European XFEL

SEMINAR

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AER 19 / Seminar Room 4.14

“Hard X-ray Emission Spectroscopy in Transition Metal Complexes at the LCLS”

by

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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 using the conventional approach of X-ray spectroscopy in the linear regime is used.We will further present very recent data on stimulated X-ray emission spectroscopy (S-XES). This FEL based technique that 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 4p 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. In S-XES an incoming X-ray pulse simultaneously excites a large number of metal atoms, creating an inverted population of 1s core-hole excited states along its beam path. The subsequent decay results in stimulated K emission along the forward beam direction and can lead to strong amplification gains along this direction. In addition to the strong directionality, the emission spectrum will change in the process, including gain narrowing. The amplification and strong directionality of the XES signal can lead to dramatic gains in signal strength and an exponential spectral sensitivity, which can be used to selectively probe subsets of emission lines. S-XES has thus the potential to be a game changer in how we do FEL based X-ray spectroscopy.

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Host: Christian Bressler