Self-assembly in Dipolar Fluids

MICHELA RONTI, SOFIA KANTOROVICH, Univ of Vienna — We are studying low temperature structural transitions in dipolar hard spheres (DHS), combining grand-canonical Monte Carlo simulations and direct analytical theoretical calculations. DHS is characterized by long-range anisotropic interactions: it consists of a point dipole at the center of a hard sphere. We are interested in low temperature and low density phase behaviour of DHS systems. From a theoretical point of view the process of self-assembly is not responsible for a phase transition; this belief was completely reverted by theoretical studies showing that the process of self-assembly is alone capable to induce phase transition. On the other hand in the last years it was proved that no sign of critical behaviour is observed, implementing efficient and tailored Monte Carlo algorithms. Moreover a theoretical approach based on Density Functional Theory was developed: a series of structural transitions were discovered providing evidence of a hierarchy in the structures on cooling. We are performing free-energy calculations in order to draw the phase diagram of DHS model. Comparing the numerical results with the theoretical ones shed light on the scenario of temperature induced structural transitions in magnetic nanocolloids.

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