103st MSS-Seminar
Wednesday, September 7th, 15:30
Nägelsbachstr. 49b

The influence of shape on the phase and vacancy behaviour of hard slanted cubes

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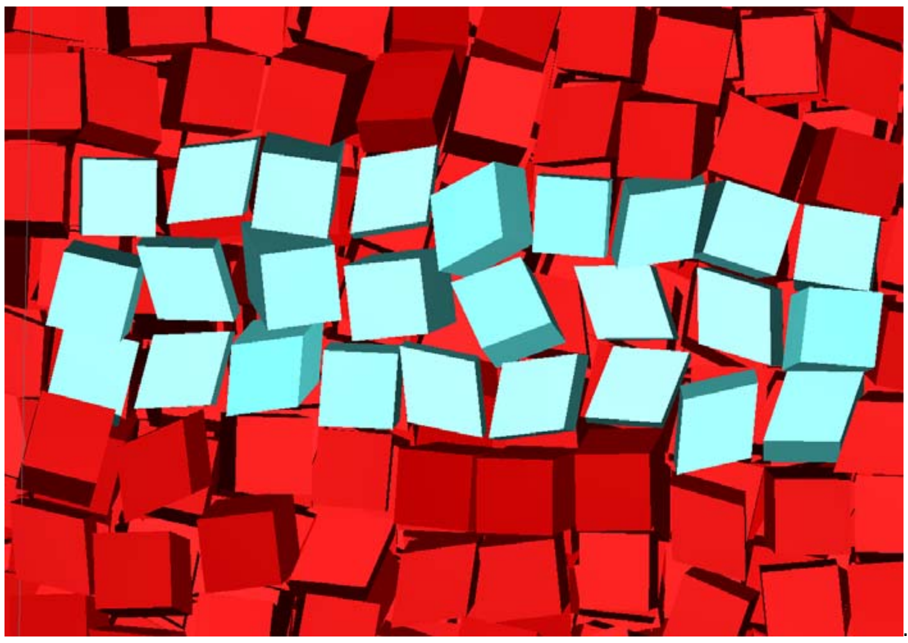

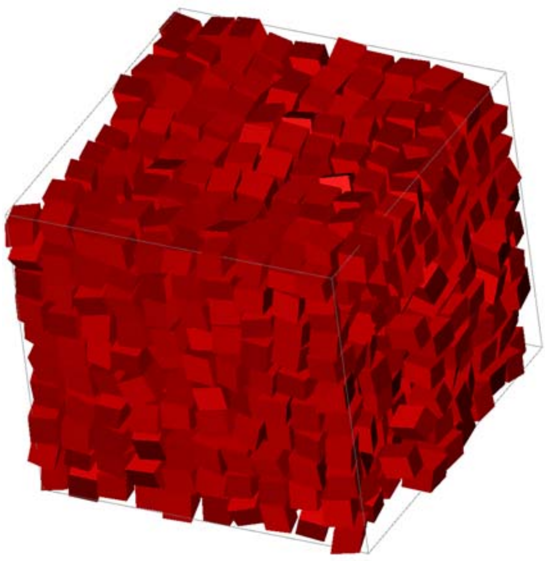

Particle shape plays a large role in the phase behaviour of colloidal particles, especially for higher densities where efficient packing of space becomes important. Advances in colloid synthesis now allow for the creation of particles with carefully tailored shapes, and interest in the phase behaviour of anisotropic particles has increased as a result. One recently-investigated case concerns vacancies in a simple cubic crystal of hard cubes (Ref. 1). Alongside a unusually high concentration of vacancies (8% of the lattice), these vacancies delocalize over multiple lattice sites. Inspired by this study, we investigate the phase and vacancy behaviour of slanted cubes: rhombus-shaped particles that for a slant angle of 90 degrees reproduce hard cubes. Primarily, we seek to find out how the vacancies in this crystal change as the shape of its constituent particles changes. To this end, we first determine the phase behaviour of the system for various slant angles through the use Monte Carlo and event-driven molecular dynamics simulations. Combining known methods of free-energy calculation we construct an efficient way of quantifying changes in free energy as a result of a change in particle shape. The equilibrium concentration of vacancies in simple cubic crystal is then derived from the free energy of the crystal at various densities and slant angles. Peculiarly, our data suggests that the vacancies in this crystal phase are wholly invariant to changes in the shape of the constituent particles.