

RECENT THEORETICAL TRENDS IN ANGLE RESOLVED PHOTOEMISSION: CORRELATION, DISORDER AND TEMPERATURE EFFECTS

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1. Abstract

Angle resolved as well as angle integrated photoemission in the soft and hard X-ray regime became a very important tool to investigate the bulk properties of various materials [1]. Contrary, bulk sensitivity can be achieved by so called threshold photoemission, e.g. by using for example laser light at 405 nm [2]. The increased bulk sensitivity might lead to the impression that the LSDA band structure or density of states can be directly compared to the measured spectra. However, various important effects, like matrix elements, the photon momentum or phonon excitations, are in this way neglected. Here, we present a generalization of the state of the art description of the photoemission process, the so called one-step model that describes excitation, transport to the surface and escape into the vacuum in a coherent way. A short introduction to the main features of the one-step model implementation within the Munich SPR-KKR program package will be given. Special emphasis will be put on the spin-polarised relativistic mode that allows to deal with magnetic dichroism. Also, the possibility to account for correlation effects and chemical disorder using the LSDA+DMFT (dynamical mean field theory) scheme in combination with the Coherent Potential Approximation (CPA) method [3] will be demonstrated by various examples [5].

References:

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