Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Diverse assembly behavior in colloidal Platonic polyhedral sphere clusters RYAN MARSON, ERIN TEICH, JULIA DSHEMUCHADSE, SHARON GLOTZER, RONALD LARSON, University of Michigan — We simulate the self-assembly of colloidal "polyhedral sphere clusters (PSCs)", which consist of equal-sized spheres placed at the vertices of a polyhedron such that they just touch along each edge. These colloidal building blocks have recently been experimentally fabricated (**DOI:** 10.1021/acsnano.5b03272)**;** here we predict crystal structures that would appear in the phase diagram of resulting particle assemblies. We use Brownian dynamics (BD) simulations of rigid body clusters performed in the open-source GPU-based HOOMD-Blue particle simulation package to show the assembly behavior of the 5 Platonic PSCs. The simulations contain as many as 4096 individual polyhedra, across over 30 different densities per cluster geometry, with some ordered phases possessing unit cells with 20 or more particles. We observe the formation of not only traditional cubic structures such as BCC and FCC, but also more complex phases having structure symmetries with Pearson symbols - hP7, cP20, cI2, mP6, and hR3. The observations reported here will serve as a guide for future colloidal assembly experiments using an expanded library of PSCs, consisting of other regular and irregular polyhedra, allowing researchers to target specific arrangements of "halo" and "core" particles for technologically relevant applications including photonics and structural color.

Ryan Marson
University of Michigan

Date submitted: 13 Nov 2016 Electronic form version 1.4