Modelling of noble anesthetic gases and high hydrostatic pressure effects in lipid bilayers. Supplemental Material.

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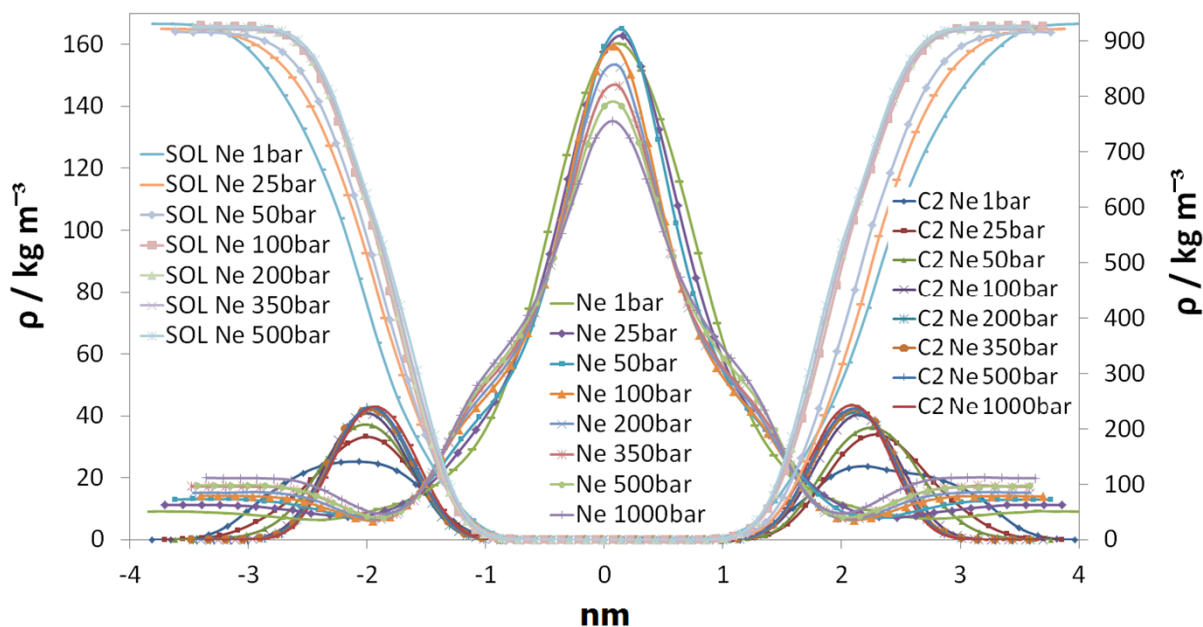
Figure S1A. Density distributions across the simulation box are shown for Ne and DOPC choline group carbon atoms (left scale) and water (right scale) at 1 - 1000 bar. The irregular DOPC-solvent boundary is traceable in the 1 - 100 bar pressure range.

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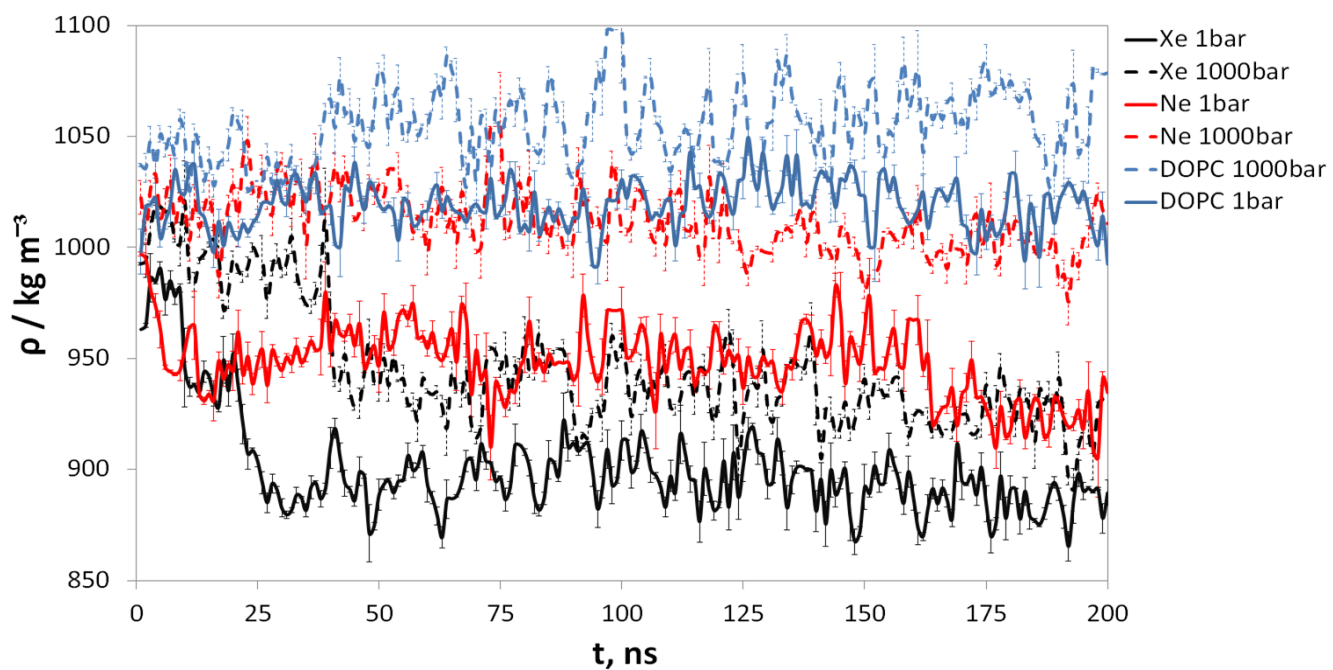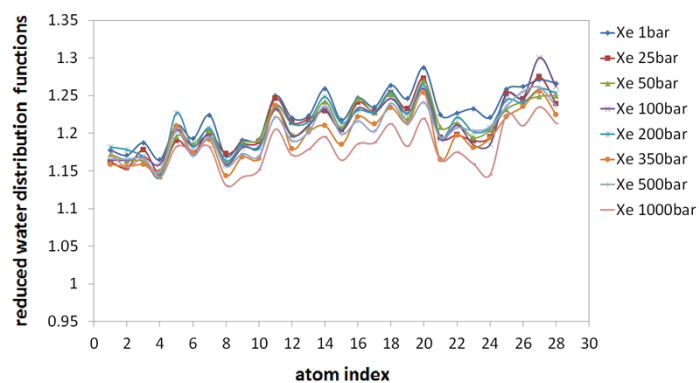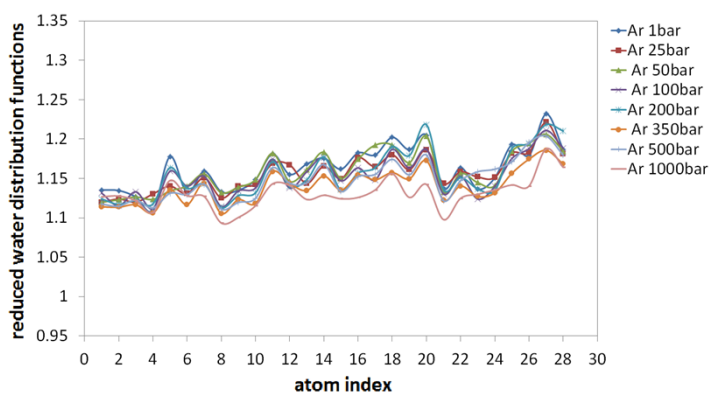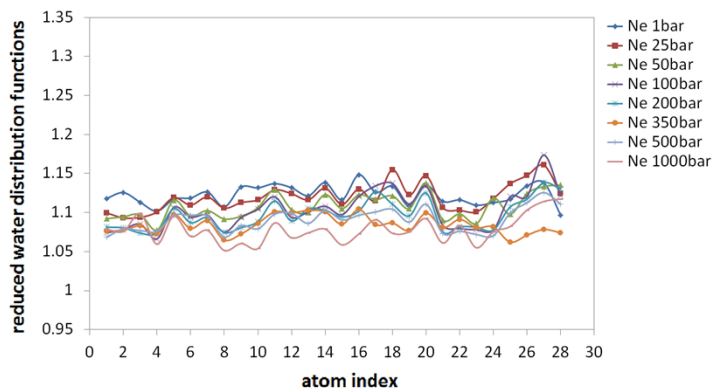
Figure S1B. The maximal densities peaks fluctuations across simulation box v. simulation time are shown for DOPC (blue lines), and DOPC saturated with Ne (red lines) and Xe (black lines), at 1bar (continuous lines) and 1000 bar (broken lines).
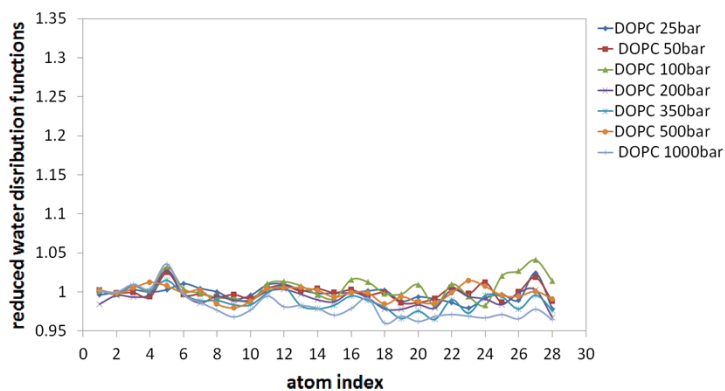
A

B

C

D

Figure S2. The relative differences in water density are presented as averaged over 0.2-1.0 nm range normalized radial distribution functions for water-headgroup DOPC atoms of the gas-saturated bilayer at 1 - 1000 bar: Xe (A); Ar (B); Ne (C); intact DOPC (D). The reference point is the water distribution of intact DOPC at standard conditions. The solvation potential of noble gases is shown as curves above 1.0. HHP demonstrates a dehydration effect.
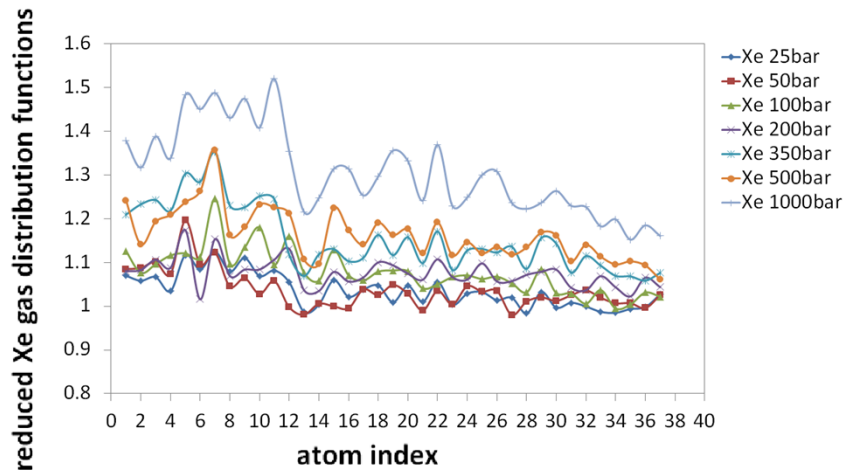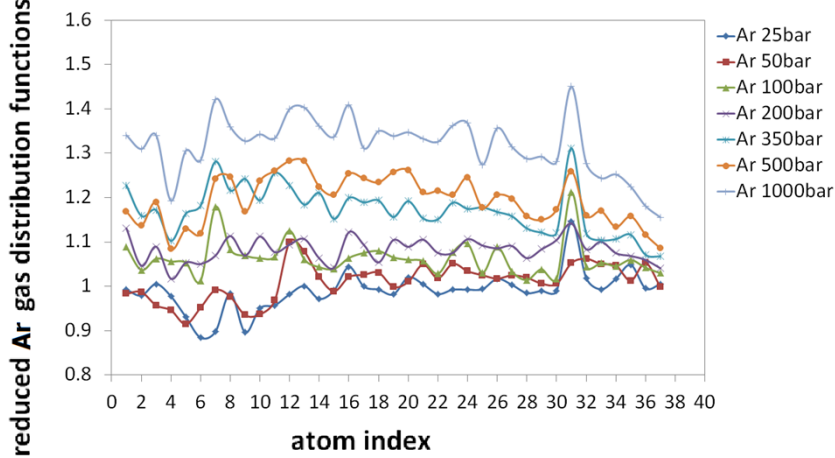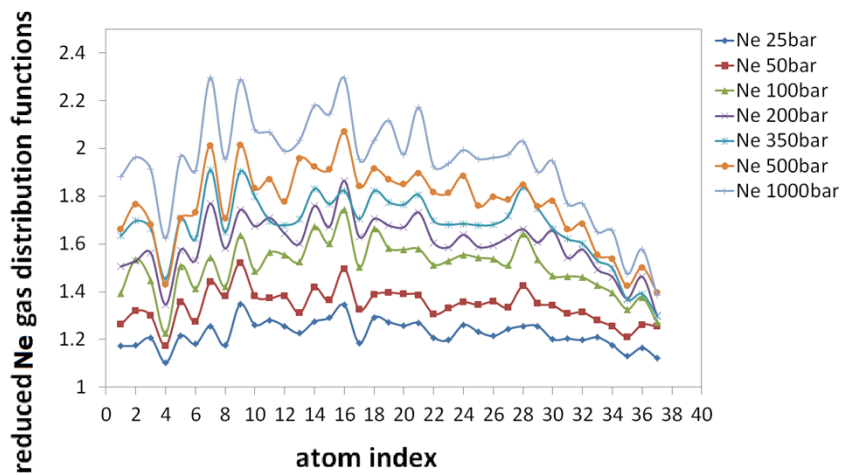
Figure S3. The relative differences in gas density are presented as averaged over 0.2-1.0 nm range normalized RDF functions of gas-DOPC atoms and shown at 1 - 1000 bar for Xe (A), Ar (B) and Ne (C). Values for the same gases at standard conditions were used as a reference. The jamming effect of the hydrophilic DOPC head group (1-10 atom indices) on gas diffusion is the most prominent for Xe at 1000 bar.
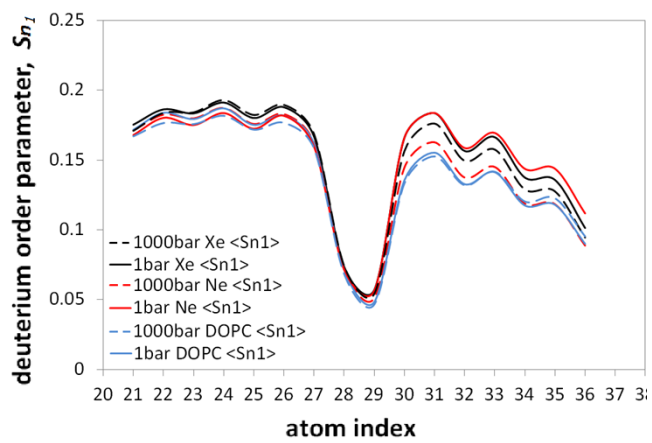
A
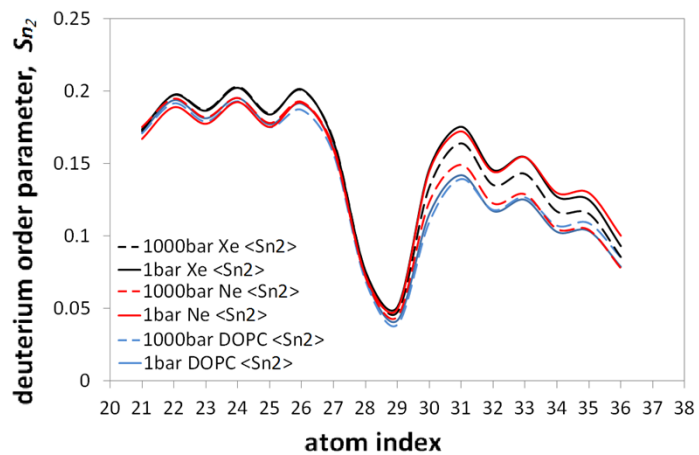
B

Figure S4. DOPC acyl chain order parameters are shown for Sn_1 (A) and Sn_2 (B) for bilayers saturated with Xe (black) and Ne (red) and the intact bilayer (blue) at 1 bar (continuous line) and 1000 bar (broken line).