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Thermodynamic stability of dense packings of hard, regular tetrahedra AMIR HAJI-AKBARI, MICHAEL ENGEL, SHARON C. GLOTZER, University of Michigan — The question of how densely regular tetrahedra can pack in three dimensions has attracted many researchers in recent years. In the first thermodynamic study of dense phases of the hard tetrahedron system, we recently reported the spontaneous formation of a dodecagonal quasicrystal [1]. The $(3.4.3^2.4)$ approximant of the quasicrystal, with an 82-particle unit cell, was compressed to a packing fraction of 85.03% [1]. Very shortly after, a much simpler crystal of tetrahedron dimers [2] with a slightly higher packing fraction of 85.63% was discovered [3], the current densest packing [3]. Since the dimer crystal packs more densely than the quasicrystal and its approximant, it is thermodynamically favored in the limit of infinite pressure. However, which structure is stable at finite pressures is an open question. Here, we explore the relative thermodynamic stability of these very different ordered phases as a function of packing density.

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