Theoretical description of angular momentum resolved photo emission on the basis of the one-step model - recent developments

PD. Dr. Jan Minar
(Department Chemie und Biochemie, Ludwig-Maximilian-Universität München)

Abstract:

Various technical developments enlarged the potential of angle-resolved photo-emission (ARPES) tremendously during the last one or two decades. In particular improved momentum, energy and spin resolution as well as the use of photon energies from few eV up to several keV makes ARPES a rather unique tool to investigate the electronic properties of solids and surfaces [1,2]. These experimental developments needs to be closely followed by corresponding theoretical description beyond simple interpretations like e.g. spectral function or DOS. 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. Within this approach we account for correlation effects by LSDA+DMFT, disorder by means of CPA and lattice vibrations by alloy analogy model. All these developments will be demonstrated by various examples.
In the last part of my talk I will show novel description of the ultrafast pump-probe experiments by means of multiple scattering Keldysh formalism [3].

[1] A. Gray, etl al., J. Minar et al., Nat. Mat. 10, 759 (2011) Minar et al., J. El. Spec. Rel. Phen. 190, 159 (2013)
[2] M. Jourdan et al., Nat. Com. 5, 3974 (2014)
[3] J. Braun et al., Phys.RevB 91, 035119 (2015), C. Cacho et al., Phys. Rev. Lett. 114, 097401 (2015)