Designing Particle Shapes for Self-Assembly of Novel Colloidal Crystals

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Abstract: When designing materials, researchers start with one of the four “pillars of materials science”—processing, structure, properties, and performance. Recently, materials research has been concerned with the “inverse design problem,” in which the desired material properties or structures motivate materials design targets and synthesis. Furthermore, nanoparticle self-assembly parallels that of materials assembly in nature, where nanoparticles or colloids spontaneously assemble into crystals like atoms do on the atomic length scale. New nanoparticle synthesis techniques enable the design of complex building blocks and lead to greater complexity—and hence functionality—in resulting materials. The recently introduced “Digital Alchemy” framework can be used to determine how to optimize building block shape for assembling crystals with target properties and structures. Using this method, I have investigated the phenomenological events that occur in shape space, the variable space which maps to a parameterization of shape. First, I will explain how this extended ensemble approach can be used to understand a core question in self-assembly science: when is self-assembly driven by the dense-packing arguments, that is, by the structure in which hard particles order most densely? Then, I will discuss how we can design reconfigurable photonic materials using tunable shape dimensions and the future of materials design through extended ensembles.