Circular dichroism in spin-resolved resonant photoemission

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Abstract

When valence band photoemission is performed at a core-level resonance, detailed chemical and site selective information on the valence electronic state can be obtained [1]. The analysis of the data is, however, complex and accurate computational methods are lacking, in particular for solid surfaces.

Here we present a first principles method for resonant valence band photoemission spectroscopy (RPES) in the participator channel, based on a real space multiple scattering approach [2,3]. The method is applied to 2p-3d RPES of itinerant magnets, either ferromagnetic (Fe(100) surface) or antiferromagnetic (Cr(110) surface).

We find strong circular dichroism in the spin-resolved RPES spectra, even for antiferromagnets and disordered ferromagnets, in agreement with experiments. It has been claimed that such dichroism is a direct measure of local magnetic moments. Our results contradict this interpretation, as we find a strong dichroic signal even for a non-magnetic ground state.

We show that circular dichroism in spin-resolved RPES is essentially due to an angular momentum transfer from the photon helicity to the photoelectron spin via the core spin-orbit coupling and the core-valence exchange interaction [2].

[1] P. Krüger et al. Phys. Rev. Lett. 108, 126803 (2012).

[2] F. Da Pieve and P. Krüger, Phys. Rev. Lett. 110, 127401 (2013).

[3] F. Da Pieve and P. Krüger, Phys. Rev. B 88, 115121 (2013).