Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effects of Interaction Range and Strength on the Phase Behavior of Small Clusters of Colloidal Particles RAY SEHGAL, DIMITRIOS MAROUDAS, Univ of Mass - Amherst — We report the findings of a computational study of the phase behavior of thermodynamically small assemblies (clusters) of colloidal particles interacting via a potential that includes electrostatic repulsion and depletion-based variable-ranged attraction. We applied the data mining technique of diffusion mapping to determine the dimensionality of an appropriate coarse-grained description of the phase behavior and to assess the suitability of chosen order parameters. The results of this technique indicate that two coarse variables, which represent metrics of assembly density and crystallinity, are required to describe the phase behavior of these colloidal assemblies. We generate free-energy landscapes (FELs) in this well-justified coarse-variable space using Monte Carlo umbrella sampling. We constructed these FELs over a range of interparticle interaction strength and range and obtained a comprehensive picture regarding the possible stable configurations of such colloidal assemblies at equilibrium and the phase changes observed between them. In particular, we observe an order-to-disorder transition between crystalline and fluid-like phases as well as a polymorphic transition between relaxed face-centered cubic and hexagonal close-packed structures.

Ray Sehgal
Univ of Mass - Amherst

Date submitted: 14 Nov 2014 Electronic form version 1.4