503b Multiscale Modeling of Structure and Phase Behavior in Heterogeneous Lipid Bilayers

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The study of lipid structure and phase behavior at the nano scale length is of main importance due to its implication in understanding the role of the lipids in biochemical membrane processes. We performed a variety of simulations of heterogeneous membrane systems to elucidate such behaviors. Our simulations demonstrate that a coarse grained simulation model can predict lipid phase separation preserving the identity of the lipids [1] as well as predict the structural changes under the influences of alcohols [2]. We apply Molecular Dynamics Simulation at different concentrations and temperatures in lipid mixtures as well as simulations under the influences of sugars and alcohols. The simulations are performed using models at different length scales ranging from the all atom scale to a scale where lipids are modeled by one interaction site. We are able to follow transformations, such as lipids phase transitions. These phase transitions were determined by analyzing parameters such as area per lipid head group, the deuterium order parameter and dynamic properties. A phase diagram of a DLPC-DSPC mixture is reproduced consistent with experiments. Additionally we characterize individual lipid molecules using rotational correlation functions to classify different dynamic populations. We moreover compare the mechanical properties of a pure lipid DPPC bilayer to a membrane composed of DPPC and ergosterol in the presence of alcohols. Ergosterol is structurally similar to cholesterol and is found in yeast membranes. The interactions between a model yeast membrane and ethanol is of interest to wine producers because of a problem known as a stuck fermentation.

[1] R. Faller and S. J. Marrink. Langmuir 20, 7686-7693 (2004). [2] A. N. Dickey and R. Faller J Pol Sci B 43, 1025-1032 (2005).