MA 42: Focus Session: Dynamical Mean-Field Approach to Correlated Electron Materials (jointly with MA)

During the last few years conventional band-structure calculations in the local density approximation (LDA) have been merged with a modern many-body approach, the dynamical mean-field theory (DMFT), into a novel computational method referred to as LDA+DMFT. This framework has proved to be a breakthrough for the realistic modeling of the electronic, magnetic, and structural properties of correlated electron materials. The Focused Session will review the significant recent progress made in this internationally active field of research.

Organizers: Ralph Claessen (University of Würzburg), Eva Pavarini (Forschungszentrum Jülich), Dieter Vollhardt (University of Augsburg)

Time: Thursday 15:00–17:45 Location: H20

Invited Talk MA 42.1 Thu 15:00 H20

How Bad Metals Turn Good: Spectroscopic Signatures of Resilient Quasiparticles — •Antoine Georges — College de France and Ecole Polytechnique, France

Many materials with strong electronic correlations display metallic-like resistivity up to very high temperature, with values exceeding the Ioffe-Regel-Mott (IRM) criterion. Yet, at low enough temperature, good metallic conductivity obeying Fermi liquid behaviour can be recovered. In this talk, I will explore how this crossover takes place. I will show that the Fermi liquid scale, which is strongly suppressed by strong correlations, should not be confused with the much higher Brinkman-Rice scale, at which incoherent transport sets in.

In between these two scales, an extended regime of metallic transport applies, in which the resistivity is smaller than the IRM value but does not follow a T^2 Fermi-liquid law. Well-defined quasiparticle excitations do exist in this regime, as manifested in the one-particle spectral function and optical conductivity, with properties distinct from Landau and Drude theories. For a hole-doped Mott insulator, a strong particle-hole asymmetry applies down to low-energy: electron-like excitations are much longer lived, placing these quasiparticle excitations on the 'dark side' for ARPES spectroscopy. This also has implications for the temperature dependence of the thermopower.

[1] X. Deng, J. Mravlje, R. Zitko, M. Ferrero, G. Kotliar, A. Georges, arXiv:1210.1769

Topical Talk MA 42.2 Thu 15:30 H20

Correlation Effects in Organic Superconductors — •Roser Valenti — Institut für Theoretische Physik, Goethe Universität Frankfurt, Frankfurt, Germany

Organic charge transfer salts are unique correlated systems with a complex phase diagram that can be finely tuned by chemical substitution or moderate pressures. Observed phases in these systems include metals, Fermi liquids, Mott insulators, antiferromagnets, spin liquids, and unconventional superconductors. A realistic description of these systems can be provided by a combination of density functional theory with dynamical mean field theory (LDA+DMFT). Such an approach has not been attempted in the past due to the complex crystal structures of these materials. Here we present recent LDA+DMFT calculations based on a new scheme to obtain molecular Wannier orbitals for a few families of organic layered conductors and discuss their spectral and optical conductivity properties.

[1] H. C. Kandpal, I. Opahle, Y.-Z. Zhang, H. O. Jeschke, and R. Valenti, Phys. Rev. Lett. **103**, 067004 (2009)
[2] J. Ferber, K. Foyevtsova, H.O. Jeschke, and R. Valenti, arXiv:1209.4466 (2012)

Topical Talk MA 42.3 Thu 16:00 H20

Photoemission Study of Correlated Oxides at High Temperatures — Jonas Weinen[1], Stefano Agrestini[1], Martin Rotter[1], Alexander Komarek[1], Yen-Fa Liao[2], Ku-Ding Tsuei[2], Chien-Te Chen[2], and •Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

Strongly correlated oxides show often quite spectacular and intriguing properties which can be traced back to the presence of several competing interactions leading to various forms of ordered phases at low temperatures. In order to unravel which of the interactions are relevant, we have set out to study the excitation spectra of the several benchmark oxides as a function of temperature. By carrying out bulk-sensitive hard-x-ray photoemission experiments at high temperatures, we can follow the changes in the spectra and thereby determine which and how local spin and orbital degrees of freedom as well as nearest neighbour spin-spin correlations influence the intricate and complex electronic structure of correlated oxides.

15 min. break

Invited Talk MA 42.4 Thu 16:45 H20

Dynamical Mean Field Theory of Collective Excitations — •Alexander Lichtenstein — University of Hamburg, Hamburg, Germany

Dynamical mean field theory (DMFT) in combination with the first-principle scheme is an optimal starting point to go beyond static density functional approximation and include effects of local spin, orbital and charge fluctuations. In order to investigate collective non-local excitations we formulate a general framework which start from the DMFT solution for strongly correlated materials within a numerically exact continuous-time Quantum Monte Carlo impurity solver[1] and use a dual-particle transformation in the path integral formalism to find an optimal diagrammatic series for the lattice Green functions.

[1] E. Gull, A.J. Millis, A.I. Lichtenstein, A.N. Rubtsov, M. Troyer, and Ph. Werner, Rev. Mod. Phys. **83**, 349 (2011)

Topical Talk MA 42.5 Thu 17:15 H20

Electronic Correlations beyond Dynamical Mean Field Theory — •Karsten Held — Institute for Solid State Physics, TU Wien

Dynamical mean field theory has been a big step forward for our understanding of electronic correlations. A major part of the electronic correlations, the local ones, are included. The arguably most fascinating physical phenomena of solid state physics, however, such as (quantum) criticality and the physics of high-T superconductors are based on non-local correlations.

To address these problems, recently diagrammatic extensions of the dynamical mean field theory have been developed, coined dynamical vertex approximation [1] and dual fermion approach [2]. Among others, these approaches allow for describing spin-fluctuation-mediated pseudogaps and for calculating critical exponents of the Hubbard model [3].

[1] A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. B **75**, 045118 (2007)
[2] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B **77**, 033101 (2008)
[3] G. Rohringer, A. Toschi, A. Katanin, and K. Held, Phys. Rev. Lett. **107**, 256402 (2011)