

Theory of resonant photo- and Auger-electron diffraction

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When the photon energy is tuned to an X-ray absorption white line, valence band photoelectrons are resonantly excited from a deep core state, resulting in an effective localization of the initial state and a chemical and orbital selectivity of the valence photoemission process [1]. Combined with photoelectron diffraction, resonant photoemission (RPES) can be used to obtain element and site-specific information of chosen valence states as we have demonstrated for in-gap states of TiO₂ [2]. After revising these findings, we present calculations of angle-resolved RPES from magnetic surfaces. First RPES of Cr and Fe surfaces is computed in the independent particle picture using a multiple scattering approach for both valence and photoelectron continuum states. The question of what information can be obtained from the combination of circular dichroism and photoelectron spin-resolution is critically examined [3]. We find that this experiment is generally not able to detect local magnetic moments in antiferromagnets or disordered ferromagnets as claimed by some authors.

Next we present a new theory of resonant photo- and Auger electron diffraction which is based on multiplet theory and multiple scattering [4]. The X-ray excitation and the Auger decay process are described in a ligand field multiplet model. For each final state channel, a real-space multiple scattering calculation is performed using a popular X-ray photoelectron diffraction code. With this approach we compute resonant photoelectron spectra and diffraction patterns from Nickel (111) and (001) surfaces, with special emphasis on the circular dichroism signal. We obtain forward focussing peak shifts (the so-called Daimon effect) in resonant photoemission, and show that its sign depends on the multiplet final state, in agreement with recent experimental findings [5]. The sign reversal is explained by analyzing the angular momentum transfer from the light to the photoelectron.

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