MM 42: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–17:45 Location: HL 001

Invited Talk MM 42.1 Wed 15:00 HL 001

Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design — •Gabriel Kotliar — Serin Physics Laboratory Rutgers University — Brookhaven National Laboratories

We will introduce a project, to build algorithms and a suite of open source codes, to compute the electronic structure of correlated materials. It involves different methods, to provide different compromises between speed and accuracy, and to treat different types of correlation (static and dynamic). The suite includes methods ranging from vertex corrected GW, rotationally invariant slave bosons and LDA+DMFT, and we will illustrate some of these methods (and their failures) in d and f electron systems.

MM 42.2 Wed 15:30 HL 001

Spectral properties of Sr2IrO4 from first principles — •Cyril Martins[1], Benjamin Lenz[2], and Silke Biermann[2,3] — [1]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin-orbit system Sr2IrO4 has raised tremendous interest recently, due to intriguing similarities to the high-Tc superconducting copper oxides.

We study the evolution of the electronic structure of Sr2IrO4 using a combination of ab-initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent photoemission data, finding good agreement with experiment.

MM 42.3 Wed 15:45 HL 001

Role of non-local correlations in doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

When doping the spin-orbit system Sr_2IrO_4 recent photoemission experiments found pseudogap behavior at low temperatures, which raises the question of its relation to the pseudogap found in high-Tc superconducting copper oxides.

Here, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron- and hole-doping by combining ab-initio density functional theory and two quantum cluster techniques. Our treatment includes the effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions on a first-principles level. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. Furthermore, pseudogap features in the momentum-resolved spectral function of the emerging exotic metallic state are analyzed and found to be in good agreement with experiment.

MM 42.4 Wed 16:00 HL 001

Describing the coupled structural and metal-insulator transition in rare-earth nickelates with DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO_3}$, display a rich phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and is related to a charge disproportionation driven by correlation effects, resulting in an insulating state. Here, we employ density functional theory together with dynamical mean field theory (DFT+DMFT) to explore the interplay between lattice distortions and electronic correlation effects in these compounds. By utilizing a symmetry-based distortion mode analysis, we are able to isolate the specific lattice distortion occurring at the phase transition. Calculating total energies within DFT+DMFT then allows us to relax the structures with respect to this distortion. We find, that the resulting distortion amplitudes and its variation across the series are in good agreement with experimental results. Our work highlights the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

MM 42.5 Wed 16:15 HL 001

Magnetocrystalline anisotropy of FePt: LDA+DMFT study — •saleem Ayaz Khan[1], Junqing Xu[2], johan Schott[3], Ondřej Šipr[1], and Jan Minár[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany — [3]Uppsala University, Sweden

In our recent work (Phys. Rev B, 94, 144436, 2016) we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

MM 42.6 Wed 16:30 HL 001

Diagnostics for plasmon satellites and Hubbard bands in transition metal oxides — •Steffen Backes[1], Hong Jiang[2], and Silke Biermann[1] — [1]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France — [2]College of Chemistry and Molecular Engineering, Peking University, China

The generally accepted picture of $SrVO_3$ is that of a correlated electron metal where a renormalized quasi-particle peak at the Fermi level coexists with upper and lower Hubbard bands, separated by Coulomb interaction U. Recently, this picture has become blurred with the rise in interest in additional plasmonic satellites. Distinguishing plasmonic features from Hubbard bands is a non-trivial question. In this talk we employ combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") to discuss the processes that give rise to these different satellites and show how to identify their origin in realistic materials. We present an application of this scheme to different transition metal oxides, which we find to exhibit both Hubbard and plasmonic satellites at similar energetic positions.

MM 42.7 Wed 16:45 HL 001

Phase transitions of the 2D Hubbard-Holstein model — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In the 2d Hubbard-Holstein model at zero temperature, a quantum phase transition between Mott and Peierls insulator can be observed. Whether a metallic phase emerges in between remains an open question [1,2]. As the emergence of the Mott phase is a many body effect, a description beyond the mean field level is crucial. At the same time, a method that can cope with two dimensions is needed.

To address this open question, we have extended Density Matrix Embedding Theory (DMET) from the purely electronic case [3,4] to coupled fermion-boson systems. DMET is an embedding theory which benefits from the exponentially decaying correlation in most quantum systems thus allowing a description beyond mean field at low cost.

We show the phase diagram of the 2d Hubbard-Holstein model at zero temperature obtained for different cluster sizes. [1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012) [2] S. Wouters, C. A. Jiménez-Hoyos, G. K.-L. Chan, arXiv:1605.05547 (2016) [3] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett 95, 096401 (2005) [4] J. Bauer, EPL 90 27002 (2010)

MM 42.8 Wed 17:00 HL 001

A quantum embedding theory combining many-body perturbation theory with configuration interaction — •Marc Dvorak and Patrick Rinke — Department of Applied Physics, Aalto University School of Science, 00076-Aalto, Finland

We present a new quantum embedding theory called dynamical configuration interaction (DCI). It captures non-local and static correlation in an orbital active space with configuration interaction (CI) and high-energy, dynamic correlation in the complementary bath space with many-body perturbation theory (MBPT). The formulation is general, but we focus on molecular systems with an *ab-initio* Hamiltonian. The conceptual key to our approach is to replace the exact electronic Hamiltonian in the bath space with one of excitations defined over the correlated ground state. This transformation is naturally suited to the language and methodology of many-body Green's functions. Correlation in the bath is therefore described at the quasiparticle level with Green's functions instead of with the many-body wave function. Our approach avoids computational and conceptual difficulties associated with Green's function embedding and improves upon wave function methods by including dynamical correlation from the bath space. A major advantage to DCI is that it naturally treats ground and excited states on equal quantum mechanical levels. For ground state properties, we present dimer dissociation curves for H_2 and N_2 in excellent agreement with exact results. Excited states of N_2 give excellent agreement with experiment, and we demonstrate the scalability of our method by computing excited states of a free-base porphyrin molecule.

MM 42.9 Wed 17:15 HL 001

Real-Structure Effects and Correlation in Layered Sodium Cobaltates — Sophie Chauvin[1,2], Silke Biermann[1], Lucia Reining[2], and •Claudia Rödl[3] — [1]Centre de Physique Théorique, École polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Na-doped layered cobaltates Na_xCoO_2 feature a rich phase diagram with a plethora of physical phenomena ranging from metal-insulator transitions over magnetism to charge ordering. These instabilities of the electronic structure are mostly attributed to correlation effects within the quasi-2D CoO_2 layers. Here, we focus on $Na_{2/3}CoO_2$, a doping for which the system is metallic and exhibits an experimentally established charge disproportionation on the Co atoms.

We study the electronic properties of the CoO_2 layers and investigate the impact of the intercalated Na atoms on the electronic structure in the ordered layered superstructure. The problem is tackled from an *ab-initio* point of view using density-functional theory (DFT) and many-body perturbation theory (MBPT). Moreover, we study the static charge-density response of the material to understand instabilities in the system. Our approach complements recent model calculations from extended dynamical mean-field theory (EDMFT). The calculated results are compared to experimental spectroscopic data.

MM 42.10 Wed 17:30 HL 001

Slave rotor approach to impurity models with correlated dp orbitals — •Jakob Steinbauer and Silke Biermann — École Polytechnique, Palaiseau, France

We propose a slave rotor method for the solution of many-orbital quantum impurity problems, which maps the original problem onto one with reduced degeneracy. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states with d-electrons are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and test the method in the atomic limit.