A deeper spectroscopic look at chemical bonding and hybridization

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Material and device development crucially depend on an in-depth characterization of the electronic and chemical properties of the involved materials and their interfaces. Traditionally, (soft) x-ray spectroscopy techniques are very powerful tools for probing the electronic and chemical structure. Many instrumental advances have been achieved over the last decades, mostly focusing on high-resolution (and thus unavoidably low-transmission) instruments, which are particularly important for fundamental studies of well-defined systems. In contrast, the investigation of real-world devices requires highly sensitive (high-transmission) probes that are able to measure trace elements, minimize the x-ray dose to prevent beam-induced changes, and are ideally also applicable in an *in situ/operando* environment. At the same time, the most relevant materials questions concern the chemical bonding present in the materials and how they react to changes in processing or operating conditions, which does not require the highest possible energy resolution. At KIT, we focus on developing x-ray spectroscopy techniques and the necessary experimental setups for this type of applications, which has led to the development of the SALSA (Solid and Liquid Spectroscopic Analysis) experimental station, novel soft x-ray spectrometer concepts, and the X-SPEC beamline and its endstations at the KIT Light Source.

This presentation discusses the experimental setups and the recent development of x-ray spectroscopy tools, in particular soft x-ray emission spectroscopy (XES) and resonant inelastic (soft) x-ray scattering (RIXS), for applied materials research. The particular focus will be on a deeper understanding of chemical bonding and hybridization. We use XES and RIXS to (1) identify chemical building blocks in liquids and solids and (2) extract information of their chemical environment from the fine structure of the spectra. The first highly benefits from the local character of the techniques that makes the spectral fingerprint characteristic of specific functional units, independent of their immediate environment, e.g., in a large molecule, a liquid solution, or other complex multicomponent systems. Secondly, high-quality data allows a detailed look at finer spectral differences that indeed carry information about the local chemical environment of individual atomic species. Using selected examples, it will be shown how XES and RIXS reveal hybridization between (a) solutes and solvents in liquids, (b) anions and cations in crystal solids, as well as (c) in the valence band structure of crystalline solids.