



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

**Dr. Peter Virnau**

Institut für Physik,  
Johannes Gutenberg-Universität Mainz

Monday, 19th of April, 4:00 p.m.  
ICAMS Seminar room UHW 11/1102

## **Monte Carlo Test of the Classical Theory for Heterogeneous Nucleation**

Flat walls facilitate the condensation of a supersaturated vapor: classical theory of heterogeneous nucleation predicts that the free energy barrier  $\Delta F_{het}^*$ , which needs to be overcome for the formation of sphere-cap-shaped nucleation seeds, is smaller than the barrier  $\Delta F_{hom}^*$  for spherical droplets in the bulk by a factor  $0 < f(\Theta) < 1$ , which only depends on the contact angle  $\Theta$ . We compute both  $\Delta F_{hom}^*$  and  $\Delta F_{het}^*$  from Monte Carlo simulations and test the theory for the lattice gas model (for which  $\Theta$  can be readily controlled). Even though the theory is only based on macroscopic arguments, it is shown to hold for experimentally relevant nanoscopic nucleation seeds ( $20 \leq \Delta F^*/kBT \leq 200$ ) if line tension effects are considered. If time allows I will also present recent work on "knotted proteins".