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Multiscale Modeling of Heterogeneous Lipid Bilayers ROLAND FALLER, UC Davis, SANDRA BENNUN-SERRANO, UC Davis, ALLISON DICKEY, UC Davis — The first line of defense for a cell against intrusive molecules is the membrane which must be resilient to prevent unwanted molecules from passing through as a change in the intracellular ion balance could be detrimental. Experimentally, it has been shown that as chain length and concentration of alcohols near a membrane increase, the area per lipid expands, increasing the likelihood of permeation. Additionally, there is evidence for pattern formation in cell membranes due to the presence of various lipids. These patterns or rafts are believed to play important roles in cell signaling. Here, we use MD to study the interactions between alcohols and pure lipid bilayers as well as pattern formation in mixed membranes using atomistic and coarse-grained models. We characterize the effect of alcohol chain-length and concentration on the lipid bilayer through area per head group, order parameter, and density profile. We also examine the effects of lipid-alcohol interactions on membrane curvature with the CG model and find satisfactory system representation. We use a mixture of DLPC and DSPC as model system for phase separation. Different concentrations and temperatures are used to reproduce phase transitions. We obtain agreement with experiments for area per lipid head group and deuterium order parameter. At high DSPC concentrations phase separation into a gel and liquid state is found. Simulations confirm that increasing DLPC concentrations lower the transition temperature.

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