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Fakultät für Physik

Isotopenforschung und **Kernphysik**

E I N L A D U N G

zum

V E R A - S E M I N A R

von

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The time scale problem in molecular simulations: nucleation of first order phase transitions

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. The free energetic cost related to the creation of an interface between the two phases prevents this process from occurring rapidly and the transition takes place only if a rare fluctuation produces a nucleus of sufficiently large size. On a molecular time scale, the transition is a rare event and the resulting long time scales present a challenge for computer simulations. Similar difficulties arise in the simulation of a variety of molecular processes ranging from protein folding to chemical reactions and transport in and on solids. In this talk, I will first give a general introduction to rare events and then discuss how the transition path sampling methodology provides a framework to address this time scale problem and to study the mechanism and the kinetics of first order phase transformations. As an illustrative example, I will report on our work on the pressure-induced transition from the four-coordinate Wurtzite structure to the six-coordinate rocksalt structure in CdSe nanocrystals studied experimentally by Alivisatos and coworkers at UC Berkeley. From our simulations we obtain the preferred transformation pathway and determine activation enthalpies and volumes, which permit to make direct contact to experimental results.

Donnerstag, 11. März 2010, 16:30 Uhr

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