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## **X-Ray Photoelectron Spectroscopy: Computational Challenges and Perspectives**

Photoelectron spectroscopy is a widely applied tool to probe the electronic structure of matter. The X-Ray energy range yields access to core excited and ionized states, the energies of which are element specific. The core holes are usually localized on single atoms and their lifetime is determined almost exclusively (light elements) by the Auger decay. Hence, X-Ray photoelectron spectroscopy (XPES) provides a local and site-specific probe of the electronic structure of molecular systems. This makes it possible to study a plethora of effects, however, this talk will focus on the L-edge XPES of  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$  complexes. The iron core-hole states are highly multi-configurational and subject to strong spin-orbit coupling. To understand and characterize the feature rich experimental spectra high level calculations need to be conducted. The backbone of the computational XPES protocol [1] that I will present is the usage of high level multi-configurational self consistent field methods to obtain the wave functions and transition energies. On top of that a Dyson orbital approach is employed to estimate the transition intensities numerically [1]. The talk will start from an XPES overview, introduce the computational procedure proposed by our group, demonstrate how this can be generalized to describe the Auger decay of core hole states and discuss the most important computational challenges that need to be solved when calculating Auger decay rates.

### **References:**

[1] G. Grell et al., J. Chem. Phys., **143**, 074104 (2015)

Talk: English

Slides: English

**Location:** Institute of Physics, Albert-Einstein-Str. 24, HS1