# X-ray Investigations on the Mechanisms of Homo- and Heterogeneous Catalysis

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In this talk we will present the ultrafast time-resolved, in-situ and / or operando X-ray view on homogeneous and heterogeneous catalysis. The experiments are based on recent developments combining liquid jet microtechnology with different types of soft X-ray spectroscopy coupled to synchrotron and free-electron laser sources. We are particularly interested in multidimensional photon-in / photon-out techniques, such as X-ray emission spectroscopy (XES) and resonant inelastic X-ray scattering (RIXS) with high time and energy resolution. As one of the first homogeneous catalysis model systems we studied the ultrafast photocatalysis of $Fe(CO)_5$ in ethanol with iron L-edge free-electron laser RIXS.

The pilot hetero catalytic systems we investigated was the highly efficient oxygen evolution reaction (OER) on perovskites surfaces. Water splitting is intensively studied for sustainable and effective energy storage in green / alternative energy harvesting-storage-release cycles. We will present our different in-situ and time-resolved RIXS studies of the manganese L-edge and oxygen K-edge of perovskites during OER. For that various X-ray photon-in / photon-out spectroscopy techniques, zone plates and gratings have been combined with liquid jet technology. The combination of liquid jet with low-resolution X-ray spectroscopy is sufficient for element- and oxidation-state-specific chemical OER monitoring. For an in-depth study of OER mechanisms, however, including charge-transfer characterization of catalyst-water adsorbates, high-resolution (grating) spectroscopy tools resolving even vibronic couplings, combined with liquid jets bear bigger potential since they allow resolution of otherwise-overlapping, ultrafast X-ray spectroscopy transitions.

The impact of polarons and whether they can contribute to OER will be discussed for our latest high-resolution RIXS studies. How they impact proto-coupled electron transfer reaction will be presented on the example of OER on ZnO. The projects are supported by the SFB1073 (“Atomic Scale Control of Energy Conversion”) and the SFB1633 (“Proton Coupled Electron Transfer”).

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