TT 100: Correlated Electrons: Other Materials

Time: Thursday 15:00–18:30 Location: H 3005

TT 100.1 Thu 15:00 H 3005

The effects of spin-orbit coupling and electron correlations on the Fermi surface of Sr_2RuO_4 — •Guoren Zhang[1], Evgeny Gorelov[1], and Eva Pavarini[1,2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425, Jülich, Germany — [2]JARA High-Performance Computing

In this work we investigate the effects of spin-orbit coupling (SOC) and electron correlations on the Fermi surface (FS) of Sr_2RuO_4. We first study the spin-orbit coupling effects by comparing the FSs obtained by local-density approximation (LDA) and LDA+SOC calculations. Then, to study the effects of electron correlations, we perform LDA + dynamical mean field theory method (DMFT) and LDA+SOC+DMFT calculations. Our LDA and LDA+SOC results are consistent with previous theoretical works [1, 2]. Our LDA+SOC+DMFT results show that, in order to reproduce the experimental FS [3], it is key to include both effects.

[1] M. W. Haverkort, I. S. Elfimov, L. H. Tjeng, G. A. Sawatzky, and A. Damascelli, Phys. Rev. Lett. **101**, 026406 (2008).
[2] E. Pavarini, and I. I. Mazin, Phys. Rev. B **74**, 035115 (2006).
[3] A. Damascelli, D. H. Lu, K. M. Shen, N. P. Armitage, F. Ronning, D. L. Feng, C. Kim, Z. X. Shen, T. Kimura, Y. Tokura, Z. Q. Mao and Y. Maeno, Phys. Rev. Lett. **85**, 5194 (2000).

TT 100.2 Thu 15:15 H 3005

LDA+DMFT calculation of optical conductivity of layered ruthenates — •Esmaeel Sarvestani, Guoren Zhang, Evgeny Gorelov, and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany

Motivated by recent precise measurements of optical conductivity of correlated metals, we have used the LDA+DMFT method to calculate the optical spectra of paradigmatic correlated metals, strontium ruthenate oxides. The optical conductivity calculation is performed via linear response theory and Kubo's formalism.
For single layer ruthenate oxide, calculations are done for various temperatures. The effects of spin-orbit coupling on the optical spectra are studied. Two sets of interaction parameters, Hubbard U and Hund*s coupling J, which are commonly employed for these systems, have been used. It is shown that for smaller value of interaction, spin-orbit coupling does not change the spectra very much. For larger value of interaction, only if spin-orbit coupling is taken into account, the main features of experimental spectra are reproduced.
By means of numerical analysis, the role of spin-orbit coupling in optical conductivity is traced back to specific elements of the self-energy matrix and single particle spectral functions.
Finally, results of conductivity for double layer ruthenate are also presented.

TT 100.3 Thu 15:30 H 3005

On the absence of an orbital-ordering transition in $KCuF_3$ — •Hunter Sims[1], Eva Pavarini[2], and Erik Koch[1] — [1]German Research School for Simulation Sciences, 52428 Jülich, Germany — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

The Mott insulating perovskite $KCuF_3$ is considered the paradigm of a long-ranged orbitally-ordered material with cooperative Jahn-Teller distortion. We have found, however, that neither the Kugel-Khomskii superexchange mechanism nor the Jahn-Teller effect can, even qualitatively, account for the observed absence of a transition to a symmetric phase at high temperature. Instead, we show that the distortion of the F-octahedra is only limited by the shortest distance between Cu and F, leading to an increased distortion for the thermally expanded material. To quantitatively understand this we calculate the temperature-dependent Born-Oppenheimer surfaces in LDA+U. Based on this we determine the temperature-dependence of the distortion using a generalization of the Halperin-Englman mean-field model.

TT 100.4 Thu 15:45 H 3005

Long-range Coulomb interaction in surface systems: From cRPA to GW+DMFT — •Philipp Hansmann[1,2], Thomas Ayral[1,3], Antonio Tejeda[4], and Silke Biermann[1] — [1]Centre de Physique Theorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [3]Institut de Physique Theorique (IPhT), CEA, CNRS, URA 2306, 91191 Gif-sur-Yvette, France — [4]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, 91192 Gif sur Yvette, France

In spectroscopic (ARPES, cPES) and STM experiments group IV adatoms on semiconductors X:Si/Ge(111) (X=Sn, Si, C, Pb) show competing ground states but are partially in strong contradiction with one another. Ab initio derivation of a low energy Hamiltonian, including constrained RPA calculation for the effective interaction, suggests i) that correlation effects are beyond a single particle treatment and ii) an effective interaction which is not of a local "Hubbard U" type, but has a long-range character. Tackling the problem with standard dynamical mean-field methods (DMFT) is, hence, rather questionable. Instead we depart from the local approximation of DMFT to include, fully self-consistently, non-local effects in a GW+DMFT scheme. We observe that the non-local interaction is responsible for (experimentally observed) charge fluctuations which in some materials (Pb:Si/Ge(111), Sn:Ge(111)) are frozen in a commensurate charge order while in others (Sn:Si(111)) they remain dynamic and explain above mentioned experimental controversies.

TT 100.5 Thu 16:00 H 3005

Structural distortions in Vanadium Sesquioxide (V_2O_3) — •Daniel Grieger and Michele Fabrizio — Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

Vanadium Sesquioxide (V_2O_3) has attracted large attention mainly because of its prototypical Mott insulating behaviour with negative (chemical) pressure/Chromium doping. Besides trying to shed some light on details of this transition, this contribution is primarily aimed at the structural distortions that accompany the electronic phase diagram. These are especially important near the transition to the low-temperature ($T < 140$K) antiferromagnetic insulating phase, as well as in a recently discovered high-pressure monoclinic metallic phase. The relation and concurrence of the former with the antiferromagnetic ordering is investigated theoretically, which also has consequences for the appearance of the high-pressure phase. Formalisms applied for this purpose are combinations of traditional electronic structure formalisms and DFT+-like approaches.

TT 100.6 Thu 16:15 H 3005

Instantaneous Band Gap Collapse in VO_2 caused by Photocarrier Doping — •Marc Herzog[1], Daniel Wegkamp[1], Lede Xian[2,3], Matteo Gatti[3,4], Pierluigi Cudazzo[2,3], Christina L. McGahan[5], Robert E. Marvel[5], Richard F. Haglund[5], Angel Rubio[1,2,3,6], Martin Wolf[1], and Julia Stähler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Univ. del País Vasco, San Sebastian, Spain — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]École Polytechnique, Palaiseau, France — [5]Vanderbilt Univ., Nashville, Tennessee, USA — [6]MPI for the Structure and Dynamics of Matter, Hamburg, Germany

We have investigated the controversially discussed mechanism of the insulator-to-metal transition (IMT) in VO_2 by means of femtosecond time-resolved photoelectron spectroscopy (trPES). Our data show that photoexcitation transforms insulating monoclinic VO_2 quasi-instantaneously into a metal without an 80 fs structural bottleneck for the photoinduced electronic phase transition. First-principles many-body perturbation theory calculations reveal an ultrahigh sensitivity of the VO_2 band gap to variations of the dynamically screened Coulomb interaction thus supporting the fully electronically driven isostructural IMT indicated by our trPES results. We conclude that the ultrafast band structure renormalization is caused by photoexcitation of carriers from localized V $3d$ valence states, strongly changing the screening before significant hot-carrier relaxation or ionic motion has occurred.

TT 100.7 Thu 16:30 H 3005

Spinon Confinement in the Quasi-1D Ising-like Antiferromagnet $SrCo_2V_2O_8$ — •Zhe Wang[1], Michael Schmidt[1], Anup Kumar Bera[2], Bella Lake[2,3], Alois Loidl[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Institut für Festkoerperphysik, Technische Universität

Berlin, Berlin, Germany

Using THz transmission spectroscopy in magnetic field, we have investigated low-energy magnetic excitations in the quasi-one-dimensional Ising-like XXZ antiferromagnet $SrCo_2V_2O_8$. Spinon-pair excitations on the antiferromagnetic ground state have been observed in the XXZ antiferromagnet. Spinon-pair bound states with entangled spin-orbit moment S = 1 are determined unambiguously. The hierarchy of the spinon-pair boundstates can be described by a one-dimensional Schrödinger equation with a linear confinement potential imposed by the interchain interaction.

15 min. break.

TT 100.8 Thu 17:00 H 3005

The influence of the phosphor z position on the Fermi surface of $SrCo_2P_2$: Experiment and theory. — •K. Götze[1,2], J. Klotz[1,2], C. Bergmann[3], C. Geibel[3], H. Rosner[3], I. Kraft[3], V. Lorenz[4], and J. Wosnitza[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörperphysik, TU Dresden, Germany — [3]Max-Planck-Institut CPfS, Dresden, Germany — [4]IFW, Dresden, Germany

The exact crystallographic and electronic structure plays an important role for the occurrence of quantum criticality, magnetic order, and superconductivity in the family of transition-metal pnictides AT_2Pn_2. The pnictide-distance z is a crucial parameter for the electronic structure because the distance between the T_2Pn_2 layers determines whether the tetragonal crystal structure is collapsed or uncollapsed and, thereby, whether pnictide bonds are formed or not.

We have investigated the influence of the P z position on the band structure of the strongly enhanced Pauli paramagnet $SrCo_2P_2$, a close relative to the superconducting iron arsenides, that is on the verge of magnetic order. The pronounced temperature dependence of the P z position influences the density of states (DOS) at the Fermi energy strongly. Therefore, we have investigated the Fermi surface of $SrCo_2P_2$ in the paramagnetic ground state with the de Haas-van Alphen effect. We compare our experimental results to band-structure calculations in order to determine the exact contribution of individual orbits to the DOS. We will also address the renormalization of the effective masses and the dimensionality of the Fermi surface.

TT 100.9 Thu 17:15 H 3005

Angle-resolved photoemission spectroscopy of correlated electron pairs on NiO and CoO — •Michael Huth[1], Cheng-Tien Chiang[1,2], Andreas Trützschler[1,2], Wolf Widdra[2,1], Jürgen Kirschner[1,2], and Frank O. Schumann[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

It is well received that the independent electron approximation breaks down in strongly correlated materials. Therefore there is a keen interest to develop a direct experimental probe to spectroscopically resolve the characteristic feature of electron correlation in those materials. One way is to explore double photoemission (DPE) where an electron pair is emitted by a single photon. We use a laboratory high-order harmonic generation light source and the electrons are detected in coincidence with a pair of time-of-flight spectrometers operated in an angle resolving mode [1]. We present DPE spectra from the valence band of strongly correlated 3d transition metal oxides such as NiO and CoO films and characterize the two-dimensional energy and momentum distributions of the photoelectron pairs. Possible signatures of the electron correlation will be discussed.

[1] Huth, Chiang, Trützschler, Schumann, Kirschner, Widdra, Appl. Phys. Lett. 104, 061602 (2014)

TT 100.10 Thu 17:30 H 3005

Ground state oxygen holes and the metal-insulator transition in rare earth nickelates — •Thorsten Schmitt[1], Valentina Bisogni[1], Sara Catalano[2], Marta Gibert[2], Raoul Scherwitzl[2], Yaobo Huang[1], Vladimir Strocov[1], Pavlo Zubko[2], Robert J. Green[3], Shadi Balandeh[3], George Sawatzky[3], and Jean-Marc Triscone[2] — [1]Research Department Synchrotron Radiation and Nanotechnology, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Département de Physique de la Matière Condensée, University of Geneva, Switzerland — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada

Perovskite rare-earth (Re) nickelates $ReNiO_3$ continue to attract a lot of interest owing to their intriguing properties like a sharp metal to insulator transition (MIT), unusual magnetic order [1] and expected superconductivity in specifically tuned super-lattices [2]. Full understanding of these materials, however, is hampered by the difficulties in describing their electronic ground state (GS). From X-ray absorption (XAS) at the Ni $2p_{3/2}$ edge of thin films of $NdNiO_3$ and corresponding RIXS maps vs. incident and transferred photon energies we reveal that the electronic GS configuration of $NdNiO_3$ is composed of delocalized and localized components. Our study conveys that a Ni $3d^8$-like configuration with holes at oxygen takes on the leading role in the GS and the MIT of $ReNiO_3$ as proposed by recent model theories [3].

[1] Medarde et al., J. Phys. Cond. Matt. 9, 1679 (1997).
[2] Chaloupka et al., PRL 100, 016404 (2008).
[3] Mizokawa et al., PRB 61, 11263 (2000);
Park et al., PRL 109, 156402 (2012).

TT 100.11 Thu 17:45 H 3005

Correlation driven charge and spin fluctuations in $LaCoO_3$ — •Michael Karolak[1], Manuel Izquierdo[2,3,6], Serguei L. Molodtsov[2,4,5], and Alexander I. Lichtenstein[6] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]European XFEL GmbH, Albert-Einstein-Ring 19, 22761 Hamburg, Germany — [3]Synchrotron Soleil, L'Orme des Merisiers St-Aubin, BP-48, 91192, Gif-sur-Yvette, France — [4]Institute of Experimental Physics, Technische Universität Bergakademie Freiberg, 09599 Freiberg, Germany — [5]ITMO University, Kronverkskiy pr. 49, 197101 St. Petersburg, Russia — [6]Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany

The spin transition in $LaCoO_3$ has been investigated within the DFT+DMFT formalism using continuous time quantum Monte Carlo. Calculations on the experimental rhombohedral atomic structure with two Co sites per unit cell show that an independent treatment of the Co atoms results in a ground state with charge imbalance induced by electronic correlations. Each atom shows a contribution from either a d^5 or a d^7 state in addition to the main d^6 state. These charged states play a relevant role in the spin transition which can be understood as a low spin-high spin (LS-HS) transition with significant contributions ($\sim$ 10%) to the LS and HS states of d^5 and d^7 states. A thermodynamic analysis reveals that the introduction of charge imbalance significantly lowers the total energy of the system.

TT 100.12 Thu 18:00 H 3005

Electronic and magnetic properties of manganese pnictides — •Manuel Zingl, Simon Erker, and Markus Aichhorn — Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

We study the electronic and magnetic properties of the manganese based compounds $BaMn_2As_2$ and LaOMnAs by combining density functional theory and dynamical mean field theory (DFT + DMFT). These systems crystallize in the same structure as the iron based pnictide superconductors and were experimentally determined to small gap semiconductors with a Néel type antiferromagnetic ground state. With our study we will clarify the importance of electronic correlations on the formation of the insulating gap. Within DMFT we consider a dp-model corresponding to the experimental crystal structure and we investigate the influence of the selected energy window, the double counting correction and the interaction parameters U and J.

TT 100.13 Thu 18:15 H 3005

Pressure-induced semimetal to semiconductor transition in bismuth. — •Konstantin Semeniuk, Philip Brown, Aleksandar Vasiljkovic, and Malte Grosche — University of Cambridge, Cambridge, The United Kingdom

The semimetal bismuth stands out among the elements for its extremely low carrier concentration. This arises from small electron and hole Fermi surface pockets, which amount to about 10^{-5} of the Brillouin zone, or one mobile electron per 100,000 atoms. Situated very close to the transition to a semiconductor, the electronic structure can be tuned further by doping with antimony or by applied hydrostatic pressure.

We investigate the electrical resistivity, Hall effect and Shubnikov de Haas oscillations of single crystal bismuth under hydrostatic pressure of up to 25 kbar in a piston cylinder pressure cell. While the temperature dependence of the resistivity is metallic at ambient pressure, it

develops a pronounced kink and subsequently a maximum near 40 K with increasing pressure. The maximum shifts towards lower temperature with further increasing pressure until, above about 20 kbar, the resistivity of bismuth resembles that of a narrow-gap semiconductor. These results suggest that the Lifshitz transition from semimetal to semiconductor can indeed be studied in bismuth at pressures less than 25 kbar, at which a structural transition into a fully metallic state takes place. This makes it possible to access ultra-low carrier density states at intermediate pressures, in which the quantum limit can be reached at very low applied fields.