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SUPPLEMENTARY INFORMATION
Structural and mechanical parameters of lipid bilayer membranes using a lattice refined Self-consistent field model

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1 Grandpotential density variations

In this section, we provide a quick overview of the changes found in the grand potential density (GPD) profiles upon a select few parameter variations. Find below in figure S1 the GPD profiles of our model lipid bilayer with various variations in χ_{CW} parameters. While discussing these results, we will be speaking in terms of various regions of this GPD profile, i.e. regions 1 to 5, which have been defined in the main article. We will first discuss the general GPD profile changes after which we will shortly discuss the consequences for the mechanical parameters $\bar{\kappa}$ and J_0^m.

As can be seen in figure S1, the effect of χ_{CW} is quite substantial, whether the interaction parameter change occurs in the tails, glycerol backbone, or in the headgroup. In the figure, the solid line represents a more hydrophilic tail, glycerol, or headgroup compared with the dashed line. The negative regions (regions 2 and 4) represent a stopping force for self-assembly, and positive regions (regions 1, 3, and 5) represent a driving force. A discussion on each region is given in the main text. As we are looking at a tensionless bilayer, the driving forces and stopping forces are equally balanced, but we observe a change in the ratio of the two stopping forces when varying the χ parameters. For all cases, we observe a decrease in region 2 and an increase in region 4. This suggests that tail stretching (region 2) becomes a more important stopping force compared to the headgroup overlap (region 4) as the lipid becomes more hydrophobic. The main driving force occurs in region 3 (the large positive peak), and it represents the hydrophobic-hydrophilic interface. The height of this peak is effectively dependent on how strong the repulsion of the hydrophobic and hydrophilic region is. The stronger the repulsion, the larger the peak. When increasing χ_{C_TW}, we observe an increase in region 3, see figure S1A, while increasing χ_{C_GW} and χ_{C_HW}, a decrease in region 3 is observed, see figure S1B and C. In short, more hydrophobic tails increase the repulsion of the hydrophilic-hydrophobic interface, whereas an increased hydrophobicity of the glycerol backbone or the headgroup, which are generally more hydrophilic in nature, decreases this repulsion.

Some individual effects are also visible and worth mentioning. For the case of varying χ_{C_TW} (figure S1A), in addition to the changes in $\omega(z)$, we observe a shift to higher z as well. This is consistent with a significant increase in the bilayer core width (d_{OO}) due to tail stretching, see main figure 5A. A different effect is seen when changing χ_{C_HW} (figure S1C) where we find a significant positive peak in region 5. For these circumstances, we expect that the bilayers are mutually attractive, as is explained in the main article.

Also discussed in the main article is that an increase in hydrophobicity of the lipid, no matter the region, leads to an increase in $\bar{\kappa}$ and a decrease in J_0^m. As these parameters directly follow from the GPD profiles, it seems like the clue to understanding these effects can thus be found in the GPD profile. Changes in $\bar{\kappa}$ and J_0^m occur when ω changes as well, and as $\bar{\kappa}$ scales with z^2 and J_0^m scales with z, increases or decreases to ω at higher z have substantially more effect compared to at lower z. Taking this into account, it thus seems like the change in ratio of the two stopping forces, are the main instigators to the changes in $\bar{\kappa}$ and J_0^m. As a lot of questions remain concerning the GPD profiles and the immense amount of information it contains, we abstain from going into too much detail. A more in-depth study is required.

2 Bilayer thickness results

The most important structural results are provided in the main article, yet for a few arguments, other structural parameters, such as the bilayer thickness (d_{NN}) are useful. Find results of d_{NN} in figure S2. As can be seen from the figure, d_{NN} increases with increasing χ_{C_TW} or tail length (figure S2A), and decreases with increasing χ_{C_HW} (figure S2B). The discussion on these results can be found in the main article.

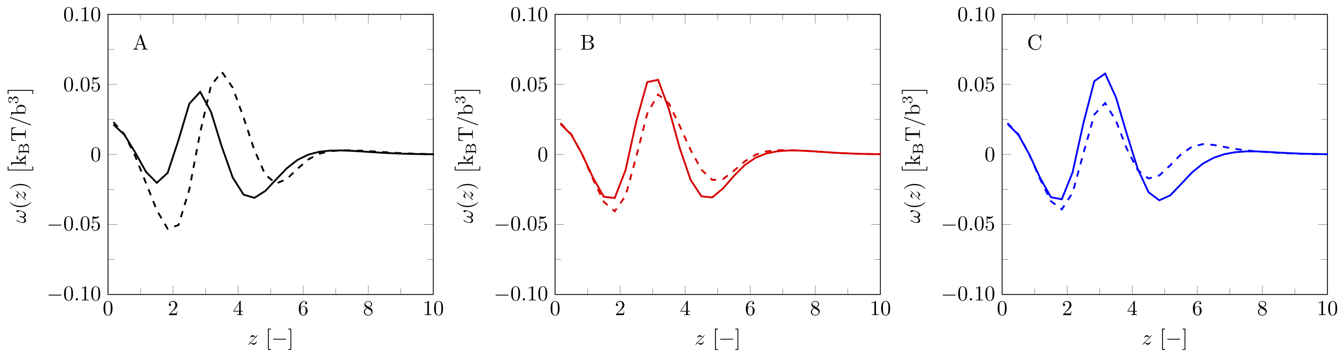

Figure S1 Grandpotential density profiles for lipid bilayers with variations in $\chi_{C_W T}$ (A), in $\chi_{C_G W}$ (B) and in $\chi_{C_H W}$ (C). Solid black line: $\chi_{C_T W} = 1.0$; Dashed black line: $\chi_{C_T W} = 1.5$; Solid red line: $\chi_{C_G W} = 1.0$; Dashed red line: $\chi_{C_G W} = 1.5$; Solid blue line: $\chi_{C_H W} = 0.4$; Dashed blue line: $\chi_{C_H W} = 0.9$;

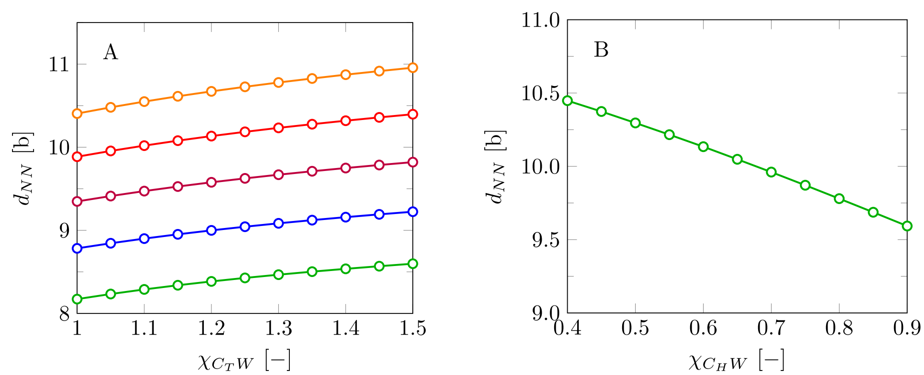

Figure S2 d_{NN} as a function of $\chi_{C_T W}$ (A) and $\chi_{C_H W}$ (B). For (A) we display the results for various tail lengths: Green: $l_t = 12$ C segments, blue: 14 segments, purple: 16 segments, red: 18 segments, orange: 20 segments.