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Prof. Marcus Lundberg

Ångström Laboratory, Uppsala University, Sweden

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Rationalizing the sensitivity of x-ray probes to electronic and structural dynamics in transition metal complexes

Date: Tue, Nov 19th, Time: 14:30 – 16:00, Venue: Room 537, ITbM

Abstract The combination of an *ab initio* philosophy and excellent accuracy has made multi-configurational wavefunction approaches powerful tools to analyze x-ray spectra of transition metal complexes. We use chemically intuitive models that describe metal-ligand interactions using at most three. Recently, we have implemented a stable and efficient algorithm to solve the configuration interaction equations when targeting a very large number of states. We have then used this algorithm to study the electron transfer cascade upon excitation of a highly efficient iron photosensitizer, which is used to convert photons into chemical energy through electron transfer reactions. The combination of different x-ray spectroscopic techniques makes it possible to probe the coherent structural dynamics in the femtosecond time scale. We rationalize the sensitivity to structural dynamics by analyzing how the core holes affect the metal-ligand bond, which leads to a relative shift of the potential energy surfaces along the coherent vibration.

Contact: Takeshi Yanai (yanait@chem.nagoya-u.ac.jp)