

Photon-Based Spectroscopy for Material and Energy Research:  
From Soft X-ray to Far Infrared

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The global need for sustainable sources of energy is an important driver for materials science. This challenge is a strong motivation to develop methods and build instrumentation exploiting the unique characteristics of modern light sources, and is at the heart of a growing energy material research program at HZB. The availability of a large range of photon energies (from IR to X-rays) at the synchrotron radiation BESSYII light source and of ultrashort light pulses in the UV/VIS to (X)EUV range in our laser lab are ideal to characterize materials, determine their static and dynamical properties, and to explore their behavior upon light-induced electronic excitation, and the following chemical reactions involving transient reactive species. Different methods typically reveal information on just selective aspects, and only taken together will we identify the complex physical and chemical interactions governing the processes in the material–energy interplay. For instance, X-ray techniques are extremely powerful in characterizing the local electronic structure of matter, and accurately sense smallest changes in the chemical environment. Here it is crucial to explore both the radiative and the non-radiative relaxation channels.<sup>[1]</sup> In fact we are beginning to realize the importance to simultaneously detect emitted photons and electrons, providing complementary information of the complex electronic-structure interactions. Most attractive techniques include Resonant Inelastic X-ray Scattering (RIXS) and Resonant Photoelectron Spectroscopy (RPES), and an interesting additional aspect is the structure information contained in the (photo)electron angular distribution (PAD). The latter, which is barely studied so far in the temporal domain or in liquid solutions, has been recently perused by us with the construction of a new high-harmonic generation (HHG) laser lab at FU Berlin.<sup>[2]</sup> In ongoing experiments (using ultrashort EUV laser pulses) we investigate the valence electronic structure of applied/catalytic materials under real conditions (e.g. ambient conditions), and this includes the study of solids, bulk liquid solutions, and the solid-liquid interface. In addition to electronic-structure investigation we will also explore in detail vibrations for material characterization. For this purpose we recently implemented infrared spectroscopy and microscopy, available at one of our beamlines at BESSY. In my talk I will present the power of these tools by highlighting several experimental activities in our group. (1) The electronic structure interaction and electron dynamics for Fe(CO)<sub>5</sub> complex in solution<sup>[3]</sup> and the biomimetic manganese oxides which are widely studied for water oxidation, exhibiting high oxygen evolution rates at the interfaces<sup>[4]</sup>. (2) Time-resolved PAD addressing the electron dynamics of the solvated electron which plays a key role in oxygen evolution rates from a wide range of nanoparticles. I will conclude by presenting current technical developments, e.g., dedicated experimental stations for X-ray spectroscopy, infrared<sup>[5]</sup> and laser lab challenging the study of dynamics particularly of materials in solution and at (liquid-solid) interfaces using time-resolved experiments in the XUV energy range.

**References:**

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