HL 38: Frontiers of electronic structure theory: Charge and spin dynamics

Time: Tuesday 14:00–15:45 Location: MA 004

Invited Talk HL 38.1 Tue 14:00 MA 004

First-principles theories of electron-plasmon and electron-spin fluctuation interactions in nanomaterials — •Johannes Lischner — Imperial College, London, United Kingdom

The GW method includes an accurate treatment of many-electron interaction effects beyond density-functional theory and is the state-of-the-art approach for computing spectral functions and quasiparticle energies in nanomaterials. These quantities are measured in photoemission and tunneling experiments. Despite its great success, the GW approach has certain shortcomings and I will discuss two topics that require going beyond GW: i) plasmon satellites in spectral functions and ii) the coupling of quasiparticles to spin fluctuations.

Plasmon satellites in recent photoemission experiments on doped graphene have been interpreted in terms of novel plasmaron excitations, strongly coupled plasmon-hole states, predicted by GW theory. Using a cumulant expansion of the Green's function to include higher-order electron-electron interaction effects and an accurate description of the substrate, I will demonstrate that no plasmaron states need to be invoked to explain the experiments. Similar conclusions are drawn for tunneling spectra of semiconductor quantum-well two-dimensional electron gases. I will also discuss the interaction of quasiparticles with spin fluctuations in iron selenide and demonstrate that significant coupling constants can give rise to superconducting transition temperatures consistent with experimental findings.

HL 38.2 Tue 14:30 MA 004

Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-C60 dyad — •Stefano Pittalis[1], Alain Delgado[1], Jörg Robin[2], Lena Freimuth[3], Jens Christoffers[3], Christoph Lienaua[2], and Carlo Andrea Rozzi[1] — [1]Istituto Nanoscienze - CNR, Modena, Italy — [2]Institut fuer Physik and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany — [3]Institut fuer Chemie and Center of Interface Science, Carl von Ossietzky Universität, Oldenburg, Germany

A novel dyad composed of a diaminoterephthalate scaffold, covalently linked to a Fullerene derivative, is explored as a nanosized charge separation unit powered by solar energy. Its opto-electronic properties are studied and the charge separation rate is determined. Simulations of the coupled electronic and nuclear dynamics in the Ehrenfest approximation are carried out on a sub 100 fs time scale after photoexcitation in order to gain insights about the mechanisms driving the the charge separation. In particular, the role of vibronic coupling and of the detailed morphology are highlighted.

HL 38.3 Tue 14:45 MA 004

Transfering spin into an extended π-orbital of a large molecule – ab-initio study of Au-PTCDA:Au(111) — •T. Deilmann[1], T. Esat[2], B. Lechtenberg[3], P. Krüger[1], C. Wagner[2], R. Temirov[2], F.B. Anders[3], F.S. Tautz[2], and M. Rohlfing[1] — [1]Institut für Festkörpertheorie, Universität Münster, Germany — [2]Peter Grünberg Institute (PGI-3), FZ Jülich, Germany — [3]Lehrstuhl für Theoretische Physik II, TU Dortmund, Germany

The combination of an organic molecule with an unpaired spin offers a large variety of interplay between spins and orbitals, with high sensitivity to structural and environmental details. Recently, a single Au atom on a PTCDA monolayer physisorbed on Au(111) has been investigated experimentally; it exhibits a Kondo peak in the STS spectrum.

In this talk we discuss ab-initio mean-field electronic spectra (which will then serve as input data for a subsequent NRG calculation to describe the Kondo effect). Based on ab-initio structural data (in agreement with observed STM images) we evaluate the electronic spectra by many-body perturbation theory within the *GW* approximation, as well as, a simplified LDA+*GdW* approach [1]. For gas-phase PTCDA and Au-PTCDA, both methods agree well with one another and with available measurements. For Au-PTCDA on Au(111), a full *GW* calculation is too expensive due to the substrate. LDA+*GdW*, on the other hand, fully allows to incorporate the substrate polarizability in the self energy inside the molecule and leads to good agreement with the experimental data.

[1] M. Rohlfing, *Phys. Rev. B* **82**, 205127 (2010).

HL 38.4 Tue 15:00 MA 004

Quasi-particle band structure of the transition-metal-based zero-gap semiconductors — •Murat Tas[1], Ersoy Sasioglu[2], Iosif Galanakis[3], Christoph Friedrich[2], and Stefan Blügel[2] — [1]Department of Basic Sciences, İstanbul Kemerburgaz University, 34217 İstanbul, Turkey — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Department of Materials Science, School of Natural Sciences, University of Patras, GR-26504 Patra, Greece

Zero-gap semiconductors (SCs) are promising materials for a variety of applications ranging from spintronics to thermoelectricity. Using the *GW* approximation within the framework of the FLAPW method, we study the quasi-particle band structure of a number of transition-metal-based zero-gap SCs XX′YZ, where X, X′ and Y are the transition metal elements, and Z is an *sp* element. We find that, in contrast to *sp*-electron based SCs such as Si and GaAs, the many-body renormalization has a minimal effect on the electronic band structure of these systems. It turns out that for many compounds the change of the band gap is less than 0.2 eV, which makes the starting point PBE a good approximation for the description of the electronic properties of these materials. Furthermore, the band gap can be tuned either by the variation of the lattice parameter or by the substitution of the Z element.

HL 38.5 Tue 15:15 MA 004

Keldysh nonequilibrium Green's function vs. Feshbach projection operator approach for plasmon-assisted photoemission — •Yaroslav Pavlyukh, Michael Schüler, and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

A unified theoretical treatment of the single and double electron emission is achieved by using the Feshbach projection method. In this formalism the final target's state fixes the projection operator which subsequently determines the effective Hamiltonian and the optical potential for emitted electrons. The method of non-equilibrium Green's functions is a complementary approach which also allows to treat such processes diagrammatically. We explicitly establish a correspondence between these two approaches and illustrate the diagrammatic technique by calculations of the two-electron emission from C_{60} assisted by the excitation of plasmons.

HL 38.6 Tue 15:30 MA 004

Inclusion of thermal lattice vibrations and spin fluctuations within transport calculations — •Sergiy Mankovsky, Kristina Chadova, Diemo Ködderitzsch, Svitlana Polesya, and Hubert Ebert — Dept. Chemie/Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Deutschland

We present an approach for the calculation of response quantities, e.g. Gilbert damping and electrical conductivity, accounting for temperature induced effects of lattice vibrations and spin fluctuations. The approach is based on the alloy analogy model with thermal vibrations and spin fluctuations modeled by random atomic displacements or magnetic moments deviations, respectively. We discuss various models to deal with spin fluctuations, determining their impact on the temperature dependent behaviour of conductivity and Gilbert damping parameter. We demonstrate the non-additivity of the separate contributions to the conductivity. The results of the calculations are compared to experimental data demonstrating a rather good agreement for the systems under consideration.