

Tracking chemical transformations of transition metal complexes

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X-ray spectroscopy tools can be utilized as powerful probes of chemical dynamics, with different sources offering access to different time scales depending on their brilliance as well as time structure. Pulsed sources allowed us to introduce such techniques as probes in time-resolved pump-probe experiments. However, synchrotron-based studies make use of picosecond-long pulses, and thus lack the necessary time resolution to unveil many of the details of electron and structural dynamics in photo-induced transformations. The very intense femtosecond pulses of X-ray free electron lasers enable us to exploit X-ray spectroscopy with the appropriate time resolution, offering direct access to the changes in the charge, spin and nuclear degrees of freedom during the elementary physical processes of a chemical reaction, photophysical transformation, or biological function. Results obtained on light-excited transition-metal-based model systems for photoswitchable or light-harvesting functional molecules will be reported.

However, developments of monochromators and detectors have also affected the possible experiments with the oldest type of sources in the laboratory. In addition to frontier research, there is high demand for routine characterization of concentrated samples with the simplest X-ray spectroscopies including XANES and EXAFS. This, together with the relatively slow access to synchrotron radiation facilities made a few groups develop novel effective laboratory spectrometers. We have developed a laboratory von Hámos X-ray spectrometer, which offers relatively rapid transmission experiments for X-ray absorption. The use of a small-radius cylindrical analyzer crystal and a position sensitive detector enabled us to build a robust but flexible setup with low operational costs, while delivering spectra with good signal to noise ratio in reasonably short acquisition times. An illustrative example of the applications of laboratory XANES will be presented. This instrument can also follow chemical transformations that are too slow to be considered at synchrotrons.