Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Polytetrahedral Frustration of Crystallization: A Study of 4d Hard Spheres PATRICK CHARBONNEAU, Duke University, JACOBUS A. VAN MEEL, FOM Institute for Atomic and Molecular Physics, DAAN FRENKEL, Cambridge University — Geometrical frustration is thought to ease the supercooling of a liquid. In $3d$ hard spheres the preferred local cluster is icosahedral and the densest packing is tetrahedral, but no periodic lattice is consistent with either symmetry in Euclidian space, so a crystal phase with a different symmetry nucleates upon compression. For $2d$ disks in contrast triangular or hexagonal order is both locally and globally preferred and crystallization of a metastable fluid is quasi-instantaneous. Yet the precise origin of geometrical frustration remains unclear, because in $2d$ and $3d$ polytetrahedral structures are often equated conceptually to the optimal local cluster. Here, we conduct a computational study of the $4d$ analogue, where the optimal local cluster and global order are commensurate, but the polytetrahedral order is not. We observe no sign of facile crystal formation, which support the polytetrahedral frustration scenario. We also find the fluid to be structurally very different from the crystal. The resulting high interfacial free energy sheds new light on $3d$ geometrical frustration and its role in glass formation.

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Date submitted: 19 Nov 2008 Electronic form version 1.4