TT 52: Focus Session: Realistic Dynamical Mean-Field Approaches to Correlated Quantum Materials

Theoretical investigations of the properties of correlated quantum materials require not only the application of electronic structure theories but also of many-body techniques. Here realistic dynamical mean-field approaches have proved to be a conceptual breakthrough, leading to important new insights into the physics of electronically correlated materials. This is a very active field of research, which will be reviewed by internationally acknowledged experts.

Organizers: Roser Valenti (Goethe-Universität Frankfurt am Main)
and Dieter Vollhardt (Universität Augsburg)

Time: Wednesday 15:00–18:15 Location: H20

Invited Talk TT 52.1 Wed 15:00 H20
Hund's Metals: a New Road to Strongly Correlated Electron Behavior — •Gabriel Kotliar — Rutgers University Piscataway NJ USA

Over the past thirty years, substantial effort has been devoted to describing materials near a Mott transition. In these systems, correlation effects (i.e. departures from free electron behavior) arise from strong on site repulsion (Hubbard U terms). Prototypical materials are V_2O_3. Recently attention has turned to a different origin of strong correlation phenomena which is rooted in the Hund's coupling J term, starting with LDA+DMFT studies in the iron based high temperature superconductors and the ruthenium oxides. We will argue that Hund's metals are well described by Dynamical Mean Field Theory, and are characterized by the phenomena of orbital spin separation[2,3]. We will present an elementary introduction to the theory of Hund's metals stressing the experimental signatures which distinguishes them from materials near a Mott transition

[1] K. Haule and G. Kotliar, New J. Phys. **11**, 025021 (2009).
[2] C. Aron and G. Kotliar, PRB **91**, 041110 (2015).
[3] K. Stadler et. al., PRL **115**, 136401 (2015)

Invited Talk TT 52.2 Wed 15:30 H20
Screened Exchange Dynamical Mean Field Theory — •Silke Biermann — Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, France

Dynamical mean field theory (DMFT), in conjunction with electronic structure techniques has led to tremendous progress in the description of excited state properties of materials with strong electronic Coulomb correlations. One of the main challenges nowadays consists in refining the interface of electronic structure and many-body theory in order to develop quantitatively accurate predictive schemes. We review recent efforts of incorporating dynamical screening effects into a DMFT-based description of correlated materials [1]. Such effects can stem either from higher energy degrees of freedom that have been integrated out [2] or from nonlocal processes that are effectively backfolded into a local description. This can be conveniently done by combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") techniques [3]. These insights lead to a simple but efficient scheme, dubbed "Screened exchange dynamical mean field theory" [4], which can be understood as an approximation to GW+DMFT, or as a non-perturbative dynamical generalization of Hedin's Coulomb-hole-screened-exchange approximation. In particular, it includes non-local exchange beyond the local density approximation and dynamical screening beyond standard DMFT techniques.

[1] S. Biermann, JPCM **26**, 173202 (2014)
[2] J. M. Tomczak et al., PRB **90**, 165138 (2014)
[3] T. Ayral et al., PRL **109**, 226401 (2012)
[4] A. van Roekeghem et al., PRL **113**, 266403 (2014);
A. van Roekeghem et al., EPL **108**, 57003 (2014)

Invited Talk TT 52.3 Wed 16:00 H20
Dynamical Screening in Correlated Electron Materials — •Philipp Werner — University of Fribourg, 1700 Fribourg, Switzerland

I will discuss efficient methods for treating dynamically screened interactions within dynamical mean field theory (DMFT). These methods allow to incorporate ab-initio estimates of the local Coulomb matrix elements into low-energy effective models, and to treat the screening from nonlocal Coulomb interactions within extended DMFT or more sophisticated formalisms. I will present results from applications to simple model systems and strongly correlated materials, and some insights into the real-time dynamics of screening obtained with a recent nonequilibrium implementation of extended DMFT.

15 min. break

Invited Talk TT 52.4 Wed 16:45 H20
Lattice stability of correlated electron materials — •Ivan Leonov — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

The theoretical understanding of the interplay of electronic correlations and lattice, and, in particular, the realistic description of strongly correlated electron materials, is one of the most challenging problems in condensed matter physics. In this talk, I will report results of the application of the LDA+DMFT computational scheme to explore the electronic and structural properties of correlated materials from first principles. Our results show that electronic correlations are crucial to explain the electronic state, equilibrium crystal structure, and lattice stability of correlated materials [1]. In addition, I discuss application of the LDA+DMFT approach to compute the interatomic forces, which makes it possible to determine the atomic displacements and to perform structural optimization of correlated materials [2].

[1] I. Leonov *et al.*, PRL **106**, 106405 (2011);
I. Leonov *et al.*, PRL **115**, 106402 (2015);
I. Leonov *et al.*, PRB **91**, 195115 (2015)
[2] I. Leonov *et al.*, PRL **112**, 146401 (2014)

Invited Talk TT 52.5 Wed 17:15 H20
Tin Foil at the Nanometer Scale - from Electronic Correlations to Topological Physics — •Ralph Claessen — Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, 97074 Würzburg, Germany

With respect to its electronic properties and compared to its semiconducting siblings C, Si, and Ge the group IV element tin (Sn) has always been a somewhat profane material. At ambient conditions Sn is a white-silverish metal (tetragonal β-Sn) and as tin foil has long been used for wrapping food (nowadays replaced by aluminum foil). At 13.2° C a structural phase transition into the diamond-like α-phase occurs, known as "tin pest" which in former times posed a severe threat to church organ pipes in the winter time.

I will report on recent studies of (ultra)thin Sn films in which this elemental material displays highly interesting topological physics and correlation effects, otherwise seen only in materials of much higher structural or chemical complexity. This includes (1) the realization of compressively strained α-Sn as 3D topological insulator (TI), (2) our attempts to grow the Sn analogue of graphene, so-called stanene, which is predicted to be a 2D TI, and (3) the formation of triangular Sn lattices on semiconductor substrates, which display Mott-Hubbard physics and even magnetic instabilities despite the frustrated geometry.

Invited Talk TT 52.6 Wed 17:45 H20
Electron Correlations in Nanosystems and 2D Materials: What's so Different from Bulk? — •Tim Wehling — University of Bremen, Bremen, Germany

To date, experimental nanofabrication techniques offer atomic scale control of correlated electron materials from Mott insulators and magnets to superconductors. Here, we discuss correlation effects in atomic scale structured systems based on a combination of first-principles and many-electron techniques. We show that substrate, environmental and doping effects can change Coulomb interactions in monolayer thin 2d

materials on the eV scale [1], which has strong influence on electronic excitations and collective modes [2]. With two sets of magnetic systems, a Cr (001) surface and hydrogenated Fe adatoms on Pt (111), we address then how electronic hybridization and kinetic terms can be manipulated at the atomic scale. These terms control in both systems a delicate interplay of charge, spin, and orbital degrees of freedom and allow us to turn electronic correlation phenomena like the Kondo effect on and off [3].

[1] M. Rösner et al., PRB **92**, 085102 (2015)
[2] A. Steinhoff et al., Nano Lett. **14**, 3743 (2014)
[3] A. Khajetoorians et al, Nature Nanotech. **10**, 958 (2015).