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DESIGN OF NOVEL MATERIALS: ARPES EXPERIMENTS AND THEORY

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Angle-resolved photoemission spectroscopy (ARPES) 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 [1]. 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 [2]. 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 excitation, 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 [3,4]. 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 [6], Rashba systems [5], topological insulator materials [1], materials relevant for photo-catalysis [8] or ultrafast femtosecond spin dynamics [7] will be shown.
In this presentation I review some of the recent ARPES results and discuss the future perspective in this rapidly developing field. In addition I will introduce our new spin polarised ARPES laboratory.

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