CFEL SCIENCE

SEMINAR

18th May 2017 - 10:00 h

CFEL – Building 99, seminar room I+II (ground floor)

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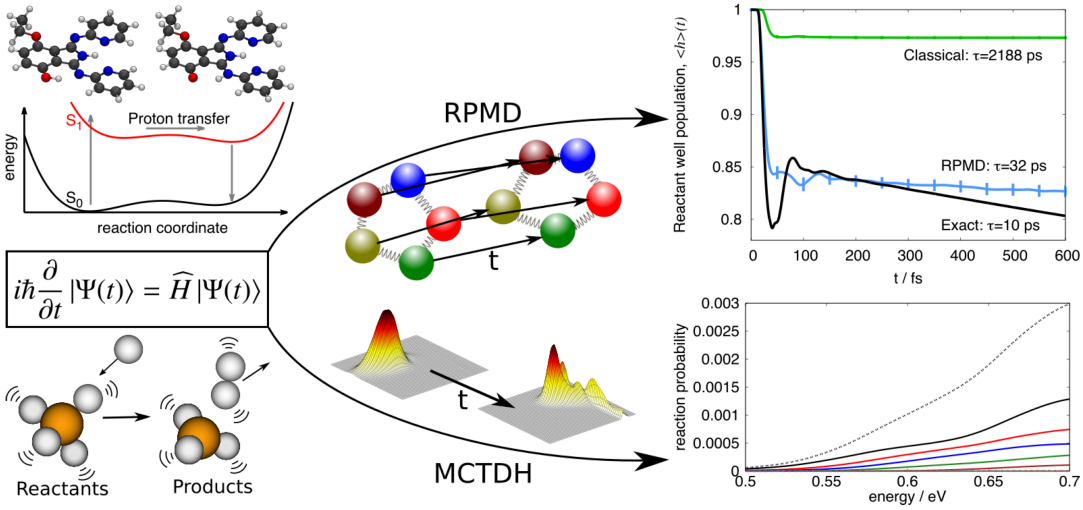
New methodologies for simulating quantum dynamics in complex chemical systems

The fundamental and detailed understanding of molecular reactions and light-molecule interactions is a central challenge in chemical physics. However, the theoretical and computational treatment of quantum mechanical effects of nuclei is a challenging task. In this talk, this challenge will be met from two complementary perspectives. First, I will present progress in advancing exact quantum dynamics methods to simulate reactive scattering processes for polyatomic systems. Specifically, full-dimensional state-resolved reaction probabilities calculated for the $H+CH_4(v, j,m) \rightarrow H_2(v')+CH_3(v'')$ reaction are presented. This is the first time exact calculations could be performed for a six-atom reaction, due to a newly developed extensions of the quantum transition state concept, the multi-layer extension of the multiconfigurational time-dependent Hartree approach and a new and efficient scheme to evaluate accurate Shepard interpolated potential energy surfaces on modern graphics processing units. Second, I will present recent advances in approximate quantum dynamics methodology. Specifically, the extension of the Ring-Polymer Molecular Dynamics (RPMD) approach to simulate processes with non-equilibrium initial conditions will be discussed. In the last decade, the RPMD approach has proven to be an efficient method to simulate the dynamics of large systems by approximately incorporating quantum effects in dynamics calculations using classical trajectories in an extended ring-polymer phase space. However, the current formalism has been limited to the calculation of correlation functions associated with the equilibrium Boltzmann distribution. Furthermore, the prospects of the approach to study photoexcited processes like excited-state proton transfer processes will be investigated.



Host: Terry Mullins / CFEL Molecular Physics Seminar