Engineering Entropy in Nanomaterials: The Bad, the Ugly, and the Good.

Speaker:
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By elucidating structure-property relationships of soft matter, molecular simulations can assist in the engineering of materials with desirable properties; e.g., properties that originate in the creation of special types of structural order or the control of phase transitions. I will focus on the use of nanoparticles as building blocks for the creation of novel ordered structures. This is motivated by the ability of current synthetic routes to generate tailor-made nanoparticles of tunable sizes, shapes, chemistry, and surface patterning, which has opened the door to a new physical-chemistry with “super atoms” as building blocks. Ordered assemblies of such super atoms can possess unique optical, rheological, and mechanical properties, making them attractive components in the preparation of novel composite, photonic, plasmonic, and photovoltaic materials. I will describe some of our attempts to formulate fundamental principles that govern the self-assembly of such super atoms, and build a sort of “metallurgy” of nanoparticles. While molecular engineering often focuses on tuning chemical interactions, I will focus first on the engineering of entropic interactions as they are often equally crucial but less appreciated. I will describe our recent efforts on the use of molecular simulations to map out the phase behavior of suspensions of particles with polyhedral shapes, including the formation of multicomponent compounds. Our results provide both a basis to existing experimental observations and predictions of novel phases yet to be seen in the lab. In particular, we predict the formation of various novel entropy-aided self-assembling liquid- and plastic-crystalline phases which are resilient to size polydispersity. We also provide guiding rules to maximize the formation of substitutionally disordered solids and compounds from binary mixtures containing particles of different shape. These and other examples illustrate the potential benefits of a more pro-active approach to harnessing the often overlooked power of entropy.