

Physics Colloquium

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Computational Design of Bioinspired Vesicles with Tunable Shape and Interfacial Characteristics

Via the use of a mesoscopic simulation technique called Dissipative Particle Dynamics, we design bioinspired vesicles with tunable shape and interfacial properties. The vesicle designs are inspired by different types of biological cells. For the first design: we create bacterial cell-mimicking hairy vesicles through the self-assembly of a binary mixture composed of amphiphilic molecular species, such as lipids grafted with poly ethylene glycol (PEG) chains, and phospholipids. We investigate the influence of the molecular stiffness, and dissimilarity in the hydrocarbon tail groups, along with the relative concentration of the species, the PEG group length and the confinement volume on the shape of the hairy vesicle. We study the interfacial adsorption of amphiphilic nanoparticles onto a hairy vesicle. The functionalized nanoparticles are modeled as patchy spheres. We examine the relation between the relative concentration and size of the OEG chains, the adsorption kinetics, life-time and post-adsorption dynamics of the nanoparticles. We also draw correspondence with experimental studies on the adsorption of proteins onto the surface of colloidal particles. For the second design: we create a multicomponent vesicle encompassing different species of phospholipids and cholesterol. We examine the interfacial adsorption of peptide-inspired nanoparticles onto the hybrid vesicle, the nanoparticle insertion and post-insertion dynamics. We present our findings on the role of cholesterol concentration and nanoparticle architecture on the pre- and adsorption processes along with the insertion and post-insertion dynamics of the nanoparticles. Results from our investigations can potentially be used for the design of novel hybrid soft materials for applications in the encapsulation, delivery of therapeutic agents and bionanoelectronics.

Dr. Meenakshi Dutt joined Rutgers University in July 2011 as a tenure-track Assistant Professor. She obtained her B.Sc. from the University of Delhi, India followed by a M.Sc. from the Indian Institute of Technology–Delhi, India and her Doctorate in Physics from Duke University, USA. She has held research positions at the Pfizer Institute of Pharmaceutical Materials Science at the University of Cambridge, UK, the University of Illinois at Urbana-Champaign and the University of Pittsburgh. She is the recipient of the Open Eye Junior Faculty ACS COMP (August 2015) and the NSF CAREER award (2017).

Thursday, March 30, 2017 at 4:10PM

In Lewis Lab. 316

Refreshments at 3:45PM