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Self-assembly of Amphiphilic Nanotubes and Lipids into Synthetic Vehicles: Computer Simulation Study MEENAKSHI DUTT, OLGA KUKSENOK, STEVEN LITTLE, ANNA C. BALAZS, University of Pittsburgh — Via Dissipative Particle Dynamics (DPD) approach, we study the self-assembly of amphiphilic nanotubes and lipids immersed into a hydrophilic solvent. Each nanotube encompasses an ABA triblock architecture, with a hydrophobic stalk and two hydrophilic ends. Individual lipids are composed of a hydrophilic head group and two hydrophobic tails. We show that an energetically unfavorable interaction between the solvent and the hydrophobic segments of the nanotube and the lipids drive them to self-assemble so as to shield the hydrophobic entities from the hydrophilic solvent. The equilibrium self-assembled structures formed depend upon the concentrations of the lipids and nanotubes, 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 formation of specific equilibrium self-assembled structures. The simulations are supported by free energy calculations for the amphiphilic nanotube-lipid-solvent system. Ultimately, these self-assembled structures of nanotube-lipid systems can be used for making hybrid control release vehicles.

Meenakshi Dutt
University of Pittsburgh

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