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Investigation of Phase Transitions of Saturated Phosphocholine Lipid Bilayers via Molecular Dynamics Simulations

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Abstract

Lipid bilayers play an important role in biological systems as they protect cells against unwanted chemicals and provide a barrier for material inside a cell from leaking out. In this paper, nearly 30μs of molecular dynamics (MD) simulations were performed to investigate phase transitions of 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC) and 1,2-dipalmitoyl-*sn*-glycero-phosphocholine (DPPC) lipid bilayers from the liquid crystalline (L_α) to the ripple (P_β) and to the gel phase (L_β). Our MD simulations accurately predict the main transition temperature for the single-component bilayers. A key focus of this work is to quantify the structure of the P_β phase for DMPC and compare with measures from x-ray experiments. The P_β major arm has similar structure to that of the L_β, while the thinner minor arm has interdigitated chains and the transition region between these two regions has large chain splay and disorder. At lower temperatures, our MD simulations predict the formation of the L_β phase with tilted fatty acid chains. The P_β and L_β phases are studied for mixtures of DMPC and DPPC and compare favorably with experiment. Overall, our MD simulations provide evidence for the relevancy of the CHARMM36 lipid force field for structures and add to our understanding of the less-defined P_β phase.

Keywords: Lipid Bilayers, Molecular Dynamics simulations, Phase transition,