Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Interplay of directional and isotropic interactions in self-assembly
DEBRA AUDUS, National Institute of Standards and Technology, FRANCIS STARR, Wesleyan University, JACK DOUGLAS, National Institute of Standards and Technology — Patchy particle models, composed of hard spheres with decorated with attractive patches, have been introduced as models of micron-sized particles with anisotropic interactions, as well as solutions of globular proteins. Here, we extend the canonical model of the patchy particles to include a short-ranged isotropic interaction in order to probe of the coupling of the directional and isotropic interactions on the self-assembly process. In particular, we evaluate basic properties characterizing self-assembly including average cluster mass and the fraction of particles in the clustered state using both Monte Carlo simulation and analytic Wertheim theory. This combination allows for validation of the theory and for insight into analyzing experimental data. We also find that Flory-Stockmayer theory describes the cluster size distribution data found in our simulations remarkably well, despite its erroneous mass-scaling exponent. This result, coupled with Wertheim theory, predicts both a master curve for the average cluster mass and a method to parameterize patchy particle models using experimental data.

Debra Audus
National Institute of Standards and Technology

Date submitted: 05 Nov 2015 Electronic form version 1.4