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X-RAY SPECTROSCOPY AND SCATTERING WITH 20~FMS TIME RESOLUTION AT SWISSFEL BERNINA ENDSTATION: PROBING ULTRAFAST DYNAMICS OF $[Fe(terpy)_2]^{2+}$

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Time-resolved X-ray spectroscopy and scattering techniques at X-ray free electron lasers (XFELs) are powerful tools for studying chemical dynamics on ultrafast timescales. Comprehensive insights of even disordered molecules in solution can be gained for the electronic state, local structure, and solvation structure using X-ray emission spectroscopy (XES), X-ray absorption spectroscopy (XAS), and X-ray solution scattering (XSS), respectively [Zhang et al. 2014].

Detailed views into ultrafast electronic dynamics, however, may be obscured through a limitation in temporal resolution. As shown in Transition metal compounds showing charge transfer as well as spin transitions upon optical excitation, valuable insights about their mechanism can be gained by especially studying the initial cascade of electronic state transitions [Lemke et al. 2017].

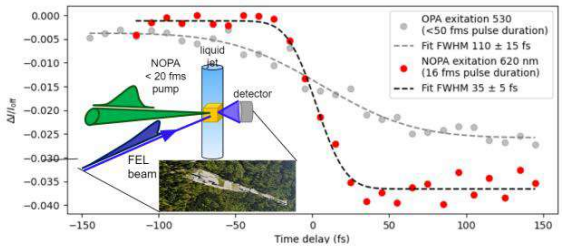

Fig. 1 Time resolved XANES measuring dynamics of the charge transfer state. at pre-edge region (7,113.5 eV) with and without ultrashort NOPA exitation performed at SwisFEL Bernina endstation

We show FEL-based results of different X-ray techniques using a newly developed NOPA laser system providing tunable pulses that allow better control of the ultrafast excitation at a timescale of the order of initial transition rates. The study has been performed on $[Fe(terpy)_2]^{2+}$, an example of molecular Iron model complexes showing ultrafast charge transfer decaying into a cascade of spin transitions. The initial subpicosecond dynamics may depend on optical excitation parameters, such as wavelength, bandwidth, and time duration. Fig. 1 shows a significant improvement in the time of transient XANES changes measured at the pre-edge region (7,113.5eV) with a tunable ultrashort NOPA.