Contribution ID: **42** Type: **Contributed talk**

High Photon Energy X-ray Absorption and Emission Spectrometers at the FXE instrument of European XFEL

Thursday 29 August 2024 12:45 (15 minutes)

X-ray probes, e.g., X-ray absorption and X-ray emission spectroscopies (XAS and XES, respectively) have the advantage of being sensitive to the electronic configurations and local structures around the absorbing element. They have routinely been employed to study photoexcited states of materials at synchrotron radiation and X-ray Free Electron Laser (XFEL) large-scale facilities. Time resolved (tr) X-ray spectroscopies have rarely been employed in very hard X-ray regimes, mainly due to the lack of X-ray sources. Femtosecond X-ray Experiments (FXE) has unique capability of delivering high photon energies, allowing X-ray spectroscopies to be performed above 18 keV 1, which covers the K-edges of 4d elements and L-edges of 5f elements. However, there are inherent challenges for high photon energy spectroscopic pump-probe techniques. To our knowledge, currently, there is no fs time resolution X-ray spectroscopic studies at such high energy. Very recently, FXE succeeded in collecting XAS spectra at niobium K edge (~19 keV). XAS at high X-ray energies is fundamentally limited by the large core-hole lifetime (CHL) broadening [2], which obscures the interpretation of near-edge features and comparison with theory. One way to overcome CHL broadening is to use high resolution detection (HERFD) mode, wherein an efficient X-ray spectrometer is necessary. Standard XES spectrometers operating in Bragg reflective geometry quickly loose efficiency at energies > 15 keV, thus new approaches are needed.

In this contribution, we will present our recent XES and XAS developments at the FXE instrument on high photon energies (>18 keV). A transmission-type spectrometer equipped with Laue analyzers made of silicon and quartz was recently commissioned at FXE, providing an energy resolution of about 2.5 eV (ΔE/E-1.2×10-4) at about 16-19 keV with improved photon collection efficiency [3,4]. Considering the natural linewidths of emission lines at 16-19 keV are usually 5-7 eV, our spectrometer will be able to well resolve the emission spectrum of 4d and 5f elements. Benefiting from the recent developments at FXE, we have recently performed tr-XAS measurements with ~100 fs time resolution on a photocatalyst nanoparticle Nb2O5 in solution. The first X-ray spectroscopic results provide a route for future tr-studies at high photon energies using high energy resolution. For example, HERFD-XAS measurements using our new Laue analyzers can enhance the XAS resolution to overcome the limitation imposed by CHL broadening, which is important for deconvoluting the states originating the pre-edge features and significantly improving the comparison with calculated spectra [2].

[[1]] D. Khakhulin et al. Ultrafast X-ray photochemistry at European XFEL: capabilities of the femtosecond X-ray experiments (FXE) instrument. Appl. Sci. 10, 995 (2020).
[2] F. Lima et al. High-resolution molybdenum K-edge X-ray absorption spectroscopy analyzed with time-dependent density functional theory. Phys. Chem. Chem. Phys. 15, 20911 (2013)
[3] P. Jagodzinski et al. A DuMond-type crystal spectrometer for synchrotron-based X-ray emission studies in the energy range of 15–26 keV. Rev Sci Instrum 90, 063106 (2019).
[4] X. Huang, et al., in preparation.

Indico rendering error

```
Could not include image: Cannot read image data. Maybe not an image file?
```

I plan to submit also conference proceedings

No

Primary authors: ALVES LIMA, Frederico (Eur.XFEL (European XFEL)); HUANG, Xinchao (Eur.XFEL (European XFEL)); UEMURA, Yohei (Eur.XFEL (European XFEL))

Co-authors: MILNE, Christopher (Eur.XFEL (European XFEL)); KHAKHULIN, Dmitry (Eur.XFEL (European XFEL)); ARDANA LAMAS, F. (European XFEL); WANG, Hao (Eur.XFEL (European XFEL)); YOUSEF, Hazem (Eur.XFEL (European XFEL)); Mr KNOLL, Martin (European XFEL); BIEDNOV, Mykola (Eur.XFEL (European XFEL)); Mr FRANKENBERGER, Paul (European XFEL); ZALDEN, Peter (Eur.XFEL (European XFEL)); Ms HEDER, Siti (European XFEL); JIANG, Yifeng (Eur.XFEL (European XFEL))

Presenter: HUANG, Xinchao (Eur.XFEL (European XFEL))

Session Classification: Mikrosymposium 6/3: FELs: New facilities and Opportunitites

Track Classification: 6. FELs: New facilities and opportunities