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Mesoscopic Simulations of the Insertion of the Amphiphilic Nanotubes into Lipid Bilayers MEENAKSHI DUTT, MICHAEL NAYHOUSE, OLGA KUKSENOK, University of Pittsburgh, ALEXANDER ALEXEEV, Georgia Institute of Technology, STEVEN R. LITTLE, ANNA C. BALAZS, University of Pittsburgh — Using Dissipative Particle Dynamics (DPD) simulations, we investigate the interactions between amphiphilic nanotubes and a lipid bilayer membrane. Each nanotube encompasses an ABA triblock (TB) architecture, with a hydrophobic stalk and two hydrophilic ends. To allow controlled transport through the nanotube, we introduce hydrophilic tethers at one or both ends of the nanotube. Individual lipids are composed of a hydrophilic head group and two hydrophobic tails. We begin with a stable lipid bilayer membrane immersed in a hydrophilic solvent, and introduce the nanotube into the surrounding solution. The energetically unfavorable interaction between the solvent and the hydrophobic segment of the nanotube could potentially drive them to penetrate the membrane, with the hydrophobic stalk being buried within the hydrophobic domains of the bilayer. This process, however, depends upon the hydrophobic fraction of the nanotube, the degree of hydrophobic mismatch between the nanotube and the bilayer, and the presence of hydrophilic end-tethers. We isolate the conditions that promote the insertion of the synthetic nanotubes into membrane. The simulations are supported by free energy calculations for the amphiphilic nanotube-lipid-solvent system. Ultimately, these embedded synthetic nanotubes could be used to regulate the passage of molecules through synthetic membranes.

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