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Size and interaction-strength effects on the phase behavior of colloidal particle assemblies RAY SEHGAL, DAVID FORD, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We report the findings of a systematic computational study of the inherently complex phase behavior of thermodynamically small assemblies (clusters) of colloidal particles interacting via a potential that includes electrostatic repulsion and depletion-based short-ranged attraction. Using Monte Carlo umbrella sampling with coarse graining in two order parameters and a biasing scheme based on a genetic algorithm, we generate free-energy landscapes (FELs) that can indicate coexistence between fluid-like and crystalline phases. We have used the data mining technique of diffusion mapping to determine the dimensionality of the order-parameter space and assess the suitability of chosen order parameters that represent metrics of cluster density and crystallinity. Evaluation of phase behavior metrics from analysis of the FELs leads to predictions of conditions for formation of stable phases of such small colloidal clusters. A stable crystalline phase emerges as the number of particles in the assembly increases beyond a critical value. We find that the critical cluster size for the onset of crystallization decreases with increasing strength of the interparticle attraction. This FEL analysis also enables a mean-field description of the phase transitions undergone by these assemblies.

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