Luigi Delle Site

Max Planck Institute for Polymer Research, Mainz

Adaptive Coupling of Different Resolution Levels in Molecular Simulations

Location: **Dahlem Center Seminar Room**

Time: Monday, February 28th, 2011, 14 h s.t.

Abstract:

Simulations that couple different molecular models in an adaptive way by changing resolution on the fly allow us to identify the relevant degrees of freedom of a system. This, in turn, leads to a detailed understanding of the essential physics which characterizes a system. While the delicate process of transition from one model to another is well understood for the adaptivity between classical molecular models the same cannot be said for the quantum-classical adaptivity. The main reason for this is the difficulty in describing a continuous transition between two different kinds of physical principles: probabilistic for the quantum and deterministic for the classical. Here we report the basic principles of an algorithm that allows for a continuous and smooth transition by employing the path integral description of atoms.