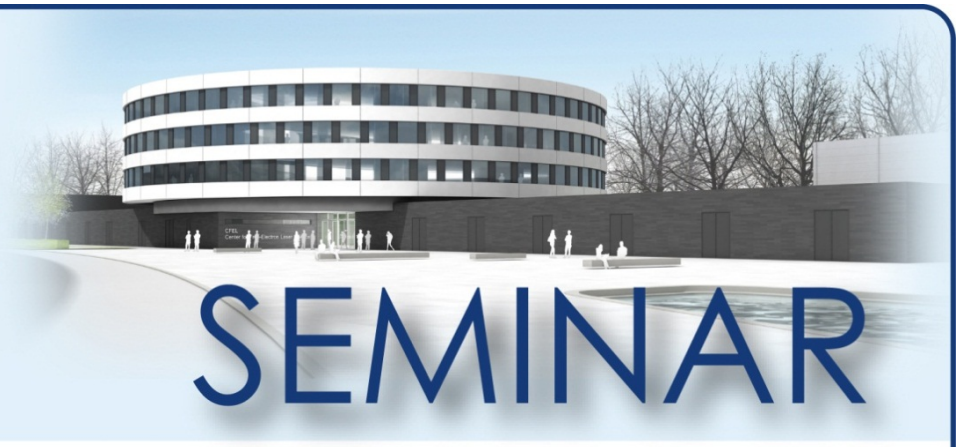
CFEL SCIENCE



SEMINAR

6th September 2023 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Centre for Free-Electron Laser Science, DESY, Germany

Studying ultrafast nuclear dynamics through non-adiabatic dynamics simulations

The advent of femtosecond lasers has opened up the possibility to follow photo-induced chemical dynamics occurring on an ultrafast timescale. With the fast growth of experimental techniques, it has become necessary, more than ever, to employ first principles simulations to explain and characterize the large amount of available experimental data. Ultrafast broadband pulses often coherently excite the system to a manifold of electronic states interacting strongly with each other, necessitating to go beyond the Born-Oppenheimer (BO) approximation. While there is a plethora of methods available, from pure quantum wavepacket dynamics to a series of mixed-quantum-classical descriptions to simulate non-adiabatic molecular dynamics (MD), the method of choice is often highly problem dependent. In close collaboration with experimentalists, we have studied ultrafast dynamics occurring in different length and timescales. We have performed quantum wavepacket dynamics simulations to study the coherent control of the first steps of vision and light-induced spin-crossover reaction in transition-metal complexes. Trajectory surface hopping dynamics simulations have been used to explore photoionization-induced hydrogen-abstraction dynamics in gaseous acetylene. DFT-based QM/MM MD simulations in addition to static quantum chemical calculations at multi-reference level reveal the underlying mechanism of the influence of pump laser fluence on the ultrafast dynamical changes in myoglobin.

Host: Robin Santra – CFEL-DESY Theory Division