Supporting Information

Effects of High Pressure on Phospholipid Bilayers

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Electron density profiles

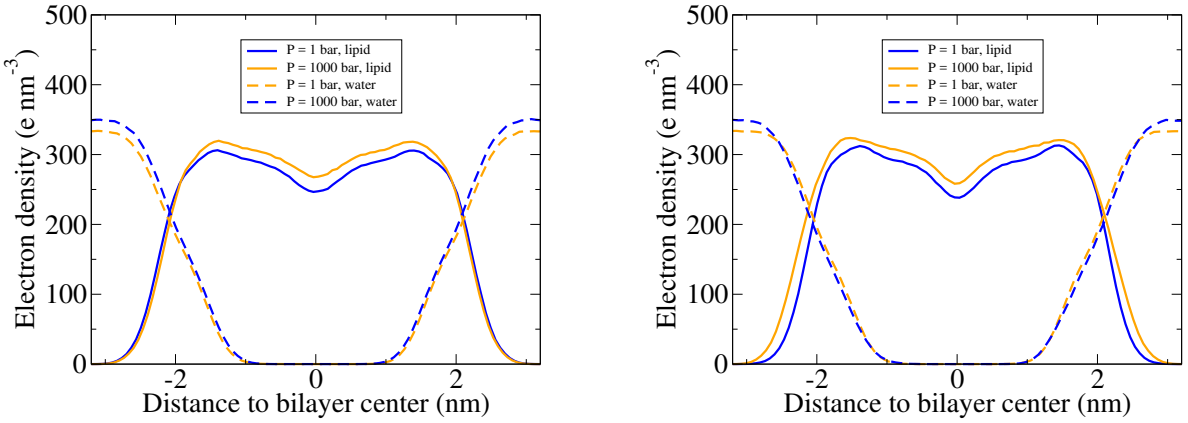

Figure S1: Electron density of the individual water and lipid components for (a) DOPC and (b) POPC bilayers at 1 bar (blue) and 1000 bar (orange).

Headgroup orientation

We calculated the angle between the lipid head P-N vector and the z-axis (i.e. the bilayer normal). For DOPC, the angle is 69.53 ± 0.20 degrees at 1 bar and 69.24 ± 0.23 degrees at 1000 bar, while for POPC it is 69.38 ± 0.22 degrees at 1 bar and 69.54 ± 0.22 degrees at 1000 bar. Statistically, the differences for both pairs are not significant ($p > 0.05$). Incidentally, the absence of a significant effect on the headgroup orientation is consistent with the results obtained for the dipole potential, when one considers that the P-N vector is the main contributor (in terms of magnitude) to the overall dipole potential.

Hydrogen bonds

The table below reports the average number of hydrogen bonds per lipid formed between lipid head groups and water molecules ("Head-Water"), and between lipid head groups themselves ("Head-Head"):

Number	DOPC		POPC	
of H bonds	1 bar	1000 bar	1 bar	1000 bar
Head-Water	6.87 ± 0.04	6.91 ± 0.03	6.60 ± 0.03	6.66 ± 0.03
Head-Head	0.34 ± 0.02	0.34 ± 0.01	0.38 ± 0.01	0.39 ± 0.01