

April 7th, 2022 10:30 AM

MPSD seminar

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Title

"Visualizing conical intersections with ultrafast X-Ray absorption spectroscopy: the signature of short hydrogen bonds"

Abstract

Conical intersections (*ConIs*) are considered one of the holy grails for photochemistry and photophysics. The presence of *ConIs* in the electronic energy landscape provides radiationless relaxation channels in which the nuclei and electrons evolve on comparable timescales becoming strongly coupled. The quest for characterizing the wavepacket dynamics around *ConIs* has been one of the most intense research lines in the field for the last 70 years. However, due to their complexity and ultrafast nature very few experimental studies have been able to observe *ConIs* directly. In this seminar, I will present our recent simulations showing the unique ability of time-resolved x-ray absorption spectroscopy (TRXAS) to probe the ultrafast nuclear and electronic dynamics around *ConIs*. As a benchmark case, two prototypical hydrogen-bonded molecular crystals were employed: L-Glutamine and L-Pyroglutamine. The TRXAS signature of the S_1-S_0 *ConI*, combined with our unsupervised machine learning approach, reveals fundamental details about the system's evolution, such as the presence of a stable or a transient strong hydrogen bond network.