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

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Comparing different approaches to follow excited state molecular dynamics: Relativistic ultrafast electron diffraction vs Time resolved photoelectron spectroscopy

Pump-probe measurements aim to capture the motion of atoms and molecules in real time as chemical and physical transformations take place, effectively making "molecular movies" with short light pulses. However, it is not possible to make movies directly from experimental observations due to a number of fundamental and technical limitations. Thus, it is through a combination of experimental measurements and theoretical calculations that one can actually construct molecular movies. I will present a combination of spectroscopic (time resolved photoelectron spectroscopy - TRPES) and structural (relativistic ultrafast electron diffraction - UED) measurements to follow the coupled electronic and nuclear dynamics involved in the internal conversion and photodissociation of diiodomethane, CH_2I_2 . The TRPES measurements provide the time-dependent energy of the molecule, and the UED measurements give the positions of the nuclei for each time. These measurements are combined with trajectory surface hopping calculations, which are capable of calculating the measured observables for both measurements from the same dynamics simulation. The measurements highlight the non-local dynamics captured by different groups of trajectories in the calculations. This is the first time that both structural and spectroscopic measurements are combined with theory capable of calculating the measurement observables in both cases, yielding an unprecedented view of the complicated quantum dynamics.