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# Wave packet observation of Cu(I) complex by ultrafast x-ray absorption spectroscopy

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Time-resolved x-ray absorption near edge structure (TR-XANES)1 is one of most promising applications of X-ray free electron lasers (XFELs): X-ray absorption measurements combining XFELs and synchronized optical lasers enable one to probe ultrafast changes in the electronic states and the local structure around the absorbing atom during photoreactions.
Here, we report on our recent TR-XANES study of a prototypical copper(I)-phenanthroline complex, [Cu(dmphen)2]+ (dmphen = 2,9-dimethyl-1,10-phenanthroline)2-4, conducted at SPring-8 Angstrom Compact free-electron Laser (SACLA). In the experiment, femtosecond transient XANES changes were measured at three different incident photon energies of 8979.5 eV, 8985.0 eV, and 8986.5 eV. Using the timing diagnostics5,6 at SACLA, the time resolution was improved to ~70 fs by suppressing influences of a timing jitter. At 8979.5 eV (1s -> 3d transition) and 8985.0 eV (1s -> 4p transition), we clearly observed oscillations originating from coherent molecular vibrations, which damp within 1 ps. On the other hand, at 8986.5 eV (1s -> 4p transition), no oscillatory feature was found. These observations umambiguously indicate that the selection of the incident photon energy is critically important to capture a nuclear wave packet in TR-XANES. We will discuss not only the mode assignments of the observed vibrations, but also the selectivity of TR-XAS to molecular vibrations.

[1] T. Katayama, et. al., Femtosecond x-ray absorption spectroscopy with hard x-ray free electron laser, App. Phys. Lett. 103, 131105 (2013).
[2] M. Iwamura, et. al., Real-time observation of the photoinduced structural change of bis(2,9-dimethyl-1,10-phenanthroline)copper(I) by femtosecond fluorescence spectroscopy: A realistic potential curve of the Jahn-Teller distortion, J. Am. Chem. Soc. 129, 5248-5256 (2007).
[3] M. Iwamura, et. al., Coherent nuclear dynamics in ultrafast photoinduced structural change of bis(diimine)copper(I) complex, J. Am. Chem. Soc. 133, 7728-7736 (2011).
[4] G. Capano, et. al., Probing wavepacket dynamics using ultrafast x-ray spectroscopy, J. Phys. B At. Mol. Opt. Phys. 48. 21, (2015).
[5] T. Katayama, et. al., A beam branching method for timing and spectral characterization of hard X-ray free-electron lasers, Struct. Dyn. 3, 034301 (2016).
[6] T. Sato, et. al., Highly efficient arrival timing diagnostics for femtosecond X-ray and optical laser pulses, Appl. Phys. Express 8, 012702 (2015).

**Primary author:** KATAYAMA, Tetsuo (RIKEN SPring-8 Center, Japan)

**Presenter:** KATAYAMA, Tetsuo (RIKEN SPring-8 Center, Japan)

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