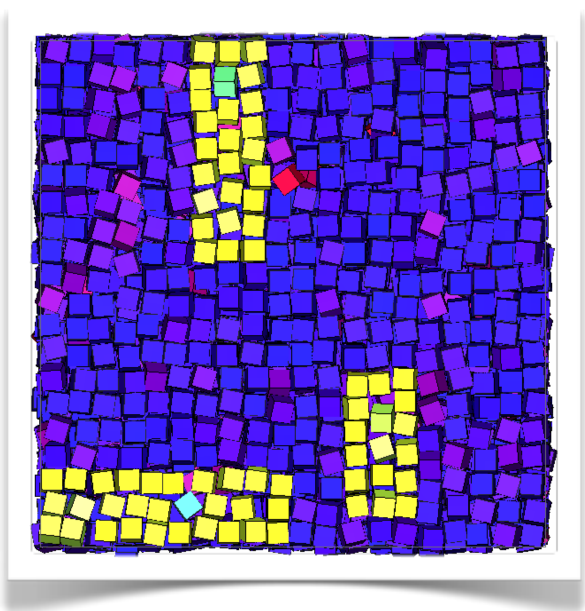
Vacancy-stabilized crystalline order in hard cubes
PNAS **109** (2012) 17886.

Authors: Frank Smallenburg, Laura Filion, Matthieu Marechal, and Marjolein Dijkstra

Recommended and a commentary by Randall D. Kamien, University of Pennsylvania

How do fluids freeze? The success of colloidal science in mimicking atomic and molecular based systems is a good starting point -- real-space, confocal, microscopy and relatively slow dynamics allows us to probe questions of phase transitions in unprecedented ways [1]. Of course, most colloidal particles are spherical and only form the simplest crystals [2]. Can we use non-spherical constituent particles to model more complex, non-isotropic interactions? Recent work has made astounding progress at studying the packing of a variety of geometrically regular polytopes [3] leading to a rich



In the defect furthest to the right, the highlighted area shows three cubes sharing four lattice sites. The uppermost defect has six cubes sharing seven lattice sites, and the bottom most defect has seven cubes sharing eight lattice sites. From recommended article. Courtesy of M. Dijkstra.

phase diagram of liquid crystals, rotator crystals, disordered packings, and periodic structures. The paper by Smallenburg, *et al*., explores the crystal phases of cubic colloids. Not only is their geometry interesting, but the topology of the lattice into which they assemble is especially interesting. It is isostatic -- unlike the FCC or HCP packing of spheres with 12 nearest neighbors, the cubes only have 6. So what? As the authors point out, if one sphere is removed from an FCC crystal, the neighbors are held in place by their other neighbors. Not true in the isostatic case where there are precisely the minimum number of neighbors to hold something in place.

The authors find that not only are the fraction of vacancies huge in comparison to spherical packings, 3-6% versus 0.01%, but that they are also delocalized, something for which lattice isostaticity is *necessary*. It makes one wonder whether the cubic anisotropy leads to extended columns associated with the vacancies. Though these columns may or may not exhibit nematic order, they certainly have a length -- a delocalization length that is somehow controlled by the volume fraction of vacancies since columns are limited by other columns. Is there a delocalizaton length scale here that could give us a clue about the onset of soft modes in near isostatic systems ? Can we use this as a "lattice" model for near isostatic structures?

---

1. J. Zhu, M. Li, R. Rogers, W. Meyer, R.H. Ottewill, STS-73 Space Shuttle Crew, W.B. Russel, and P.M. Chaikin, Nature **387** (1997) 883.
2. U. Gasser, E.R. Weeks, A. Schofield, P.N. Pusey, and D.A. Weitz, Science **292** (2001) 258.
3. P.F. Damasceno, M. Engel, and S.C. Glotzer, Science **337** (2012) 453.