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. Andreas Tröster

Johannes Gutenberg – Universität Mainz, Germany

Monte Carlo Simulation of Curved Interface Free Energies

The computation of interface free energies is of fundamental importance in understanding nucleation processes in metastable phases at first order phase transitions. Interestingly, despite decades of theoretical and computational research, our understanding of the curvature dependence of the interface tension between coexisting phases is still far from being complete. In particular, the reliable determination of the so-called Tolman length, which is believed to govern the curvature dependence of the interface tension of spherical droplets and bubbles, remains a highly controversial subject.

In this talk I will discuss to which extent the study of phase separation in finite systems by Monte Carlo simulations can allow for a direct thermodynamic analysis of the free energy barriers associated with different interface topologies. An effort will be made to explain both the underlying theoretical concepts as well as our computational approach. Recent results on Lennard-Jones fluids and the q-state Potts model illustrate both the insights as well as the limitations of the present methods.

Date: Monday, May 30, 2011 16:00

Location: Josef-Stefan-Hörsaal,
Strudlhofgasse 4, 3rd floor, 1090 Wien