RESOLVING ULTRAFAST PHOTOCHEMISTRY OF COORDINATION COMPLEXES USING HIGH HARMONIC GENERATION XANES SPECTROSCOPY

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Extreme ultraviolet (XUV) spectroscopy is an inner shell technique that probes the $M_{2,3}$ -edge excitation of atoms. Absorption of the XUV photon causes a $3p \rightarrow 3d$ transition, the energy and multiplet of which is directly related to the element and ligand environment. This in-lab technique is thus element-, oxidation state-, spin state-, and ligand field specific and is a useful tool for the study of electron and energy transfer processes in materials and chemical biology.

With the use of this technique and semi-empirical simulations, I have collected ultrafast transient $M_{2,3}$ -edge absorption data of four different metalloporphyrinates (M = Fe, Co, Ni, Mn) in order to resolve the early time relaxation mechanism of these catalytically-relevant coordination complexes with femtosecond time resolution. This is the first instance of using tabletop transient XUV/VUV spectroscopy on coordination complexes and furthermore highlights the importance of directly probing of the metal center in these systems. I will additionally present ongoing work on applying this technique to the study of heterobimetallic systems with directly-interacting dual metal centers within a non-innocent ligand scaffold. The relation of function to metal-specific photodynamics will help lay essential groundwork for the development of multimetallic catalysts with efficiencies comparable to those found in nature.