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Translational diffusion in two-component lipid membranes close to phase transition: A Monte Carlo study

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The intriguing phenomenon of subdiffusion frequently observed in cell membranes in SPT, FCS, and FRAP experiments is usually ascribed to the presence of membrane heterogeneities with dimensions below the optical resolution limit. In order to understand how the submicrometer-scale phase separation in the cell membrane can affect the lipid diffusion and manifest itself experimentally, we carry out dynamic Monte Carlo simulations of a two-lipid membrane (DMPC/DSPC) with the size on the micrometer scale over time intervals of order of a second. To be able to do that with reasonable computational efforts, we simplify the traditional lattice model of a membrane – coupled lipid chains on a triangular lattice – and represent the membrane as a square lattice of lipid molecules. By comparing our simulation results with differential scanning calorimetry data for DMPC/DSPC membranes, we demonstrate that, with a proper choice of the lipid interaction parameters, our model correctly reproduces the thermodynamic properties, as well as the phase diagram of the lipid mixture. For certain ranges of the membrane compositions and temperatures we find that the Brownian motion of lipid molecules shows strong deviations from the normal diffusion law. Possible effects of the dynamic phase separation in SPT, FCS, and FRET experiments will be discussed.