O 2: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles I (jointly with TT)

Time: Monday 10:30–13:15 Location: HE 101

Topical Talk O 2.1 Mon 10:30 HE 101

Non Uniform Polarizability and Coulomb interactions in Compounds and Interfaces — •George Sawatzky — Physics department University of British Columbia 6224 agricultural road Vancouver BC Canada

The polarizability of relatively ionic compounds like the transition metal or rare earths exhibit quite non uniform polarizabilities requiring a full treatment of the non local field effects when studying the the details of especially relatively short range electron -electron interactions. We discuss how this affects the effective on site Coulomb interactions and show that the intermediate range interactions are not monotonically decreasing with distance even for insulating materials. this has important consequences for the use of models like the Hubbard model especially in low dimensional systems. We will use examples of low dimensional systems as well as the Cuprates, Manganites, Fe Pnictides with strongly polarizable anions in this discussion. We suggest that for the Fe Pnictides the Fe-Fe nearest neighbor coulomb interactions can be much smaller than the next nearest neighbor ones and may turn out to be slightly attractive. Similar non local effects are present at surface and interfaces which can lead to band gap closing rather than conventional band bending for semiconductor metal interfaces. In view of this it is rather important to revisit simple on site only based models and to develop first principles approaches taking into account the non uniform polarizability of the systems studied.

O 2.2 Mon 11:00 HE 101

Adatom systems on the silicon 111-surface: Mott or not? — •Philipp Hansmann, Loig Vaugier, and Silke Biermann — Centre de Physique Theorique, Ecole Polytechnique, CNRS-UMR7644, F-91128 Palaiseau, France

For more than a decade now the interest in adsorbate systems on semiconducting substrates has increased due to exotic ground state features among which one finds charge-density waves[1] and even superconductivity[2]. Associated are often surface states with rather small bandwidths and the question about the role of electronic correlations arises naturally. Especially for akaline-metal adatoms on the Si(111) surface such correlations have been claimed to be essential for an explanation of the insulating ground state within a Mott scenario[3]. However, recent experimental findings [4] challange this theory and have reignited the "surface-correlation-controversy". In order to resolve the issue from a state-of-the-art theoretical point of view, the mere solution of an effective many-body problem is only one part of the answer. As long as the interaction parameters for such calculations are not determined in an ab initio way, there cannot be any definitive conclusions. In our work we outline the procedure of the so called constrained random phase approximation to calculate interaction parameters for the semiconductor surface systems in order to promote methods like the merger of density functional- and dynamical mean field theory to be truly ab initio.[1]J.M.Carpinelli et al., Nature 381,398(1996); [2] T. Zhang et al.,Nat.Phys. 6,104(2010); [3]H.H. Weitering et al.,PRL 78,1331(1997); [4]C. Tournier-Colleta et al.,PRB 84,155443(2011)

O 2.3 Mon 11:15 HE 101

Hubbard U and Hund's J from the constrained Random Phase Approximation within a full-potential linearized augmented plane wave approach: trends for 3d and 4d transition metal perovskites — •Loig Vaugier[1], Hong Jiang[2], and Silke Biermann[1] — [1]CPHT, Ecole Polytechnique, Palaiseau, France — [2]College of Chemistry, Peking University, Beijing 100871, China

Determining the Coulomb interactions in real materials presents a serious challenge for first principles approaches. In 2004, a systematic way - called constrained-RPA (cRPA) - of calculating the Hubbard U and Hund's rule J parameters from first-principles has been proposed by Aryasetiawan and coworkers [1]. We have implemented the cRPA method in the framework of the Full Potential Linear Augmented Plane Waves method as implemented in the Wien2k code [2]. Our scheme permits us to calculate the Hubbard interactions in the same basis in which combined LDA+DMFT calculations are performed within the implementation of [3], yielding a fully consistent first-principles scheme. As an application of cRPA, we have calculated Hubbard U's and Hund J's for cubic 3d and 4d transition metal perovskites [4]. In contrast to what is usually assumed, the trend is not necessarily monotonic. Our work emphasizes the dependence of U and J on the choice of the one-electron part of the Hamiltonian.

[1] Aryasetiawan et al. PRB 70, 195104 (2004)
[2] Blaha et al., Wien2k, (2001)
[3] Aichhorn et al., PRB 80, 085101 (2009)
[4] Vaugier, Jiang and Biermann, in preparation

O 2.4 Mon 11:30 HE 101

Strength of the Hubbard U at metal and insulator surfaces — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The effective on-site Coulomb interaction (Hubbard U) between localized electrons at surfaces of solids is expected to be enhanced since the effective screening volume of the surface is reduced with respect to the bulk. By means of first-principles calculations in conjunction with the constrained random-phase approximation (cRPA) [1] within the full-potential linearized augmented-plane-wave (FLAPW) method [2] we show that this is indeed the case for simple metals and insulators but not necessarily for transition metals and insulators that exhibit pronounced surface states. In the latter case, the screening contribution from surface states as well as the influence of the band narrowing can increase the electron polarization to such an extent that the expected decrease resulting from the reduced effective screening volume is overcompensated. In some cases, the Hubbard U parameter is substantially reduced, e.g., by around 30% for the (100) surface of bcc Cr, contrary to the conventional wisdom. We show a systematic study for prototype materials including transition-metal surfaces.

[1] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011).
[2] http://www.flapw.de

O 2.5 Mon 11:45 HE 101

Multi-orbital Kondo physics of Co in Cu hosts — •Tim Wehling[1], Brigitte Surer[2], Matthias Troyer[2], Philipp Werner[2], Andreas Läuchli[3], Aljoscha Wilhelm[1], and Alexander Lichtenstein[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [2]Theoretische Physik, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zürich, Switzerland — [3]Institut für Theoretische Physik, Universität Innsbruck, Technikerstrasse 25/2, A-6020 Innsbruck, Austria

We investigate the electronic structure of cobalt atoms on a copper surface and in a copper host by combining density functional calculations with a numerically exact continuous-time quantum Monte Carlo treatment of the five-orbital impurity problem. In both cases we find low energy resonances in the density of states of all five Co d-orbitals. The corresponding self-energies indicate the formation of a Fermi liquid state at low temperatures. Our calculations yield the characteristic energy scale – the Kondo temperature – for both systems in good agreement with experiments. We quantify the charge fluctuations in both geometries and suggest that Co in Cu must be described by an Anderson impurity model rather than by a model assuming frozen impurity valency at low energies. We show that fluctuations of the orbital degrees of freedom are crucial for explaining the Kondo temperatures obtained in our calculations and measured in experiments.

Topical Talk O 2.6 Mon 12:00 HE 101

Actual theoretical trends in angle resolved photoemission: correlation, disorder and temperature effects — •Ján Minár — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany

The fully self-consistent combination of local spin-density approximation (LSDA) and dynamical mean field theory (DMFT) provide a powerful tool to treat correlations beyond plain LSDA. The KKR or multiple scattering approach implemented on this basis allows among others to deal with alloy and surface systems as well as to study various spectroscopic properties on equal footing [1]. The latter feature is of particular interest because a direct comparison with experimental data reveal the impact of correlation effects unambiguously as matrix element, surface and temperature effects are included [2]. Here, we present a generalisation of the state of the art description of the pho-

toemission process, the so-called one-step-model of photoemission that describes the photoemission process in a coherent way. To illustrate the applicability of this formalism several examples of ARPES calculations from simple transition metals (Fe, Co), transition metal oxides (NiO, VO_2) as well as from complex disordered alloys (Ni_xPd_{1-x}, GaMnAs, $SrTiO_3/La_xSr_{1-x}MnO_3$) will be presented [3].

[1] J. Minár, J. Phys.: Cond. Mat. (Topical Review) **23**, 253201 (2011).
[2] H. Ebert,D. Ködderitzsch and J. Minár, Rep. Prog. Phys. **74**, 096501 (2011).
[3] A. Gray et al., J. Minar et al., Nature materials **10**, 759 (2011); J. S. Barriga et al., Phys. Rev. B **82**, 104414 (2010)

O 2.7 Mon 12:30 HE 101

Valence-band correlations and core hole effects in the x-ray absorption and magnetic circular dichroism spectra — •Ondřej Šipr[1], Stephan Borek[2], Angelika Chassé[2], Hubert Ebert[3], and Jan Minár[3] — [1]Institute of Physics AS CR v.v.i., Praha, Czech Republic — [2]Institut für Physik, Martin-Luther-University Halle-Wittenberg, Germany — [3]Department Chemie, Universität München, Germany

A quantitative description of the x-ray absorption spectra (XAS) and x-ray circular magnetic dichroism spectra (XMCD) should account for correlations between valence electrons in the initial state and for a core hole in the final state. We employ the local spin density approximation (LSDA) plus dynamical mean field theory (DMFT) formalism to describe the correlations between the d electrons and the linear-response theory within the time-dependent density-functional-theory (TDDFT) to describe the core hole. The most important effects beyond the LSDA are thus included and yet the scheme is computationally tractable.

The impact of many-body effects on XAS and XMCD is assessed by investigating $L_{2,3}$-edge spectra of $3d$ transition metals. We find that the LSDA+DMFT alone improves the LSDA results, in particular concerning the asymmetry of the L_3 white line. To get more accurate results, particularly concerning the ratio of the intensities of the L_3 and L_2 peaks, the dynamic aspects of the core hole have to be included via the TDDFT linear response framework. Similar conclusions follow also from our study of Heusler alloys (Cu_2MnAl).

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O 2.8 Mon 12:45 HE 101

Progress and problems of DFT+DMFT approach — •Alexander Lichtenstein — Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg

Effects of strong electron correlations in real materials can be described within the QMC, GW or DFT+DMFT methods. We discuss recent progress of realistic Dynamical Mean Field Theory of complex systems including oxides and magnetic nanomaterials. Possible future directions to overcome standard problems of the DFT+DMFT scheme and to include non-local correlation effects will be reviewed.

O 2.9 Mon 13:00 HE 101

GW+EDMFT simulation of the U-V Hubbard model — •Thomas Ayral[1], Silke Biermann[2], and Philipp Werner[1] — [1]Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France

We study the extended Hubbard model with on-site and nearest-neighbor repulsion on a square lattice within a GW+EDMFT scheme at finite temperature and half-filling. This technique combines the successful description of screening effects due to non-local interactions within Hedin's GW approximation with the dynamical mean field description of strong local interactions. We analyze the role of the frequency-dependence of the local interactions in the formation of the charge-ordered phase and show that non-local contributions to the self-energies generated via the GW approximation have a substantial impact on the local observables and on the phase diagram, depending on the interaction parameters. Our work thus has implications for electronic structure techniques based on Hedin's GW approximation in that it demonstrates a local many-body vertex to be sufficient for fully self-consistent GW calculations.