Contribution ID: **135** Type: **Talk**

X-ray femtochemistry: Mapping the valence electronic structure of dissociating molecules with femtosecond RIXS at the free electron laser LCLS

Saturday, 17 September 2011 12:00 (20 minutes)

We present our recent results on how we follow both the occupied and unoccupied valence orbitals of dissociating Fe(CO)5 molecules in solution with femtosecond RIXS at the free electron laser LCLS (Stanford, USA).

A pump-laser wavelength of 267 nm is used for resonant metal-to-ligand charge transfer excitation. The evolution of the valence electronic structure is probed with RIXS at the Fe L-edge as Fe(CO)5 dissociates into Fe(CO)4 and CO in ethanol solution. We use a recently built set up with a liquid jet in vacuum and a soft x-ray RIXS spectrometer. Our results reveal the coupling of orbital population, chare transfer and structural dynamics during dissociation and solvation of the photoproducts up to 3 picoseconds after initiating the reaction. They give unique insight into the coordinatively unsaturated carbonyl intermediate Fe(CO)4 and give complete access to the dissociation dynamics of a fundamentally important chemical bond with sigma-donation and pi-back donation between the metal center and the carbonyl groups. We believe that femtosecond RIXS gives unique access to the coupling of transient electronic structure and nuclear dynamics during chemical reactions.

This contribution will conclude with recent and complementary results with steady-state RIXS on liquids and solutions obtained with the same experimental set up at BESSY II.

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Talk

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