

Abstract Submitted
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Assembly precursors in fluids of hard polyhedra M. ERIC IR-
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— The role of shape in entropy-driven self-assembly has recently been highlighted
in computer simulations of hard anisotropic particles. A rich diversity of crystal
and other solid-like phases has been demonstrated in particular for hard polyhedra.
Moreover, a correlation has been observed between local structure in the fluid phase
and structure of the solid-like phase[1]. Here we investigate the question of when the
fluid first “recognizes” particle shape and anticipates a pending phase transition. We
present equations of state for systems of hard polyhedra spanning the low-density
fluid to high- density solid states, obtained numerically from equilibrium Monte
Carlo simulations. We discuss trends in the behavior for different shapes, and show
some general features common to all systems. [1] P. F. Damasceno, M. Engel, and
S. C. Glotzer, Science 337, 453 (2012)

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