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Directed Self-Assembly of Spherical Particles NATALIE ARKUS,
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We examine the kinetics and energetics of self-assembly in systems containing a small number of spherical colloidal nanoparticles using a combination of theory, simulation, and experiment. We then explore how the addition of spherically symmetric binding specificity can be used to direct the self-assembly of a given structure.

Using graph theoretic, numerical, and algebraic geometric techniques, we denumerate all possible packings for a system of n particles. We map out the energy landscape of these packings, which is determined not only by the value of the potential energy at these minima, but also by the vibrational normal modes of the structures. Experiments for a 6 particle system show that the likelihood of a given packing follows this expected equilibrium distribution.

To explore the kinetics of packing formation, we simulate the self-assembly of these systems in the irreversible binding limit. For the 6 particle system, this reveals that the kinetics required to form one of the packings is highly unlikely, resulting in the other packing forming with 100% probability. With the addition of binding specificity however, we can cause the unlikely packing to form with 100% probability. We show how the addition of binding specificity effects the energetic landscape of these systems, and that it alone is sufficient to direct self-assembly.

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