

Abstract Submitted
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Structural and dynamical properties of water at the bilayer DPPC membrane interface JIANPING GAO, CHARLES CLEVELAND, UZI LANDMAN, School of Physics, Georgia Institute of Technology — The properties of interfacial water near the DPPC lipid bilayer surface are probed by a nano-size quartz tip through large scale atomistic molecular dynamics simulations. The water films confined between the bilayer membrane surface and a crystalline wetting quartz surface are kept in contact with a water reservoir at 293K. The distance between the solid tip and the gel phase membrane is varied between 0.5 to 2 nanometers. Layering of the confined water film is found near the solid tip while the water at the membrane surface remains unlayered. Some water is trapped in the cavities between the head groups of the lipid molecules. The recorded solvation force does not show oscillations due to the rough nature of the membrane surface.

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