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Multiscale Modeling of supported bilayers ROLAND FALLER, CHENYUE XING, MATTHEW I. HOOPES, 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. We studied systematically the changes that a support induces on a phospholipid bilayer using coarse-grained molecular modeling on different levels. We characterize the density and pressure profiles as well as the density imbalance inflicted on the membrane by the support. 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 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.

Roland Faller
UC Davis

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