University of Texas at San Antonio

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Friday, December 7, 2011
3:15 p.m.-4:15 p.m.
BB 3.04.18*

Nanoparticles in Solution: From Spontaneous Asymmetry to Surface Film Self-Assembly and Structure using Atomistic Simulation

Nanoparticles and nanoscience are increasingly critical to a host of energy and technology applications. I'll talk about strategies and some roadblocks in understanding how we can organize nanoparticles, focusing on our work with coated nanoparticles. In solution, nanoparticles are often stabilized with functional coatings to prevent aggregation. I'll discuss the use of explicit-atom molecular dynamics simulation to determine how these coatings affect the forces between nanoparticles and present recent simulation results showing that small (2-8 nm diameter) spherical nanoparticles spontaneously produce highly asymmetric coating arrangements, when coated with commonly-used simple polymer chains. These asymmetric coatings often fail to encapsulate the particle and strongly affect the shape. At the liquid/vapor interface, these coating asymmetries are amplified and oriented by the surface, and play a significant role in the interactions between aggregating nanoparticles. Using many-nanoparticle simulations we demonstrate that the self-assembly of nanoparticle films and the resulting structure within these many-nanoparticle surface aggregations can be controlled by manipulating these very simple functionalized coatings.
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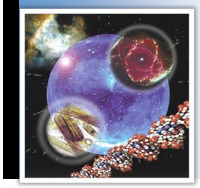

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*Please DO NOT enter this room prior to 3:00pm. Doing so will disrupt another class.