

Abstract Submitted
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What is the difference between a supported and a free lipid bilayer? ROLAND FALLER, UC Davis — Supported Lipid Bilayers are an abundant research platform for understanding the behavior of real cell membranes as they allow for additional mechanical stability and enable characterization techniques not reachable otherwise. However, in computer simulations these systems have been studied only rarely up to now. Here we present a systematic study of the changes that a support inflicts on a phospholipid bilayer using coarse-grained molecular modeling. We characterize the density and pressure profiles as well as the density imbalance induced by the support. It turns out that the changes in pressure profile are strong enough that protein function should be impacted leading to a previously neglected mechanism of transmembrane protein malfunction in supported bilayers. We also determine the diffusion coefficients and characterize the influence of different corrugations of the support. We then determine the free energy of transfer of phospholipids between the proximal (close to the surface) and distal leaflet of a supported membrane using the coarse-grained Martini model. It turns out that there is at equilibrium about a 2-3% higher density in the proximal leaflet. These results are in favorable agreement with recent data obtained by very large scale modeling using a water free model where flip-flop can be observed directly. We compare results of the free energy of transfer obtained by pulling the lipid across the membrane in different ways. There are small quantitative differences but the overall picture is consistent. We are additionally characterizing the intermediate states which determine the barrier height and therefore the rate of translocation. Simulations in atomistic detail are performed for selected systems in order to confirm the findings.

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