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How do hard, regular tetrahedra pack? MICHAEL ENGEL, AMIR HAJI-AKBARI, AARON S. KEYS, University of Michigan, XIAOYU ZHENG, Kent State University, ROLFE G. PETSCHEK, Case Western Reserve University, PETER PALFFY-MUHORAY, Kent State University, SHARON C. GLOTZER, University of Michigan — We simulate a system of hard tetrahedra using Monte Carlo simulations and determine the density-pressure equation of state by compressing an initially disordered fluid. Depending on the speed of the compression, the system either jams or spontaneously orders to a quasicrystal. By compressing a crystalline approximant of the quasicrystal, the highest packing fraction we obtain is 0.8503. We show that the system is able to achieve such high densities by the local ordering of tetrahedra into certain favorable motifs, forming larger structures that pack efficiently in both jammed and ordered structures. Jamming and crystallization are preceded by an entropy-driven transition from a simple fluid of independent tetrahedra to a complex fluid characterized by tetrahedra arranged in densely packed pentagonal pyramids that form a percolating network at the transition. Our results demonstrate how particle shape and entropy may be exploited to achieve highly complex structures. [1] A. Haji-Akbari, M. Engel et al., Disordered, quasicrystalline and crystalline phases of densely packed tetrahedra, Nature, in press (2009).

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