Seminar of the Department. 26
Thin Layers and nanostructures

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

Date : 29. 01. 2019 Tuesday
Time : 10:00 am
Place : Library,Building A, 1st floor

Topic

Nuclear quantum effects in the condensed phase through path integrals

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Methodology based on the path integral formulation of quantum mechanics offers a computationally tractable way to include nuclear quantum effects in atomistic simulations of extended condensed-phase systems. Here, we will review some of the required theoretical and algorithmic ingredients, with focus on ab initio molecular dynamics simulations. While all static quantities can be calculated numerically exactly, dynamical information can be obtained from these simulations approximately within the framework of centroid or ring polymer molecular dynamics. Equilibrium isotope effects are accessible through the thermal expectation values of the quantum kinetic energy. Ring polymer contraction is a controlled approximation which allows for an efficient evaluation of physical interactions in a path integral system. It is especially useful with our recent extension to ab initiointeractions, where it accelerates practical simulations by up to two orders of magnitude. Importantly, it can be combined with centroid and ring polymer molecular dynamics to obtain approximate dynamics from path integral simulations in a computationally efficient way. We will illustrate the use of this methodology with results of ab initio path integral molecular dynamics simulations of aqueous solutions.

Professional guarantor: *Ing. Pavel Jelínek, Ph.D.*