

Monte Carlo lattice modelling of a bilayer system

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Recently, a lattice model has been developed which allows one to describe the properties of lipid bilayer mixtures, containing DPPC and/or DLiPC [1]. It was introduced to examine the local phase separation and aggregation behavior of the respective lipids. The free energy functional is based on the lipid interaction enthalpy and lipid conformational chain entropy. All contributions can be extracted from short atomistic simulations. The model approach has proven to be able to correctly reproduce phase separation behavior and predict melting temperatures of gel phases for the lipid binary mixtures.

As cholesterol plays a crucial role in the dynamics of lipid bilayers, especially being prominent for its property to form the basis of lipid rafts, we present an extension of the lattice model by incorporation of cholesterol. We have to deal with different challenges, related, e.g., to the different sizes of cholesterol and DPPC/DLiPC. Adding cholesterol to the model will allow one to gain deeper insight into the fundamental mechanics of lipid raft formation and the basics of lipid-cholesterol interaction.

[1] D. Hakobyan, A. Heuer, *J. Chem. Phys.* **146**, 064305 (2017)