

Abstract Submitted
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Interactions of End-Functionalized Nanotubes with Lipid Vesicles: Spontaneous Insertion and Nanotube Self-organization MEENAKSHI DUTT, OLGA KUKSENOK, University of Pittsburgh, MICHAEL NAYHOUSE, University of California at Los Angeles, STEVEN R. LITTLE, ANNA C. BALAZS, University of Pittsburgh — Via Dissipative Particle Dynamics (DPD) approach, we study the self-assembly of amphiphilic nanotubes into a lipid vesicle, which is immersed in a hydrophilic solvent. Individual lipids are composed of a hydrophilic head group and two hydrophobic tails. Each nanotube encompasses an ABA architecture, with a hydrophobic shaft (B) and two hydrophilic ends (A). To allow controlled transport through the nanotube, we also introduce hydrophilic tethers at one end of the tube. We show that nanotubes initially located in the outer solvent spontaneously penetrate the vesicle's membrane and assume a trans-membrane position, with the hydrophilic tethers extending from the surface of the vesicle. We add nanotubes one at a time after the previous nanotube has been inserted. We characterize the interactions among the nanotubes that have self-assembled into the vesicles' membrane and focus on their clustering within the membrane. We also show that the nanotube insertion and clustering within the vesicle strongly affects the vesicle shape in cases of a sufficiently large number of tubes. Ultimately, these nanotube-lipid systems can be used for making hybrid controlled release vesicles.

Meenakshi Dutt
University of Pittsburgh

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