



SEMINAR

18th September 2019 - 2:00 p.m.
CFEL-bldg. 99, seminar room IV

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Light-Matter Interaction and 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. Theoretical considerations and atomistic simulations can foster the understanding and complement detailed experiments performed, e.g., at free-electron laser facilities. However, the theoretical and computational treatment of quantum mechanical effects of nuclei and of non-Born-Oppenheimer effects is a challenging task. In this talk, I will discuss these challenges and different methods to treat the coupled nuclear-electronic molecular dynamics exactly or approximately. To this end, several important chemical processes are discussed, e.g., ultrafast proton transfer in liquid water, ultrafast electronic decoherence, excited-state proton transfer, and state-selective reactive scattering events..