MS06-2-8 Combining X-ray emission spectroscopy with X-ray crystallography to study metalloprotein catalysis at synchotron sources
#MS06-2-8

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Abstract
Understanding enzyme structure in atomic detail is vital to understanding the mechanisms governing enzyme function. However, high spatial resolution provides only a partial picture of an enzymes chemistry. The XFEL-hub at Diamond Light Source (DLS) is designing and commissioning a von Hàmos spectrometer to combine time-resolved X-ray emission spectroscopy (tr-XES) and time-resolved crystallography (tr-XRD). XES is a bulk sensitive element specific spectroscopy that probes orbital configuration and is therefore sensitive to the metals oxidation, spin state and ligand bonding[1]. This setup allows in-depth studies of metalloenzymes where protein function is closely tied with, typically, first-row transition metals electronic configuration.
Building on previous seminal work[2,3], the spectrometer will accommodate 16 crystals at 400mm to provide high spectral resolution, improved solid-angle per eV, and large total solid angle. Multiple crystal mounting positions allows configurations for improved resolution or signal-to-noise, and the possibility to perform multiple simultaneous spectral measurements (Kα and Kß spectral lines)[4]. Importantly, the spectrometer will be able to integrate with a drop-on-tape sample delivery system, also under development at DLS, targeted towards sample efficient tr-XRD mixing experiments. This sample delivery system will facilitate mixing or pumped-probe time-resolved experiments in both aerobic and anaerobic environments. Together this provides a comprehensive setup for tr-XRD/tr-XES measurements for metalloenzymes. Initial commissioning will be for iron and copper spectra with deployment at the VMXi beamline at DLS. Future work includes use at other beamlines, deployment at XFELs and more elements (e.g. Nickel). Here we present the optical and design work, and on-beam benchmarking tests at VMXi.

References
References:
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