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Monday, 31th of Januar, 4:30 p.m.
ICAMS Seminar room UHW 11/1102

Dr. Christoph Dellago
Faculty of Physics, University of Vienna

Nucleation in small systems: studying pressure induced phase transformations in nanocrystals with transition path sampling

Under suitable conditions, first order phase transitions such as the freezing of a liquid or the structural transformation of a solid occur via a nucleation and growth mechanism, in which a nucleus of the stable phase is formed in the metastable phase. For systems with sizes in the nanometer regime, the nucleation mechanism and its kinetics are strongly affected by finite size effects. I will address this issue using the Wurtzite-to-rocksalt transition in CdSe nanocrystals as illustrative example. In this system, studied experimentally by Alivisatos and coworkers, the activation enthalpy determined from the temperature dependence of the transition rate constant scales linearly with the size of the crystal. Based on the results of transition path sampling simulations, we provide an explanation for this observation and relate it to the particular structure of the critical nuclei. The role of the reaction coordinate in the investigations of the transition mechanism is discussed.