X-ray Emission Spectroscopy in Transition Metal Systems using an X-ray Free Electron Laser

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A molecular level understanding of how transition metal complexes catalyze reactions has long been a grand challenge that is not only critically important for advancing efforts in developing a new generation of environmentally sustainable industrial catalysts, including the fields of solar energy conversion, fuel cells and nitrogen fixation, it is central to the study of many important metalloenzymes in biology. Synchrotron radiation (SR) based X-ray spectroscopy methods have been at the center of studying transition metal complexes for many years, specifically their electronic structure and ligand environment. Recently this research has been extended to X-ray free electrons lasers (XFELs), where ultrashort and ultra-bright X-ray pulses have opened the door to investigate ultrafast phenomena as well as systems beyond the reach of the SR-based probe. We will review some of the recent studies where Kβ X-ray emission spectroscopy (XES) has been applied to various transition metal systems, at times simultaneously with scattering/diffraction techniques.

We will further present recent data obtained at LCLS on stimulated X-ray emission spectroscopy (S-XES). This XFEL based technique has the potential to overcome two of the main limitations of X-ray emission spectroscopy, namely the lack of efficiency of the X-ray optics needed to capture a small fraction of the 4π solid angle of emitted photons, and the lack of spectral sensitivity to small changes, limited by the 1s core-hole lifetime broadening as well as the multitude of spectral features in the X-ray emission signal.

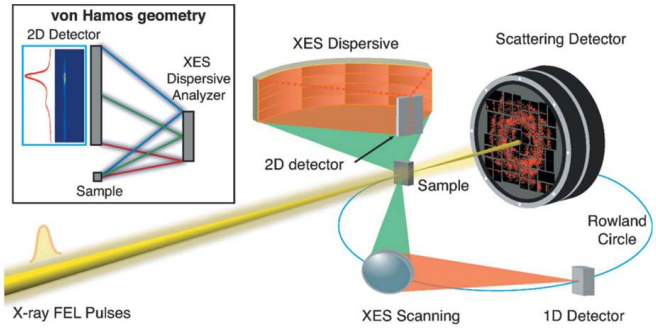

Figure 1: Schematic for simultaneous collection of photon-in photon-out and scattering signals.

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