Beating complexity through the selectivity of X-rays

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Chemistry as well as materials' functionality are determined by the potential energy surface of a systems electronic ground state and its excited states. This makes the potential energy surface a central and powerful concept in physics, chemistry and materials science. However, direct experimental access to the potential energy surface around selected atomic centers and to its long-range structure are lacking. Sub-natural linewidth resonant inelastic soft x-ray scattering at vibrational resolution is utilized to determine ground state potential energy surfaces locally and detect long-range changes of the potentials. Even directional cuts through a complex potential energy surface are possible due to highly defined wave packet dynamics during the core-excited state. In a next step, the investigation of excited state dynamics at the transform limit in energy and time will become accessible combining Anti-Stokes features with potential energy mapping. This will allow to determine also the potential energy surfaces of excited states and their crossings. Examples of selective bond modifications as well as charge separation will be discussed.