Phase Behavior of Thermodynamically Small Clusters of Colloidal Particles

RAGHURAM THYAGARAJAN, DIMITRIOS MAROUDAS, DAVID FORD, Univ of Mass - Amherst — The self-assembly of finite clusters of colloidal particles into crystalline objects is a topic of technological interest, as a route to produce photonic crystals and other metamaterials. Such assembly problems also are fundamentally interesting because they involve thermodynamically small systems, with number of particles between 10 and 1000 that is far below the bulk limit. In contrast to bulk systems, these colloidal assemblies exhibit phase coexistence over a finite range of physical conditions. Here, we report the results of a computational study of phase behavior of small colloidal clusters interacting via the Asakura-Oosawa depletion pair potential. We conducted Monte Carlo simulations for various levels of the osmotic pressure that controls the strength of the interparticle interactions, using potential energy histograms to identify distinct phases. Over a narrow but finite range of the osmotic pressure, we find bimodal distributions in the potential energy space that are indicative of coexistence between fluid-like and crystalline configurations. We also report systematic quantitative comparisons of the phase behavior observed here with results from a Fokker-Planck order-parameter approach.

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