Abstract Submitted
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Structure and dynamics of a hydrated phospholipid bilayer in the presence of a silica substrate[1] MATTHEW MCCUNE, IOAN KOSZTIN, University of Missouri — We study the structure and dynamics of a hydrated diyristoylphosphatidycholine (DMPC) lipid bilayer supported on a silica substrate using all-atom molecular dynamics (MD) simulation. A similar MD simulation of a freestanding DMPC bilayer is used as a reference to determine changes to both lipid and hydration water properties due to the introduction of the substrate. Long time (0.1 microsecond) MD trajectories were used to investigate the effect of the substrate on the structure and dynamics of the lipid bilayer by determining (i) the spatial distribution of water molecules and selected lipid atoms; (ii) the out of plane fluctuations of the lipid molecules; (iii) the dipole moment orientation of hydration waters; and (iv) the lateral mean-square-displacement of both lipid and water molecules. The obtained results suggest that (i) at equilibrium the space between the substrate and lipid bilayer is filled by only hydration water; (ii) the presence of the substrate has no major influence on the structure of hydration water layers and on the out-of-plane fluctuations of the lipids; and (iii) the silica substrate alters considerably the lateral diffusion of the lipids in the closest bilayer leaflet and the hydration waters between the substrate and DMPC membrane. The reported results appear to be consistent with previous MD and neutron scattering studies.

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