

Simulating mixing and demixing in lipid bilayers

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Biomembranes typically contain dozens of different species of lipids, each with a distinct combination of several polar headgroup with hydrocarbon tails that vary in length and degree of unsaturation. While overall membrane composition is under active regulation by the cell, heterogeneity in lipid composition on the nanoscale will be influenced by lipid interactions with each other or with other membrane components, and by variations in local curvature and tension. This talk will present our work in developing atomistic simulation methods specifically for the efficient modeling of structure and thermodynamics in lipid mixtures. Results from several simulation studies will be discussed, including local composition variations associated with bilayer edges, with transmembrane peptides, and with regions of high cholesterol.