

Abstract Submitted
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Multiscale Modeling of supported lipid bilayers ROLAND FALLER,
CHENYUE XING, MATTHEW HOOPES, UC Davis — The study of lipid structure
and phase behavior at the nano scale length is of importance due to implications in
understanding the role of the lipids in biochemical membrane processes. We per-
formed a variety of simulations in homogeneous and heterogeneous membrane sys-
tems to elucidate such behaviors. Our simulations demonstrate that various coarse
grained simulation models can predict different aspects of lipid phase separation and
describe the change of the system under the influence of a support. The simulations
are performed using models at different length scales ranging from the all atom scale
to a scale where lipids are modeled by only three interaction sites. We are able to
follow transformations, such as lipids phase transitions. These phase transitions are
determined by analyzing parameters like area per lipid head group, the deuterium
order parameter and dynamic properties. Additionally, we characterize individual
lipid molecules using rotational correlation functions to classify different dynamic
populations and we study the stability of artificially designed patterns. We discuss
the changes of the system phase behavior as well as differences between the two
leaflets as induced by the support.

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