Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Design Rules for the Self-Assembly of Voronoi Particles[1] BENJAMIN SCHULTZ, University of Michigan, Dept. of Phys., PABLO DAMASCENO, University of Michigan, Dept. of App. Phys., MICHAEL ENGEL, University of Michigan, Dept. of Chem. Eng., SHARON GLOTZER, University of Michigan, Dept. of Phys., App. Phys., Chem. Eng. — Recent theoretical advances have developed methodologies for predicting the assembly of hard, polyhedral particles. In this work, we use the Voronoi tessellation to generate polyhedral shapes that form space-filling superlattices that are isostructural to well-known atomic crystals. We focus on the assembly of these polyhedra into crystalline superlattices with orientational and positional order. Analogous to potentials designed to stabilize crystals at zero temperature, these particles are designed to stabilize the space-filling tiling at infinite pressure. We study a set of these particles in simulation and characterize how their symmetry and other geometric features affect their assembly characteristics at finite pressure. We calculate the relative stability of competing structures for several shapes that do not assemble their target structure and discuss how features of the shape affect this stability. From our conclusions, we demonstrate how to move beyond the concept of Voronoi tessellation for the design of hard polyhedral particles targeted for self-assembly.

[1]This material is based upon work supported by, or in part by, the U. S. Army Research Office under Grant Award No. W911NF-10-1-0518.

Benjamin Schultz
University of Michigan, Dept. of Phys.

Date submitted: 28 Nov 2012 Electronic form version 1.4