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

Dipl.-Ing. Günther Doppelbauer
Institute of Applied Physics, Vienna University of Technology

Crystals, Clusters and Energy Landscapes of Patchy Particles

We have investigated self assembly scenarios of patchy particles [1], which are (spherical) colloids with discrete, mutually attractive or repulsive regions on their surface and therefore anisotropic interactions. For this purpose, we have used methods suitable for exploring the rugged potential energy landscape of such systems, in particular basin hopping Monte Carlo and transition state searches [2] for patchy particle clusters of different size and an evolutionary algorithm [3] for crystalline systems. I will present results on different building patterns, namely five- and sixparticle rings, making up clusters and how their competition is reflected in the energy landscapes of such systems. For crystals made of patchy particles, I will show how the competition between packing (minimizing the volume) and bonding (minimizing the energy) leads to a very rich variety of equilibrium structures, including open (staggered honeycomb), body-centered and close packed (face-centered and hexagonal) lattices, in dependence on the system pressure and the geometry of the particles.

References

[1] E. Bianchi, R. Blaak, and C. N. Likos, Phys. Chem. Chem. Phys. **13**, 6397 (2011).
[2] D. J. Wales, *Energy Landscapes*, Cambridge University Press, Cambridge (2003).

Date: Monday, June 27, 2011 16:00
Location: Josef-Stefan-Hörsaal,
Strudlhofgasse 4, 3rd floor, 1090 Wien