Monte Carlo Simulation of Dense Packings of Hard Tetrahedra

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The densest packing of tetrahedra remains an unsolved problem, and there has been much recent debate. We simulate dense packings of mathematically smooth, hard regular tetrahedra using NPT Monte Carlo simulations and determine the density- pressure equation of state. We find disordered packings with densities that significantly exceed the hard-sphere FCC packing density of 0.740480490. Our findings thus demonstrate that tetrahedra obey Ulam's conjecture that spheres pack with a lower maximum packing density than any other hard convex object, despite recent conjecture to the contrary. The dense packings that we have found do not seem to be crystalline but are instead dense random packings. We show that the system is able to achieve such high packing densities by the local ordering of tetrahedra into certain favorable motifs, forming larger structures that pack efficiently but are overall jammed. We speculate that one or several denser crystalline packings exist.