P.14 Nucleation of hard colloidal cubes

C Karner and C Dellago

University of Vienna, Austria

Currently, research on hard anisotropic colloids is receiving a lot of attention from various experimental and theoretical groups in the soft matter community, partly due to the emergence of new fabrication techniques making it possible to produce colloidal particles with various anisotropic shapes or interactions [1]. Recent results obtained from computer simulations and theory indicate that many three dimensional hard anisotropic particles of polyhedral shape exhibit a first order phase transition from an unordered fluid to an ordered crystal.

Unlike hard spheres, the simple cubic crystal lattice of hard cubes exhibits a reasonable amount of vacancies near coexistence. Smallenburg et al. [2] showed that this finite vacancy concentration in fact stabilizes the crystal and by doing so, lowers the melting point. In addition to the high vacancy concentration, the crystal is characterized by relatively fast diffusion near coexistence. Hence, coming from the liquid phase, hard cubes will nucleate into this dynamic, vacancy rich crystal.

In this poster we will present the dynamics of the freezing transition of hard colloidal cubes. To study the properties of the transition we used kinetic Monte Carlo, combined with rare event sampling techniques such as Transition Interface Sampling.

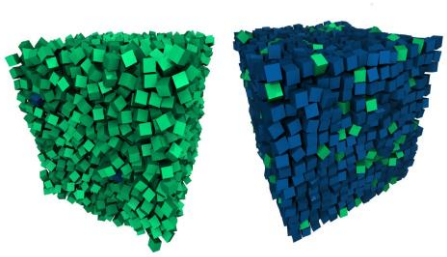

Figure 1: Cubes at packing fractions ϕ = 0.44 close to freezing point (left) and ϕ = 0.52 close to melting point (right). The cubes are colored according to the value of an order parameter that measures the relative orientations, blue denoting cubically ordered and green denoting unordered.

[1] Stefano Sacanna and David J. Pine. Shape-anisotropic colloids: Building blocks for complex assemblies. Current Opinion in Colloid & Interface Science, 16(2):96–105, 2011

[2] Frank Smallenburg, Laura Filion, Matthieu Marechal and Marjolein Dijkstra. Vacancystabilized crystalline order in hard cubes. Proceedings of the National Academy of Sciences, 109(44):17886–17890, 2012