Title: "Optimizing the Ordered Self-Assembly of Soft and Hard Nanoscale Building Blocks: Pure Components and Alloys"

Abstract:

As meso-scale building blocks, oligomers, polymers, and nanoparticles can be tailored in ways that atomic or small-molecule building blocks cannot. Recent progress in synthesis and fabrication methods allow the creation of multi-block oligomers and nanoparticles that vary not only in size and chemical composition but also in shape, rigidity, branching topology, and spatial functionalization. A key challenge that such boundless possibilities present to modelers is the ability to predict the assembling patterns of novel building blocks, and thus potentially identify phases with desirable structures and physical, optical, electronic, catalytic or mechanical properties for emerging applications.

I will describe our efforts to optimize the formation of different types of colloidal alloys, which can be seen as the analog of strategies that have already developed to make useful salts or doped solids from inorganic elements or alloys and intermetallic compounds from metals, the goal is to advance general principles and approaches to design the inter-species interactions between nanoparticles that optimize the formation of either substitutionally disordered alloys or substitutionally ordered alloys. The work focuses on binary mixtures consisting of nanoparticle components whose interactions can be characterized by asymmetries in entropic and energetic characteristics. We have formulated variational principles for enhancing co-assembly behavior with the target type of substitutional order and tested those principles by application to mixtures containing components of diverse size and shape (including polyhedral) and selective interactions that mimic the hybridization of complementary short DNA strands grafted to the nanoparticle surfaces. Some of our specific predictions are consistent with results of nanoparticle alloys already realized.

I will also briefly describe our work on the phase behavior of polyphilic oligomers, i.e., molecules consisting of several block types, focusing on cases where a rigid core is one of the constituent blocks. We focus on architectures that can create complex bicontinuous structures, filling some of the gaps in the rich phase behavior that has already been mapped experimentally. As in the case of nanoparticles, we touch on the free-energy methods used to study some of these systems and how binary alloys provide a powerful means to access new phase behaviors.