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The orbital-based view on reaction dynamics: ligand exchange of $Fe(CO)_5$ in solution ALEXANDER FÖHLISCH, Helmholtz-Zentrum Berlin für Materialien und Energy, Potsdam University

Time resolved soft X-ray spectroscopy has proven recently, that it can beat the complexity of dynamics in materials and chemical processes by its high selectivity towards elemental, chemical, and magnetic properties. Changes in chemical bonding, in particular bond breaking and bond creation seem conceptually simple, but as a result of coherent wave packet motion it is difficult to catch the dynamic pathways in a multidimensional potential energy landscape. In this contribution we exploit the unique approach of femtosecond time resolved resonant inelastic X-ray scattering at LCLS to derive how ultrafast spin-crossover and ligation determines the pathways of ligand exchange of Ironpentacarbonyl ($Fe(CO)_5$) in solution. As an outlook, it will be discussed, how non-linear X-ray processes can push time resolved soft X-ray spectroscopy in a new phase. In particular, stimulated Raman scattering and amplified spontaneous emission can overcome the weak scattering cross-sections of spontaneous processes, help to suppress sample damage and increase spectral resolution and excited state selectivity through the exploitation of Anti-Stokes Raman Scattering.