

393f Structural and Dynamic Properties of Mixed Bilayer Systems with Cryoprotectants

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Phospholipids bilayers constitute the primary structural element in biological membranes and their physical properties are of considerable experimental and theoretical interest. Membrane physical properties are presumed to influence processes such as intercellular interactions, trans-membrane transport, changes in cell surface morphology, and the functioning of membrane-associated proteins. The thickness of an interfacial region is in the nanometer range, making experimental studies of such a thin region extremely difficult. Although there are many experimental works on the lipid bilayer system, physical understanding of interfacial phenomena still relies heavily on theoretical analysis and numerical simulations. Application of molecular dynamics (MD) simulations can yield detailed information on the structure and dynamics of the bilayer. Here we describe our atomistic MD simulations of dipalmitoylphosphatidylcholine (DPPC) and dipalmitoylphosphoethanolamine (DPPE) bilayers, as well as their behavior in the presence of cryoprotectants, such as trehalose and dimethylsulfoxide.