European XFEL

THEORY GROUP MEETING

Thursday, 07th July 2016

15:00

XHQ Seminar Room E1-096

Valence State Photoemission Spectra of Solids and Possibilities for X-ray Spin Microscopy

by

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Variations of the photoionization cross section of valence states as a function of interatomic distance are studied by means of atomic and solid-state density functional approaches and compared with photoemission data. In contrast to the free atom case, a series of Cooper minima (CM) is found for 4d, 5d, and 5f states in Pd, Ag, Au, and U metals. It is shown that the translational symmetry may cause a series of Cooper minima in solids instead of a single one known to exist in the free atom. Detailed analysis of ionization spectra from 4d, 5d, and 5f states in Pd, Ag, Au, and U metals confirm the concept of the single-particle excitation and demonstrate the relationship between the lattice parameter, quality of crystalline ordering and structure of the PE spectra around the solid state CM. The spectrum of hcp U is analyzed in greater details as there are additional effects such as many body Fano and Auger processes involved in the ionization process. It is found that a cross-section minimum of the Fermi-energy feature at 90- 94 eV, which previously was assigned to a Fano anti-resonance at the 5d➔5f excitation threshold, is mainly caused by a Cooper minimum. Analogous 5f cross-section variations in the region of the 5d➔5f resonances were obtained for other 5f-element containing compounds. While the focus is on how the analysis of the X-ray PE spectra may serve as a powerful tool for investigation of the valence state wave function spatial structure in solids, there is also a discussion on the additional information about the electronic structure hidden in the spin-resolved spectra. Particular emphasis is on the magnetic structure including periodic non-collinear alignment in solids which is shown to be encoded in the spin-resolved X-ray emission. Possibilities for the decoding of the spin-structure information and concepts of the X-ray microscopy are briefly discussed as well.