On behalf of the

Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

Dr. Franzisco Martinez

Department of Chemistry, University of Cambridge, UK

Unusual Phase Behavior of Binary Mixtures DNA-Functionalized Particles

We report a Monte Carlo study of a 1:1 binary mixture of particles functionalized with DNA chains with “sticky” ends. The system was modeled using a coarse-grained representation. In order to map out the phase diagram of this model system, we combined biased Monte Carlo simulations with histogram reweighting techniques. We find that, below a critical temperature this system undergoes a phase separation between a dilute vapor-like phase and a dense network-forming liquid-like phase. We observe a surprising non-monotonic dependence of the coexistence pressure on the temperature. This anomalous liquid-vapor phase behavior can be understood in terms of a cross-over between two distinct regimes for the driving force of the phase transition: a hybridization-free-energy-driven regime and an entropy-driven regime.

An important qualitative change appears in the phase diagram when the number of DNAs per colloid (i.e., the valence κ) reaches a threshold value. Above this threshold, the system can exhibit direct vapor-liquid-crystal coexistence, but below it, the triple point disappears completely. In this case, the condensed phase that coexists with the vapor at low temperatures and low osmotic pressures is always the liquid and crystallization can therefore only take place under applied pressure. Such behavior is well known for Helium but is, to our knowledge, unprecedented for soft matter. Thus, our simulations provide an explanation for the experimental observation that dilute solutions of colloids coated with a small number of DNA strands do not crystallize. This inability to crystallize is a direct consequence of the discrete nature of DNA binding and this allows us to formulate a simple rule of thumb to estimate whether a given system of DNA-coated colloids can crystallize.

Date: Monday, April 11, 2011 16:00
Location: Josef-Stefan-Hörsaal,
Strudlhofgasse 4, 3rd floor, 1090 Wien