

COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

Molecular design of protein-mimetic nanostructures

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ABSTRACT:

Gold nanoparticles functionalized with an amphiphilic monolayer of alkanethiol ligands can insert into lipid membranes through a non-disruptive pathway that has been well-characterized using a combination of experiments and atomistic molecular dynamics simulations. The physiochemical similarity between these nanoparticles and amphiphilic membrane-bound and free-circulating proteins suggests a possibility for designing nanostructures that can function as biomimetic proteins. In this talk, I will present an overview of how molecular simulation techniques have allowed us to tackle this engineering challenge and develop nanoparticles that can modulate fusion between lipid membranes, transport hydrophobic small molecules to lipid-bound compartments, and induce transient curvature for sculpting lipid membranes into organelles. These studies point to a unique opportunity for utilizing monolayer-protected nanoparticles as a versatile platform for engineering targeted nano-bio interactions.

FRIDAY, APRIL 7, 2017

12:00 PM – 1:00 PM

Building 32, Room 155

(STATA)

Pizza and beverages will be provided.

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