TT 101: Correlated Electrons: Other Materials

Time: Thursday 15:30–18:15 Location: HFT-FT 101

TT 101.1 Thu 15:30 HFT-FT 101

Proximity-induced spin-valley polarization in silicene or germanene on F-doped WS_2 — •Udo Schwingenschlögl, Shahid Sattar, and Nirpendra Singh — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Silicene and germanene are key materials for the field of valleytronics. However, interaction with the substrate, which is necessary to support the electronically active medium, becomes a major obstacle. In the present work, we propose a substrate (F-doped WS_2) that avoids detrimental effects and at the same time induces the required valley polarization, so that no further steps are needed for this purpose[1]. The behavior is explained by proximity effects on silicene or germanene, as demonstrated by first-principles calculations. Broken inversion symmetry due to the presence of WS_2 opens a substantial band gap in silicene or germanene. F doping of WS_2 results in spin polarization, which, in conjunction with proximity-enhanced spin-orbit coupling, creates sizable spin-valley polarization.
[1] Phys. Rev. B **94**, 205415 (2016).

TT 101.2 Thu 15:45 HFT-FT 101

An optical study of the electrically driven insulator-metal transition in V_2O_3 — •Matthias Lange[1], Dennis Schwebius[1], Stefan Guénon[1], Yoav Kalcheim[2], Ilya Valmianski[2], Marcelo Rozenberg[2], Ivan K. Schuller[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut - Experimentalphysik II and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, D-72076 Tübingen — [2]Department of Physics and Center for Advanced Nanoscience, University of California - San Diego La Jolla, CA 92093, USA

The strongly correlated oxide V_2O_3 undergoes an insulator-metal transition (IMT) from a low-temperature antiferromagnetic insulating phase to a paramagnetic metallic phase at around 160 K, resulting in a several orders-of-magnitude change in resistivity. We investigated the electrical breakdown of a V_2O_3 thin film, grown by rf-sputtering on a r-cut sapphire substrate, by concomitantly measuring the electrical properties as well as the spatially resolved optical reflectivity. At temperatures near the IMT, the current voltage characteristics show jumps to lower voltages, indicating electrical breakdown of the insulating phase. Whether this electrically driven IMT is electric-field induced or caused by the creation of electro-thermal domains through Joule heating is in focus of recent research. The reflectivity measurement reveals that the breakdown is accompanied by a change in reflectivity, which can be attributed to the formation of spatially confined metallic filaments.

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TT 101.3 Thu 16:00 HFT-FT 101

Thermodynamics and transport properties of oxygen-deficient $EuTiO_3$ — •Johannes Engelmayer[1], Christoph Grams[1], Xiao Lin[1], Kamran Behnia[1,2], Joachim Hemberger[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Laboratoire Physique et Etude de Matériaux, PSL Research University, 75005 Paris, France

Various perovskite titanates $ATiO_3$ are known to undergo ferroelectric phase transitions, e.g., for $A = \mathrm{Ba, Pb, Cd}$. In contrast, $SrTiO_3$ shows quantum paraelectric behavior, that is, ferroelectric long-range order is suppressed by quantum fluctuations. A partial substitution of Sr with Ca ($Sr_{1-x}Ca_xTiO_3$) induces ferroelectricity. On the other hand, the insulating $SrTiO_3$ becomes metallic upon electron doping via oxygen deficiencies ($SrTiO_{3-\delta}$) and furthermore shows superconductivity for certain carrier concentrations. If both—Ca and electron doping—is combined ($Sr_{1-x}Ca_xTiO_{3-\delta}$), even a coexistence of ferroelectricity and superconductivity seems to be possible [1]. $EuTiO_3$ is a promising candidate for comparable phenomena, since Eu^{2+} and Sr^{2+} have the same ionic radii, which results in identical structural characteristics. However, Eu^{2+} has a large magnetic moment of $7\mu_B$, in contrast to nonmagnetic Sr^{2+}. Here, we present a detailed investigation of $EuTiO_{3-\delta}$ with $|\delta| \leq 10^{-2}$ based on thermodynamic and transport measurements.
[1] C. W. Rischau et al., *Nat. Phys.* **13**, 643 (2017)

TT 101.4 Thu 16:15 HFT-FT 101

The c-axis dimer and its electronic break-up: the insulator-to-metal transition in Ti_2O_3 — •chun-fu chang[1], thomas c. koethe[2], zhiwei hu[1], jonas weinen[1], stefano agrestini[1], jan gegner[2], holger ott[2], giancarlo panaccione[3], hua wu[4], maurits w. haverkort[5], holger roth[2], alexander c. komarek[1], francesco offi[6], giulio monaco[7], yen-fa liao[8], ku-ding tsuei[8], hong-ji lin[8], chien-te chen[8], arata tanaka[9], and liu hao tjeng[1] — [1]MPI CPfS, Dresden, Germany — [2]IOP II, Cologne, Germany — [3]TASC Laboratory, Trieste, Italy — [4]DOP, Shanghai, P.R. China — [5]Institute for Theoretical Physics, Heidelberg, Germany — [6]CNISM and DOS, Rome, Italy — [7]ESRF, Grenoble, France — [8]NSRRC, Hsinchu, Taiwan — [9]DOQM, ADSM, Hiroshima, Japan

We report on our investigation of the electronic structure of Ti_2O_3 using (hard) x-ray photoelectron and soft x-ray absorption spectroscopy. From the distinct satellite structures in the spectra we have been able to establish unambiguously that the Ti-Ti c-axis dimer in the corundum crystal structure is electronically present and forms an $(a_{1g})(a_{1g})$ molecular singlet in the low temperature insulating phase. Upon heating we observed a considerable spectral weight transfer to lower energies with orbital reconstruction. The insulator-metal transition may be viewed as a transition from a solid of isolated Ti-Ti molecules into a solid of electronically partially broken dimers where the Ti ions acquire additional hopping in the a-b plane via the e_g^π channel, the opening of which requires the consideration of the multiplet structure of the on-site Coulomb interaction.

TT 101.5 Thu 16:30 HFT-FT 101

Spin-polarized ballistic conduction through correlated Au-NiMnSb-Au heterostructures — Cristian Morari[3], •Wilhelm Appelt[1,4], Andreas Östlin[2], Ulrich Eckern[1], and Liviu Chioncel[2] — [1]Theoretical Physics II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania. — [4]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany

We examine the ballistic conduction through Au-NiMnSb-Au heterostructures consisting of up to four units of the half-metallic NiMnSb in the scattering region, using density functional theory (DFT) in combination with dynamical mean-field theory (DMFT). For a single NiMnSb unit the transmission function displays a spin polarization of around 50% in a window of 1 eV centered around the Fermi level. By increasing the number of layers, an almost complete spin polarization of the transmission is obtained in this energy range. Supplementing the DFT calculations with local electronic interactions, of Hubbard-type on the Mn sites, leads to a hybridization between the interface and many-body states. The significant reduction of the spin polarization seen in the density of states is not apparent in the conduction electron transmission, which suggests that the hybridized interface and many-body induced states are localized.

15 min. break.

TT 101.6 Thu 17:00 HFT-FT 101

Orbital disproportionation of electronic density is a universal feature of alkali-doped fullerides — •Naoya Iwahara and Liviu Chibotaru — Theory of Nanomaterials Group, University of Leuven, Leuven, Belgium

Alkali-doped fullerides A_nC_{60} show a remarkably wide range of electronic phases in function of A = Li, Na, K, Rb, Cs and the degree of doping, n = 1-5. While the presence of strong electron correlations is well established, recent investigations give also evidence for dynamical Jahn-Teller instability in the insulating and the metallic phase of A_3C_{60} [1, 2]. To reveal the interplay of these interactions in fullerides with even n, we address the electronic phase of A_4C_{60} with accurate many-body calculations within a realistic electronic model including all basic interactions extracted from first principles [3]. We find that the Jahn-Teller instability is always realized in these materials too. More remarkably, in sharp contrast to strongly correlated A_3C_{60}, A_4C_{60} displays uncorrelated band-insulating state despite pretty similar in-

teractions present in both fullerides. Our results show that the Jahn-Teller instability and the accompanying orbital disproportionation of electronic density in the degenerate LUMO band is a universal feature of fullerides.

TT 101.7 Thu 17:15 HFT-FT 101

Doping and magnetic field induced spin gaps in spin chains explored by NMR — •Hans-Joachim Grafe[1], Yannic Utz[1], Franziska Hammerath[1,2], Lena Spillecke[1], Margarita Iakovleva[1], Evgeniya Vavilova[1], Vladislav Kataev[1], Tobias Ritschel[2], Jochen Geck[2], Chritian Hess[1], Livio Hozoi[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany

We present NMR measurements on the Heisenberg spin chain $SrCuO_2$ doped with Pd and Ni impurities [1], and on the frustrated edge-sharing $S = 1/2$ chain $LiCuSbO_4$ [2]. In $SrCuO_2$, the dopants cut the chains into segments which leads to strongly decaying spin lattice relaxation rates T_1^{-1} at low temperatures, indicating the opening of a spin gap. Thereby, it turned out that Ni is in a $S = 0$ state instead of a $S = 1$ state, which has been confirmed by x-ray absorption spectroscopy and quantum chemistry calculations. In $LiCuSbO_4$, we observe a strongly field dependent spin lattice relaxation rate at low temperatures: at magnetic fields below 13T, T_1^{-1} is dominated by a power-law increase, whereas above 13T, we observe a field induced spin gap-like decrease of T_1^{-1}. The former behavior is ascribed to diverging longitudinal spin correlations typical for a multipolar spin density wave liquid, whereas the latter is due to gapped transverse spin correlations characteristic for a spin-nematic liquid.

[1] Y. Utz et al., Phys. Rev. B 96, 115135 (2017)
[2] H.-J. Grafe et al., Scientific Reports 7, 6720 (2017)

TT 101.8 Thu 17:30 HFT-FT 101

Magnetic Properties and Spin Dynamics of Defects in Organic Spin Chain Systems as Probed by ESR Spectroscopy — •Julian Zeisner[1,2], Sylvain Bertaina[3], Olivier Pilone[3], Hervé Vezin[4], Olivier Jeannin[5], Marc Fourmigué[5], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]IFMP, TU Dresden, D-01069 Dresden, Germany — [3]Aix-Marseille Université, CNRS, IM2NP UMR7334, F-13397 Marseille, France — [4]LASIR, UMR-CNRS 8516, Université de Lille 1, F-59655 Villeneuve d Ascq, France — [5]ISCR, Université de Rennes 1, UMR-CNRS 6226, F-35042 Rennes, France

Defects in 1D spin systems continue to be an active field of solid state research as they are able to alter magnetic properties of the hosting materials drastically. In this work we studied the spin dynamics of defects in the spin chain compounds (o-DMTTF)$_2X$ (X = Br, Cl) by means of ESR spectroscopy. Both materials exhibit spin-Peierls transitions at temperatures around 60 K, which allow a separation of the properties of defects inside the chains from the magnetic response of the spin chains. Temperature dependent CW ESR measurements evidence the evolution of spin dynamics from being governed by the spins in the chains at elevated temperatures to a low-temperature regime which is dominated by defects within the chains. Moreover, details of spin dynamics deep in the spin-Peierls phase were investigated by pulse ESR experiments which revealed Rabi-oscillations as well as anisotropic relaxation behaviour of the spins. We discuss the obtained results in terms of solitons localized at the defect sites.

TT 101.9 Thu 17:45 HFT-FT 101

Magnetic phase diagram and magneto-structural effects in tetra-$LiCoPO_4$ — •Changhyun Koo[1], Waldemar Hergett[1], Christoph Neef[1], Georg Bothmann[2], Anton Jesche[2], Alexander Tsirlin[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany. — [2]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The magnetic phase diagram of a new $LiCoPO_4$ polymorph with tetrahedrally coordinated Co^{2+}-ions and $Pn2_1a$ symmetry is built-up based on magnetisation, thermal expansion, specific heat and muon spin rotation data. The system evolves long-range antiferromagnetic order at $T_N = 7$ K. The magnetic phase diagram shows a variety of competing antiferromagnetic phases. While the Weiss temperature is low, $\Theta \approx T_N$, our data imply large magnetostriction and anomalous contributions to the specific heat up $\sim$160 K. The presence of spin fluctuations up to $20T_N$ is further confirmed by μSR- and previously published NMR data. The nature of the complex magnetic phase diagram and of the spin fluctuation up to high temperatures will be discussed.

TT 101.10 Thu 18:00 HFT-FT 101

Competing phases in the model of Pr-based cobaltites — •Andrii Sotnikov and Jan Kuneš — Institute of Solid State Physics, TU Wien, Austria

Motivated by the physics of Pr-based cobaltites, we study the effect of the external magnetic field in the hole-doped two-band Hubbard model close to instabilities towards the excitonic condensation and ferromagnetic ordering. Using the dynamical mean-field theory we observe a field-driven suppression of the excitonic condensate. The onset of magnetically-ordered phase at the fixed chemical potential is accompanied by a sizable change of the electron density. This leads us to predict that Pr^{3+} abundance increases on the high-field side of the transition.