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Ultrafast X-ray Laser Studies of Chemical Dynamics

KELLY GAFFNEY, SLAC National Accelerator Laboratory and Stanford University

First light at the LCLS x-ray free electron laser at the SLAC National Accelerator Laboratory marked the beginning of hard x-ray laser science 2009. With pulse energies in excess of a milliJoule and pulse durations as short as 5 femtoseconds in duration, the LCLS provides a novel and potentially transformative approach for investigating chemical dynamics in complex systems. Understanding the coupled evolution of electrons and nuclei during chemical transformations remains the central and vexing challenge in the study of chemical reaction dynamics. Ultrafast optical electronic spectroscopy can monitor both the nuclear and the electronic evolution that occurs during a chemical reaction, but this joint sensitivity often impedes the robust interpretation of experimental measurement. The LCLS provides the opportunity to simultaneously measure electronic dynamics with x-ray fluorescence and nuclear dynamics with elastic x-ray scattering, providing a robust means for disentangling the coupled motions of electrons and nuclei during excited state internal conversion and intersystem crossing. These exciting new opportunities will be discussed in the context of recent studies of photo-induced spin crossover dynamics in iron(II) tris-bipyridine. $[\text{Fe}(\text{bpy})_3]^{2+}$.