

Charge transfer and dissociation from a femtosecond electronic-structure perspective

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Abstract

Photochemically activated molecules catalyze chemical reactions, but a molecular-level understanding of how these short-lived and reactive intermediates catalyze reactions has remained elusive. A lack of suitable probes has limited the detail of our understanding due to the difficulties related with characterizing electronic excited states.

The aim of this lecture is to discuss the new opportunities provided by time-resolved x-ray spectroscopy to reveal the coupling of nuclear dynamics and transient electronic structure in the electronic excited states of molecular systems. Time-resolved x-ray spectroscopy enables a novel characterization of chemical interactions on atomic length and time scales of Ångströms and femtoseconds. The question about “Where are the electrons?” during a chemical reaction can be answered by directly addressing the valence electrons and their evolution as the reaction proceeds. Examples will be discussed for how chemical reaction dynamics can be probed with time-resolved x-ray spectroscopy from small molecules in the gas phase to coordination complexes in solution.

