Abstract Submitted
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Mobility of water and selected atoms in DMPG lipid bilayer membranes[1] F.Y. HANSEN, A. ROENNEST, G.H. PETERS, Tech. U. of Denmark, H. TAUB, A. MISKOWIEC, U. Mo. — Molecular dynamics simulations have been used to study the structure and mobility of water and selected atoms in dimyristoyl-phosphoglycerol (DMPG) lipids forming a fully hydrated free standing bilayer membrane at 310 K. The effect of the anionic headgroup in DMPG on structure and dynamics has been studied by comparison with simulation[2] and experimental[3] results for bilayer membranes of dimyristoyl-phosphorylcholine (DMPC) lipids, which have a neutral head group and the same aliphatic tails. The membrane is found to be in the fluid phase with monovalent sodium counter ions and in the gel phase with divalent calcium counter ions as evidenced by an area/lipid change and the NMR order parameter. The simulation results are compared with preliminary neutron scattering results.

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[2]F.Y. Hansen *et al.*, J. Chem. Phys., in press.
[3]M. Bai *et al.*, Europhys. Lett. **98**, 48006 (2012).

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