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TÉMA

KKR-Green's function method - recent developments and applications to ARPES

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The modern version of the KKR (Korringa–Kohn–Rostoker) method represents the electronicstructure of a system directly and efficiently in terms of its single-particle Green's function. Direct access to the Green function results in several appealing features. In particular the description of the electronic correlations, disorder and electronic spectroscopies for the nanosystems and surfaces has been developed in the recent years. In the first part of my talk I will review basic ideas of the multiple scattering KKR formalism. Second part will be devoted to the Angle-resolved photoemission spectroscopy (ARPES) which is a leading experimental probe for studying the electronic structure and complex phenomena in quantum materials. Modern experimental arrangements consisting of new photon sources, analyzers and detectors supply not only spin resolution but also extremely high angle and energy resolution. Furthermore, the use of photon energies from few eV up to several keV makes this experimental technique a rather unique tool to investigate the electronic properties of solids and surfaces. On the theoretical side, it is quite common to interpret measured ARPES data by simple comparison with calculated band structure.

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. Nowadays, the one-step model allows for photocurrent calculations for photon energies ranging from a few eV to more than 10 keV, for finite temperatures and for arbitrarily ordered and disordered systems, and considering in addition strong correlation effects within the dynamical mean-field theory. Application of this formalism in order to understand ARPES response of new materials like low-dimensional magnetic structures, Rashba systems, topological insulator materials or high TC materials will be shown.

In this presentation I review some of the recent ARPES results and discuss the future perspective in this rapidly developing field.

odborný garant: *Ing. Pavel Jelínek, Ph.D.*