Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Self Assembly of Hard, Space-Filling Polytopes[1] BENJAMIN SCHULTZ, University of Michigan, Dept. of Physics, PABLO DAMASCENO, University of Michigan, Dept. of Applied Physics, MICHAEL ENGEL, SHARON GLOTZER, University of Michigan, Dept. of Chemical Engineering — The thermodynamic behavior of systems of hard particles in the limit of infinite pressure is known to yield the densest possible packing [1,2]. Hard polytopes that tile or fill space in two or three spatial dimensions are guaranteed to obtain packing fractions of unity in the infinite pressure limit. Away from this limit, however, other structures may be possible [3]. We present the results of a simulation study of the thermodynamic self-assembly of hard, space-filling particles from disordered initial conditions. We show that for many polytopes, the infinite pressure structure readily assembles at intermediate pressures and packing fractions significantly less than one; in others, assembly of the infinite pressure structure is foiled by mesophases, jamming and phase separation. Common features of these latter systems are identified and strategies for enhancing assembly of the infinite pressure structure at intermediate pressures through building block modification are discussed.

[1] P. F. Damasceno, M. Engel, S.C. Glotzer arXiv:1109.1323v1 [cond-mat.soft]

[2] A. Haji-Akbari, M. Engel, S.C. Glotzer arXiv:1106.4765v2 [cond-mat.soft]

[3] U. Agarwal, F.A. Escobedo, *Nature Materials* **10**, 230–235 (2011)

[1]Supported by the DOD/DDRE under Award No. N00244-09-1-0062 and by the U.S. ARO under Grant Award No. W911NF-10-1-0518

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Date submitted: 08 Dec 2011 Electronic form version 1.4