Modeling Resonant Inelastic X-ray Scattering and Resonant X-ray Emission in the LDA+DMFT framework

J. Kolorenč

Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha, Czech Republic,
kolorenc@fzu.cz

I will introduce a theoretical description of photon-in/photon-out resonant X-ray spectroscopies, which is based on the Anderson impurity model. The parameters of the model are determined with the aid of the material-specific LDA+DMFT electronic-structure calculations and the spectra themselves are evaluated using a combination of the Krylov subspace methods [1].

As an application, I will discuss the valence-to-core resonant inelastic X-ray scattering (RIXS) at the europium L_3 edge in the ferromagnetic semiconductor EuS. In this setup, the main signal comes from the direct RIXS: an Eu 2p core electron is excited to an empty Eu 5d band above the Fermi level, and then another electron from an Eu 5d state hybridized with the S 3p bands (located below the Fermi level and hence occupied) fills back the Eu 2p core hole. I will analyze if one can expect to detect also indirect RIXS processes where additional excitations are induced by the Coulomb potential of the 2p core hole.

In the EuS example, the multiplet coupling between the deep Eu 2p core hole and the open Eu 4f shell in the intermediate state of the RIXS process is negligible. The same, however, is not true for resonant X-ray emission (RXES) when a shallower core hole (3d or 4d) is present in the final state. I will illustrate these core-hole effects, relate them to effects seen in the core-level photoemission [2,3], and discuss them also in the context of the high-resolution fluorescence-detected X-ray absorption spectroscopy (HERFD-XAS).

References

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