CEA - Saclay 91191 Gif-sur-yvette Cedex

Service de Physique de l'Etat Condensé

SÉMINAIRE

Mardidi 03 juin 2014 à 11h15

Orme des Merisiers SPEC, Salle Itzykson, Bât.774

One step model description of HAXPES: Correlation, matrix elements and temperature effects

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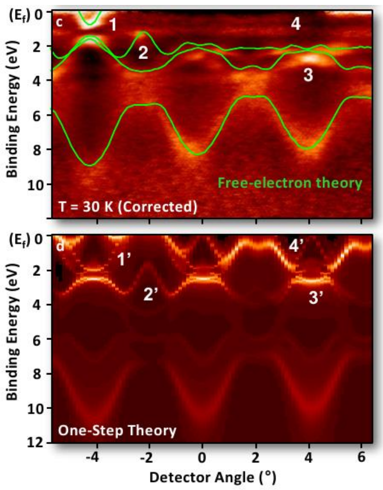
Angle resolved as well as angle integrated photoemission in the soft and hard X-ray regime became a very important tool to investigate the bulk properties of various materials [1]. Contrary, bulk sensitivity can be achieved by so called threshold photoemisison, e.g. by using for example laser light at 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 photoemisison 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. For photon energies, even in the soft-x-ray regime, a considerable effect of lattice vibrations is present [4]. Here, we discuss a theoretical description of lattice vibrations which is based on the CPA. These aspects will be discussed in an detail using various examples [5]. In the last part of my talk I will show prediction that HAXPES is possibly valuable tool to study topological surface states and rashba effect [6].

1. A. Gray, etl al., J. Minar et al., Nat. Mat. 10, 759 (2011).
2. M. Kronseder, Ch. Back, J. Minar et al., Phys. Rev. B 83, 132404 (2011)
3. J. Minar, J. Phys.: Cond. Mat. Topical review 23, 253201 (2011), H. Ebert et al., Rev. Prog. Phys. 74, 096501 (2011)
4. J. Braun, J. Minar et al., Phys. Rev. B 88, 205409 (2013)
5. A. Gray, J. Minar et al., Nature materials 11, 957 (2012), Fujii et al., Phys. Rev. Lett. 111, 097201 (2013)
6. J. Braun et al., New J. Phys 16, 015005 (2014)



A coffee break will be served at 11h00. The seminar will be given in English.