Fritz-Haber-Institut der Max-Planck-Gesellschaft

Physikalische Chemie — Direktor: Prof. Dr. Martin Wolf

MAX-PLANCK-GESELLSCHAFT

Department Seminar:

Tuesday, October 1, 2019, at **11:00** a.m.;
— all are invited to meet at around 10:40 for a chat with coffee & cookies —

Apl. Prof. Dr. Jürgen Braun

Department Chemie,
Ludwig-Maximilians Universität
München.

The one-step model of 2PPE combined with inverse photoemission: applications to simple metals and complex compounds

PC Seminar Room G2.06, Building G, Faradayweg 4 A. Paarmann

Abstract:

A brief introduction to the theory of angle-resolved photoemission spectroscopy (ARPES) of solids is given with an emphasis on the so-called one-step model of photoemission that describes excitation, transport to the surface and the escape to the vacuum in a coherent way. As the latest development a theoretical frame for the description of pump-probe photoemission is presented. The approach is based on a general formulation using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives the system out of equilibrium [1,2,3]. The theory is implemented within the fully relativistic spin-density matrix formulation [4], and is part of the Munich SPR-KKR program package [5].

As a first application, the theoretical description of two-photon photoemission (2PPE) for Ag(100) within the SPR-KKR-approach is introduced [2]. Furthermore, first examples of angular-resolved 2PPE calculations on Fe(100) will be presented where correlation effects are accounted for by means of a static self-energy $\Sigma^{DMFT}(E)$ obtained for Fe from dynamical mean-field theory. At last the impact of relativistic effects on image potential states on the ferromagntic metals Fe, Co and Ni will be discussed within a combined IPE and 2PPE analysis..

[1] J. Braun, R. Rausch, M. Potthoff, J. Minar, and H. Ebert, Pump-probe theory of angle-resolved photoemission, Phys. Rev. B 91, 035119 (2015).
[2] J. Braun, R. Rausch, M. Potthoff , and H. Ebert, One-step theory of two-photon photoemission, Phys. Rev. B 94, 125128 (2016).
[3] J. Braun and H. Ebert, Relativistic theory of 2PPE from ferromagnetic materials, Phys. Rev. B 98, 245142 (2018).
[4] J. Braun, K. Miyamoto, T. Okuda, M. Donath, A. Kimura, H. Ebert, and J. Minar, Topological behavior of d-like surface resonances: the one-step model in its density matrix formulation applied to W(110), New Journal of Physics 16, 015005 (2014).
[5] H. Ebert et al., The Munich SPR-KKR package, version 8.4, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2019).