

## 2D Monte-Carlo Model of Lipid Bilayers

Davit Hakobyan and Andreas Heuer

*WWU Münster, Institut für Physikalische Chemie, Münster, Germany*

The phenomenon of lipid rafts where different liquid phases are formed remains one of the major topics in biophysics of the last two decades. In model membranes the raft formation was explicitly shown *in-silico* with coarse-grained Molecular Dynamics (MD) simulation [1]. Nevertheless, for large systems the coarse-grained technique require significant computational power.

Here a 2D Monte-Carlo (MC) lattice model of a lipid bilayer is presented. The order parameter is defined as the main characteristic property of a lipid [2,3]. As an example, the functional form of conformational entropy is explicitly calculated for saturated DPPC and polyunsaturated DLiPC lipids based on the enthalpy term and order parameter distributions obtained from all-atom MD simulations. The proposed 2D MC model is based on a very small input data set which is taken, exclusively, from MD simulations. Although, the conformational entropy is determined only from data of pure MD systems, nevertheless, the model demonstrates extreme predictive power not only for similar pure MC systems at different temperatures and sizes but also for heterogeneous systems. The excellent agreement of phase and aggregation properties of binary MC systems with respective all-atom MD systems makes the proposed approach very promising in studying raft formation of large heterogeneous systems composed of different types of lipids and sterols.

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[3] D. Hakobyan and A. Heuer. PLoS ONE 9, e87369 (2014).