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Molecular dynamics simulation study of structural changes and pore formation in phospholipid bilayers in the presence of dimethylsulfoxide[1] DOREL MOLDOVAN, RAGHAVA ALAPATI, JIEQIONG LIN, BRIAN NOVAK, RAM DEVIREDDY, Mechanical Engineering Department, Louisiana State University, Baton Rouge, Louisiana — Understanding the structure and properties of cell membranes in the presence of various chemicals is of great importance for numerous applications in pharmaceuticals and biosciences. We present molecular dynamics simulations that delineate with atomistic details the effect of dimethylsulfoxide (DMSO) at various concentrations on dimyristoylphosphatidylcholine (DMPC) lipid bilayers. The simulations show that at low concentrations DMSO leads to bilayer thinning and increases permeability. When the DMSO concentration increases above a critical value ($\sim$6.0 wt%), even in the absence of an external stress, our simulations show that hydrophilic pores are thermally nucleated and grow. We rationalize the nucleation process in terms of a simplified free energy model that includes the entropy of the pore shape. By estimating the line tensions within the lipid bilayers with and without DMSO, our simulations corroborate the pore growth model.

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