Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Computer Simulation Study of the Nucleation of Rotator Phases in Hard Polyhedral Particles VIKRAM THAPAR, FERNANDO ESCOBEDO, Cornell University — The nucleation kinetics of the rotator phase in hard cuboctahedra, truncated octahedra, and rhombic dodecahedra is simulated via a combination of forward flux sampling and umbrella sampling. We compute the degrees of supersaturation at their corresponding pressures by improving upon the interfacial method used to estimate the liquid-rotator coexistence pressure. The nucleation rates are obtained by calculating the mean first passage time from liquid to rotator phase using forward flux sampling, and the free-energy barriers are estimated using umbrella sampling. For comparable degrees of supersaturation, the polyhedra are found to have significantly lower free-energy barriers and faster nucleation rates than hard spheres. This difference primarily stems from localized orientational ordering, which steers polyhedral particles to pack more efficiently. Orientational order hence fosters here the growth of orientationally disordered nuclei. The results are compared to preliminary data for the disorder-to-order transition for other polyhedral systems including systems pinned on a 2D interface.

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Date submitted: 13 Nov 2014 Electronic form version 1.4