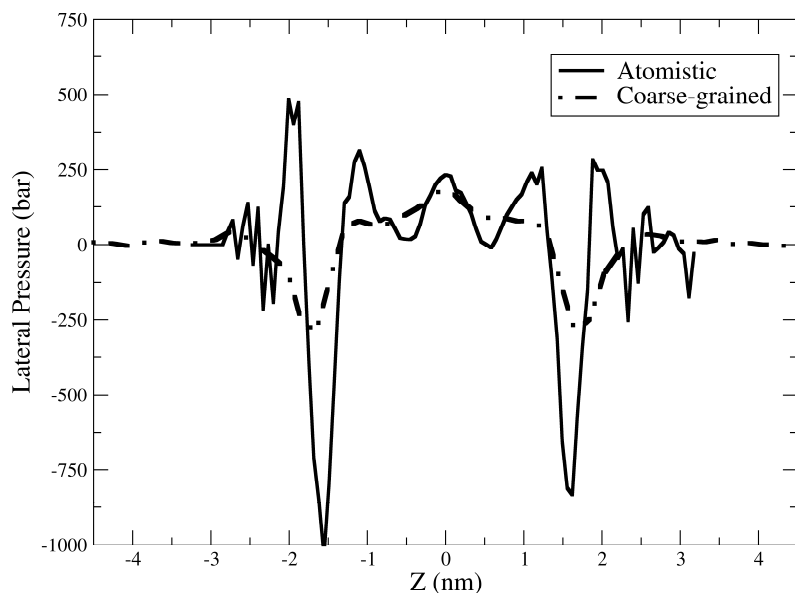Figure S1. Snapshot of supported DPPC bilayer (128 lipids).

Figure S2. Comparison of lateral pressure profiles of free-standing DPPC bilayers in CG and atomistic simulation models. Note that the scales are here not fully comparable to those in Figure 1, since in this figure the water-water interaction was not adjusted to account for substrate in order to be closer to the atomistic system.
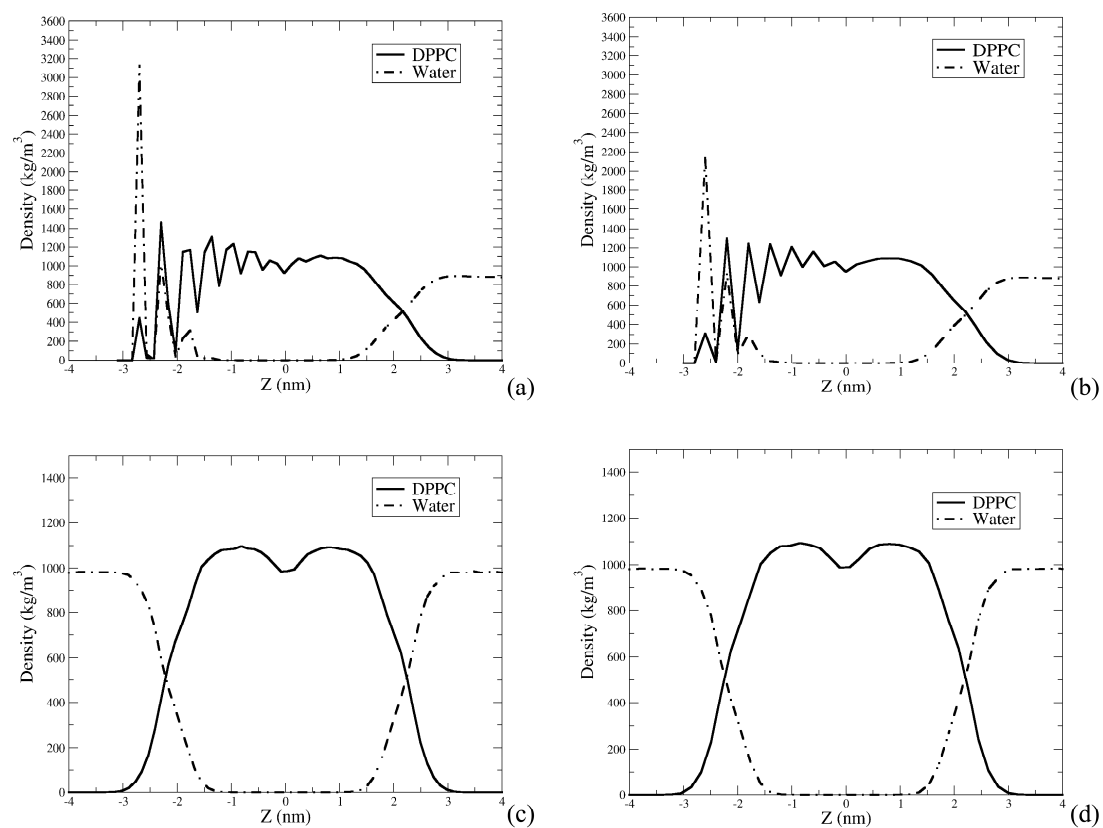
Figure S3. Density profiles of supported and free standing DPPC bilayer of 128 lipids, CG model. (a) supported, slab size = 0.1 nm; (b) supported, slab size = 0.2 nm; (c) free-standing, slab size = 0.1 nm; (d) free-standing, slab size = 0.2 nm.
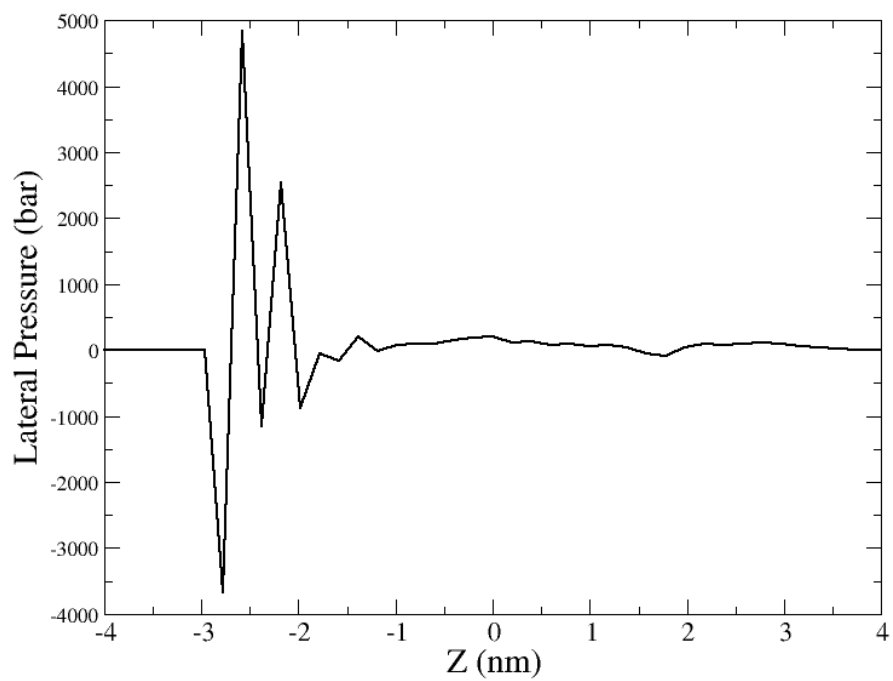
Figure S4. Lateral pressure profile of supported DPPC bilayer with 512 lipids, CG model.
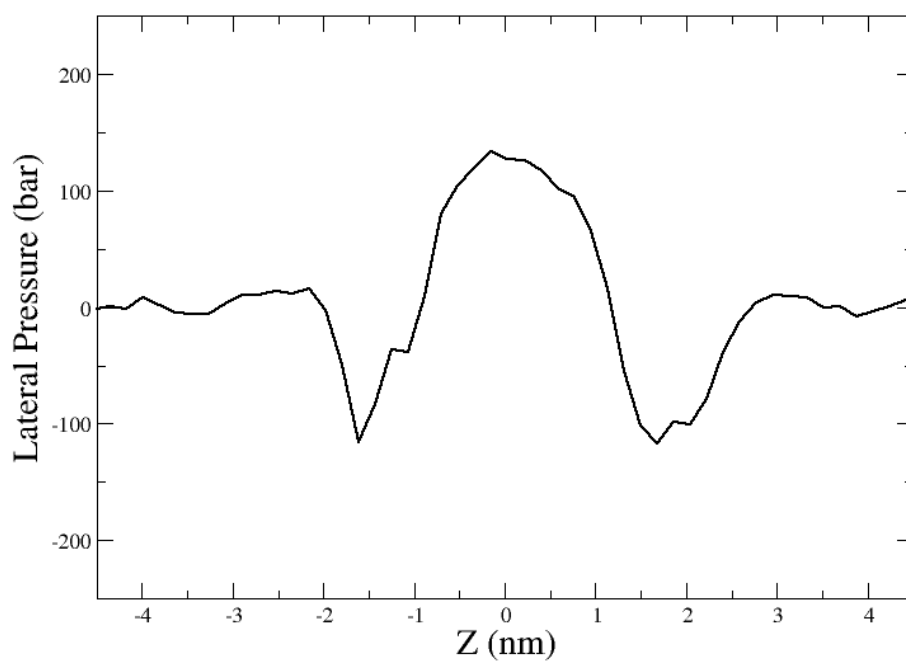
Figure S5. Lateral pressure profile of free standing DPPC bilayer of 512 lipids, CG model.

1.   S. J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman and A. H. de Vries, *Journal of Physical Chemistry B*, 2007, **111**, 7812-7824.
2.   S. J. Marrink, A. H. de Vries and A. E. Mark, *Journal of Physical Chemistry B*, 2004, **108**, 750-760.
3.   S. V. Bennun, M. Longo and R. Faller, *Journal of Physical Chemistry B*, 2007, **111**, 9.
4.   S. V. Bennun, M. L. Longo and R. Faller, *Langmuir*, 2007, **23**, 12465-12468.
5.   S. J. Marrink, J. Risselada and A. E. Mark, *Chemistry and Physics of Lipids*, 2005, **135**, 223-244.
6.   S. V. Bennun, A. N. Dickey, C. Y. Xing and R. Faller, *Fluid Phase Equilibria*, 2007, **261**, 18-25.
7.   C. Xing and R. Faller, *Journal of Physical Chemistry B*, 2008, **112**, 7086-7094.
8.   A. N. Dickey and R. Faller, *Biophys J*, 2007, **92**, 2366-2376.