Public Abstract

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Title: **Computational and theoretical study of water and lipid dynamics in biomolecular systems**

This PhD thesis describes three research projects in theoretical and computational biophysics aimed at studying the dynamics of water and lipid molecules in two distinct biomolecular systems. In the first project the energetics and dynamics of water transport through the aquaglyceroporin (GlpF) channel protein is studied by a combination of all-atom molecular dynamics (MD) simulations (both equilibrium and non-equilibrium MD) and stochastic modeling. The MD results are used to determine the potential of mean force and the diffusion coefficient of water molecules crossing the channel. Then, the latter quantities are used to estimate the intrinsic water flux through GlpF, and the corresponding channel permeability. In the second project, by employing a 0.1 micro second long, all-atom MD simulation, the self and correlated dynamics of lipid atoms and molecules in a fully hydrated DMPC lipid bilayer is investigated. The MD simulation results are used to develop a memory function based approach for accurately calculating the lateral self-diffusion coefficient of lipids. In some cases, the proposed memory function method provides a better approach than the currently used ones for determining the lateral diffusion coefficient of lipids in lipid bilayers from the dynamic structure factor measured in inelastic neutron scattering experiments. The purpose of the third project is to investigate the dynamics of water molecules in a hydrated lipid membrane. Using the same MD simulation as in the second project, the anomalous properties of buried and hydration waters (located at the proximity of the fluctuating surface of the lipid membrane) are revealed and contrasted to the properties of bulk water.