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**Characterization of phase behavior in assemblies of colloidal nanoparticles** RAY SEHGAL, Chemical Engineering, University of Massachusetts Amherst, DANIEL BELTRAN-VILLEGAS, MICHAEL BEVAN, Chemical and Biomolecular Engineering, Johns Hopkins University, DIMITRIOS MAROUDAS, DAVID FORD, Chemical Engineering, University of Massachusetts Amherst — We report results of a systematic investigation of the phase behavior of clusters of colloidal nanoparticles, which interact via a hard core and depletion attraction potential, as a function of system size and inter-particle interaction strength. To describe the various phases that may be present in such nanoparticle assemblies, we carry out a set of windowed Monte Carlo umbrella sampling (MC-US) simulations to generate free energy landscapes (FELs). For the MC-US generation of the FELs, we use the diffusion mapping method to identify the system's underlying dimensionality and define the dynamically relevant coarse variables. The resulting set of FELs samples broad ranges of the system size and interaction potential strength. These computed FELs describe the phase behavior of the nanoparticle assemblies and allow us to analyze the effects of interaction strength and system size as these assemblies approach the bulk thermodynamic limit. In very small clusters, only a single stable liquid-like phase exists. However, as the number of nanoparticles in the cluster increases, a second crystalline phase emerges in coexistence with the liquid-like phase. The corresponding critical cluster size marks the onset of nucleation of crystalline assemblies of colloidal nanoparticles.

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