TT 25 Correlated Electrons - Poster Session

Time: Wednesday 14:30–18:30 Room: P1

TT 25.1 Wed 14:30 P1

Charge-order metal-insulator transition in the two-dimensional α- (BEDT-TTF)$_2$I$_3$: a Raman scattering study — •M. Masino[1], N. Drichko[2], M. Dressel[2], D. Schweitzer[2], C. Ulrich[3], and B. Keimer[3] — [1]Dip. Chimica GIAF, Universitá di Parma, Italy — [2]Physikalisches Institut, Univetsität Stuttgart, Germany — [3]MPI für Festkörperforschung, Stuttgart, Germany

A charge order metal-insulator transition is a widely studied phenomenon in low-dimensional solids. Two-dimensional organic conductor α-(BEDT-TTF)$_2$I$_3$ (T_{CO}=135 K) is a model compound to investigate the change of the vibronic and electronic Raman response on this transition. We studied polarized Raman spectra of the single crystals as a function of temperature. We focus our attention on the low-frequency spectral region (10-500 cm^{-1}) where the insulating single particle gap is expected in the electronic response. We found a strong dependence of the spectra on excitation-line and polarization: resonant behavior of the linear I_3 anion is found with λ=514 nm excitation polarized parallel to I_3 axis (*i.e.* approximately parallel to the *a* axis); while the Raman response from the BEDT-TTF conducting layer is seen with the λ=647 nm polarized in the perpendicular direction. This allows us to improve the assignment of the BEDT-TTF phonons. In the charge ordered phase the most strongly coupled molecular vibrations split due to the different charge distribution on the molecules. Moreover, the overall spectral background decreases, and a broad band at 400 cm^{-1} appears below T_c. The nature of these anomalous spectral features is discussed in terms of electronic scattering response, and vibronic Raman enhancement.

TT 25.2 Wed 14:30 P1

Optical response of the low-dimensional organic compound (TMTTF)$_2$AsF$_6$ at the pressure-induced deconfinement transition — •A. Pashkin, C. A. Kuntscher, and M. Dressel — 1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

The organic (TMTTF)$_2X$ salts consist of weakly coupled, half-filled molecular stacks and are prime examples of one-dimensional Mott-Hubbard insulators. In the (TMTSF)$_2X$ analogs, where sulfur is substituted by selenium, the coupling along and between the stacks is enhanced, causing a deconfinement transition, i.e., a crossover from a Mott-Hubbard insulator to a higher-dimensional metallic state. Optical spectroscopy was shown to be a key tool to monitor such a deconfinement transition induced by chemical pressure. Similar effects as induced by chemical pressure can also be achieved by applying external pressure.

We studied the pressure dependence (< 6 GPa) of the mid-infrared reflectivity of (TMTTF)$_2$AsF$_6$ for the polarization of the incident radiation along and perpendicular to the molecular stacking axis *a*. With increasing hydrostatic pressure the infrared response along the stacking axis *a* approaches that of the highly-conducting TMTSF analogs. The onset of an appreciable Drude-like response for the b' direction, along which the interstack hopping occurs, is observed above 2.5 GPa suggesting a deconfinement transition. The pressure dependence of the transfer integral $t_{b'}$ has been extracted. Furthermore, the pressure-dependent optical response along the least conducting axis, c^*, is presented.

Supported by the DFG, Emmy Noether-program.

TT 25.3 Wed 14:30 P1

Charge order fluctuations in 1/4- filled conductors α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ (M=NH$_4$,K,Tl,Rb) investigated by infrared spectroscopy. — •Natalia Drichko[1], Martin Dressel[1], Jaime Merino[2], and Andres Greco[3] — [1]1. Physikalisches Institut Universität Stuttgart, Germany — [2]UAM, Spain — [3]UNR-CONICET, Argentina

Electron-electron interactions determine the properties of the two-dimensional organic conductors α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ in a wide temperature range and can be tuned by variation of the charge reservoir layer: M=NH$_4$, K, Tl, Rb. We study electronic properties of these compounds by infrared reflectance spectroscopy and compare our results with calculations performed for strongly correlated 1/4-filled conductors close to charge order transition. The observed Drude-like peak has only 10 % of the total spectral weight; we assign the shift of the spectral weight to higher frequencies to the fluctuations of charge order. For NH$_4$ compound, influence of electronic correlations decrease with temperature. For the stronger correlated K and Tl salts, spectral indications of the short-range charge order at low temperatures are observed. The charge-carriers scattering rate exhibits the temperature dependence as predicted for fluctuating charge order. We suggest a generic phase diagram for α-(BEDT-TTF)$_2M$Hg(SCN)$_4$ compounds depending on the strength of the electronic correlations. We further discuss its relevance to the superconducting ground state observed in NH$_4$ material below 1 K and the density-wave ground state, observed below 10 K for the other members of this family.

TT 25.4 Wed 14:30 P1

Spin-zero anomaly in the magnetic quantum oscillations of a two-dimensional metal — •B. Bergk[1], O. Ignatchik[2], M. Jäckel[1], J. Wosnitza[2], V. M. Gvozdikov[3], J. A. Schlueter[4], J. Mohtasham[4], R. W. Winter[5], and G. L. Gard[5] — [1]Institut für Festkörperphysik, Technische Universität Dresden — [2]Dresden High Magnetic Field Laboratory, Forschungszentrum Rossendorf — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [4]Materials Science Division, Argonne National Laboratory, Argonne, Illinois, USA — [5]Department of Chemistry, Portland State University, Portland, Oregon

We present de Haas–van Alphen (dHvA) and Shubnikov-de Haas (SdH) measurements on the quasi-two-dimensional organic superconductor β''-(BEDT-TTF)$_2$SF$_5$CH$_2$CF$_2$SO$_3$. The measurements were carried out by the torque method and by four-point low-frequency ac-resistance measurements in magnetic fields up to 15 T. Unlike theoretical expectations for two-dimensional metals the dHvA signal shows an unconventional sawtooth wave-form, i. e., an 'inversed sawtooth' wave form is observed. In order to investigate the behaviour in more detail we performed angle-dependent dHvA and SdH measurements. The SdH effect displays the behaviour predicted by the grand-canonical Lifshitz-Kosevich theorie. In contrast, the dHvA signal can be explained by a theory, which includes a slightly oscillating chemical potential. Even for simultaneous measurements of both effects the behaviour does not change. This means that the dHvA signal is not affected by an external charge carrier reservoir.

TT 25.5 Wed 14:30 P1

Field-induced charge-density-wave transitions under pressure in the organic metal α-(BEDT-TTF)$_2$KHg(SCN)$_4$ — •Werner Biberacher[1], Dieter Andres[1], Mark Kartsovnik[1], Ilya Sheikin[2], Harald Müller[3], and Natalia Kushch[4] — [1]Walther-Meissner-Institut, Garching, Germany — [2]LNCMI, CNRS, BP 166, Grenoble, France — [3]ESRF, BP 220, Grenoble, France — [4]Institute of Problems of Chemical Physics, Chernogolovka, Russia

Hydrostatic pressure is a parameter that tunes the nesting conditions of the charge-density-wave (CDW) state existing in the organic metal α-(BEDT-TTF)$_2$KHg(SCN)$_4$. With pressure the CDW gradually becomes suppressed and above 2.5 kbar it does not exist any more at zero magnetic field. The orbital effect of the magnetic field is demonstrated to re-establish the density wave, while the orbital quantization induces different CDW states in different field intervals. In particular, we have found that hysteretic features characteristic of the first order field-induced CDW transitions become visible at much higher temperatures at certain orientations of the magnetic field. This is a direct evidence for the existence of this theoretically predicted effect.

TT 25.6 Wed 14:30 P1

Anomalous magnetoresistance of a layered conductor in the weakly incoherent interlayer coupling regime — •Mark Kartsovnik[1], Dieter Andres[1], Sergei Simonov[2], Werner Biberacher[1], Harald Mueller[3], Natalia Kushch[4], and Ilya Sheikin[5] — [1]Walther-Meissner-Institut, Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]Institute of Solid State Physics, 142432 Chernogolovka, Russia — [3]ESRF, BP 220, F-38043 Grenoble, France — [4]Institute of Problems of Chemical Physics, 142432 Chernogolovka, Russia — [5]LNCMI, CNRS, BP 166, F-38042, Grenoble, France

Owing to a high crystal quality and an extremely weak interlayer coupling in the layered organic conductor α-(BEDT-TTF)$_2$KHg(SCN)$_4$, it is possible to realize, by selecting a sample with an appropriate electron scattering rate, either the coherent or incoherent interlayer transport regime while the strong-field criterion, $\omega_c\tau > 1$, is achieved at conventional magnetic fields of a few tesla. We report on striking differences

in the angle-dependent interlayer resistance of this compound observed on samples characterized by different sample quality. In the cleanest samples, the magnetoresistance is a complex function of the magnetic field orientation, bearing the information about the geometry of the well defined three-dimensional Fermi surface. By contrast, the lower quality samples are essentially insensitive to the strength and orientation of the magnetic field component lying in the plane of the conducting layers. We attribute this anomalous behavior to the breakdown of the coherent charge transport across the layers in the lower quality samples.

TT 25.7 Wed 14:30 P1

Determination of the phase diagram of the spin ladder system $(C_5H_{12}N)_2CuBr_4$ by caloric and magnetic measurements — •Klaus Kiefer[1], Christian Rüegg[2], Thomas Wand[1], Michael Meissner[1], Des McMorrow[2], Karl Krämer[3], Daniel Biner[3], and Hans U. Güdel[3] — [1]BENSC, Hahn-Meitner-Institut Berlin — [2]Department of Physics and Astronomy, University College London, UK — [3]Universität Bern

The phase diagram of the S=1/2 spin ladder system $(C_5H_{12}N)_2CuBr_4$ was determined by measurements of the specific heat, the magnetocaloric effect and the magnetisation in magnetic fields up to 14.5 T. The exponential temperature dependence of the low temperature specific heat clearly reveals the existence of an energy gap between the non magnetic ground state and the magnetic excitations. The field driven closing of this gap is found to occur at about 7 T. In the Luttinger liquid regime the expected linear temperature dependence of the specific heat was confirmed. Down to the lowest accessible temperature of 0.3 K no additional transition to long-range 3D-order could be detected.

TT 25.8 Wed 14:30 P1

Collective modes in electron Fermi-liquid of organic layered conductors — •Dmitrii Stepanenko, Olga Kirichenko, and Valentin Peschansky — B.I.Verkin Institute for Low Temperature Physics and Engineering,

We have studied theoretically the propagation of electromagnetic waves in organic layered conductors at low temperature, when the charge carriers mean free path is the largest parameter of the dimensionality of length. It is shown that the specific of the Q2D charge carriers energy spectrum in layered conductors results in the oscillatory dependence of the electron drift velocity v_D upon the angle θ between the magnetic field vector and the normal to the layers. In a strong magnetic field, when the cyclotron frequency of electrons is much greater than their collision frequency, for the entire series of the values $\theta = \theta_c$ the velocity v_D is vanishingly small everywhere at the Fermi surface. This is the case when the collisionless absorption of the wave is absent and propagation of weakly damping modes is possible for an arbitrary orientation of the wave vector. The spectrum of the collective modes have been analyzed with regard to the Fermi liquid interaction between electrons.

TT 25.9 Wed 14:30 P1

Electron Spin Resonance in sine-Gordon Spin Chains in the Perturbative Spinon Regime. — •S. Zvyagin[1], J. Wosnitza[1], A. Kolezhuk[2], J. Krzystek[3], and R. Feyerherm[4] — [1]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Rossendorf, 01314 Dresden, Germany — [2]Institut fuer Theoretische Physik, Universitaet Hannover, 30167 Hannover, Germany — [3]National High Magnetic Field Laboratory, Tallahassee, FL 32310, USA — [4]Hahn-Meitner-Institut (HMI), 14109 Berlin, Germany

We report on low-temperature multi-frequency ESR studies of copper pyrimidine dinitrate, a spin-1/2 antiferromagnetic chain with alternating g-tensor and the Dzyaloshinskii-Moriya interaction, allowing us to test a new theoretical concept proposed recently by Oshikawa and Affleck [Phys. Rev. Lett. 82, 5136 (1999)]. Their theory, based on bosonization and the self-energy formalism, can be applied for precise calculation of ESR parameters of S = 1/2 antiferromagnetic chains in the perturbative spinon regime. Excellent quantitative agreement between the theoretical predictions and experiment is obtained. Results of the presentation are published in: S.A. Zvyagin et al., Phys. Rev. Lett. 95, 017207, 2005.

TT 25.10 Wed 14:30 P1

Heat transport in one-dimensional quantum magnets — •C. Hess[1], P. Ribeiro[1], A. Waske[1], N. Wizent[1], R. Klingeler[1], D. Elefant[1], C. Sekar[1], G. Krabbes[1], B. Büchner[1], H. ElHaes[2], G. Roth[2], F. Heidrich-Meisner[3], and W. Brenig[3] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany — [3]Institut für Theoretische Physik, TU-Braunschweig, Germany

We present experimental results for the magnon thermal conductivity $\kappa_{\rm mag}$ of several one-dimensional S=1/2 spin systems, like spin ladders and chains. We put a focus on spin chain materials such as $SrCuO_2$ and $CaCu_2O_3$. $SrCuO_2$ exhibits a strong signature of $\kappa_{\rm mag}$ from spinons. However, the size of $\kappa_{\rm mag}$ is difficult to determine due to its coincidence with the peak of the phonon thermal conductivity $\kappa_{\rm ph}$. In order to obtain a better separation of $\kappa_{\rm mag}$ and $\kappa_{\rm ph}$ we selectively suppress $\kappa_{\rm ph}$ by substituting Ca for Sr. A strong signature of magnetic heat transport is also present in $CaCu_2O_3$ along its chains. Since $\kappa_{\rm ph}$ is strongly suppressed in this material the temperature dependence of $\kappa_{\rm mag}$ can be well extracted. We estimate the magnetic mean free path which turns out to be of the order of 25 Å.

TT 25.11 Wed 14:30 P1

Magnetic heat conduction in Ca-doped $SrCuO_2$ spin chains — •P. Ribeiro[1], A. Waske[1], C. Hess[1], G. Behr[1], R. Klingeler[1], D. Elefant[1], B. Büchner[1], and G. Roth[2] — [1]IFW Dresden, Germany — [2]RWTH Aachen, Germany

We present new results on the heat conduction of the spin-chain system $Sr_{1-x}Ca_xCuO_2$. The structure of this material contains two parallel antiferromagnetic $S = 1/2$ copper chains with a $J_\parallel \approx 2100$ K. They are decoupled from each other due to a frustration arising from the displacement of half a Cu-Cu distance between them. In addition to the regular phonon heat conduction this material possesses spinon contributions in the chain direction. A separation of both contributions is most ambiguous, since the spinon contribution appears in form of a shoulder on the low-temperature phonon peak. In order to achieve a better separation of both contributions we isovalently substituted Ca for Sr, which leads to a suppression of the phonon heat conduction, while a strong affect on the magnetic system in the substance is not expected.

TT 25.12 Wed 14:30 P1

Quantum Critical Spin Dynamics of a Cu(II) S=1/2 antiferromagnetic Heisenberg chain studied by ^{13}C-NMR spectroscopy — •H. Kuehne[1], J. Litterst[1], H.-J. Grafe[2], C. Baumann[2], J. Haase[2], B. Buechner[2], C. P. Landee[3], M.M. Turnbull[3], and H.-H. Klauss[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Leibniz-Institut für Werkstoffforschung, Dresden, Germany — [3]Departments of Physics and Chemistry, Clark University, Worcester, USA

The antiferromagnetic S=1/2 Heisenberg chain is a model system for quantum many-body physics. It allows a direct comparison between exact theoretical results and experiment for ground state properties and excitations. In this work we study the spin dynamics of a Cu(II) S=1/2 spin chain system by means of ^{13}C-NMR. The actual compound, $Cu(C_4H_4N_2)(NO_3)_2$ (CuPzN), is one of the best experimental realizations of an unperturbed S=1/2 chain [1]. It has been characterized by thermodynamic measurements as well as inelastic neutron scattering [1,2]. The full parameter range from the low field limit to beyond the critical magnetic field strength of H_{crit} =13.9 Tesla for ferromagnetic polarization can be accessed. We present field and temperature dependent studies of the T_1 relaxation rate at the Carbon site.

[1] P. Hammar et al., PRB. 59, 1008 (1999).
[2] M.B. Stone et al., PRL 91, 037205 (2003).

TT 25.13 Wed 14:30 P1

$Sr_2Cu(PO_4)_2$: A real material realization of the 1D nearest neighbor Heisenberg chain — •M.D. Johannes[1], J. Richter[2], S.-L. Drechsler[3], A. A. Belik[4], E. Takayama-Muromachi[4], S. Uji[4], and H. Rosner[5] — [1]Naval Research Laboratory, Washington D.C — [2]Institute for Theoretical Physics, Magdeburg, Germany — [3]Liebnitz Institute for Solid State and Materials Research, Dresden, Germany — [4]National Institute for Materials Science, Ibaraki, Tsukuba, Japan — [5]Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany

The search for one-dimensional magnets began with the advent of quantum mechanics and the discovery that fluctuation effects, enhanced by low-dimensionality, could lead to novel ground states and exotic effects not accessible in higher dimensions. We present evidence that

$Sr_2Cu(PO_4)_2$ is a nearly perfect one-dimensional (1D) spin 1/2 Heisenberg chain with nearest neighbor only interactions. Combining experimental measurements down to T=30mK with first principles and model calculations, we demonstrate that the one dimensionality of $Sr_2Cu(PO_4)_2$, as measured by the ratio k_BT_N/J_1, exceeds that of prototype 1D compound Sr_2CuO_3 by an order of magnitude. Surprisingly, $Sr_2Cu(PO_4)_2$ lacks clear structural chains, achieving magnetic one-dimensionality instead via isolated CuO_4 plaquettes coupled along a single direction. This unusual geometry also strongly suppresses frustrating interactions between second neighbors along the spin chain direction, thereby providing an ideal physical realization of an exactly solvable theoretical model.

TT 25.14 Wed 14:30 P1

Structural and magnetic properties of oxalate-bridged low-dimensional Cu^{2+} spin systems — •Katarina Remović-Langer[1], Volodymyr Pashchenko[1], Andrey Prokofiev[1], Bernd Wolf[1], Michael Lang[1], Jürgen Schreuer[2], Leonore Wiehl[2], Eiken Haussühl[2], and Björn Winkler[2] — [1]Physikalisches Institut, J. W. Goethe-Universität, FOR 412, Max-von-Laue-Str. 1, D-60438 Frankfurt(M), Germany — [2]Institut für Mineralogie/Kristallographie, J. W. Goethe-Universität, FOR 412, Senckenberganlage 30, D-60054 Frankfurt(M), Germany

Our study focused on the structural and magnetic properties of two 1,1′-bicoordinated oxalate-bridged Cu^{2+} spin chains, $[Cu(\mu\text{-ox})\text{-}(H_2O)(4\text{-apy})_2]_n$ (**1**) and $[(pyOH)Cu(ox)\text{-}H_2O]_n$ (**2**). While in **1** all oxalate molecules are in the bis-monodentate configuration, compound **2** is built from two non-equivalent ox molecules which alternate in the bis-bidentate form along the chain. The Cu atoms of compound **1** are in a distorted square-pyramidal environment while those in compound **2** are in a distorted octahedral configuration. Magnetic measurements reveal the behavior of a uniform Heisenberg spin chain with a small antiferromagnetic (AF) exchange coupling constant of $J \approx 3K$ for **1**, consistent with [1], and that of a dimer system with predominant AF intradimer interaction of $J \approx 403K$ and only weak interdimer couplings for **2**. The nature and magnitude of the magnetic coupling through the oxalate bridges in **1** and **2** will be discussed in the light of available structural data.

[1] O. Castillo et al., Inorg. Chem. 39, 6142 (2000).

TT 25.15 Wed 14:30 P1

High-field ESR study of the quantum spin magnet $CaCu_2O_3$ doped with nonmagnetic Zn — •U. Schaufuss, C. Sekar, G. Krabbes, N. Tristan, S.-L. Drechsler, V. Kataev, and B. Büchner — Leibniz Institute for Materials Research IFW Dresden

$CaCu_2O_3$ is a low-dimensional $s = 1/2$ antiferromagnet with a structurally well defined two-leg ladder topology. However, no spin gap characteristic of a two-leg $S = 1/2$-ladder is observed in this material. Instead, $CaCu_2O_3$ orders antiferromagnetically at $T_N = 25\,K$ and exhibits a small magnetic anisotropy gap at $T < T_N$ [1]. Our recent high-field ESR study of a single crystal of $CaCu_2O_3$ reveals an important role of a few percent of 'extra' spins residing at the structural imperfections for the low-temperature magnetism of the bulk spin lattice in this compound [1]. To obtain a deeper insight into a complex interplay between the host and the 'extra' spins we studied static magnetization and high-field ESR of a series of $CaCu_2O_3$ single crystals doped with nonmagnetic Zn. We discuss the influence of the nonmagnetic defects on the properties of the strongly correlated low-dimensional spin lattice focussing on the doping dependence of T_N and of the anisotropy gap.

[1] M. Goiran *at al.*, cond-mat/0501647.

TT 25.16 Wed 14:30 P1

Excitation spectrum and magnetic properties of the layered $Na_5RbCu_4(AsO_4)_4Cl_2$ — •V. Gnezdilov[1], P. Scheib[2], P. Lemmens[2], Yu. Pashkevich[3], D. Chervinskii[3], K. Lamonova[3], S. Zvyagin[4], M. Ulutagay-Kartin[5], S.-J. Hwu[5], and J.A. Clayhold[5] — [1]B.I. Verkin Inst. for Low Temp. Physics, NASU, Ukraine — [2]IPKM, TU Braunschweig, D-38106 Braunschweig, Germany — [3]A.A. Galkin Donetsk Phystech, NASU, Ukraine — [4]Hochfeld-Magnetlabor, Forschunszentrum Rossendorf, 01328 Dresden, Germany — [5]Dept. Chem., Clemson Univ., Clemson, South Carolina 29634, USA

We report on a Raman scattering study on the $Na_5RbCu_4(AsO_4)_4Cl_2$ compound with a remarkable layered lattice structure comprised of antiferromagnetically coupled square Cu_4O_4 tetramers and a magnetic transition at T_N=17K. Due to the asymmetric exchange paths and the missing inversion centers an unique spectrum of magnetic excitations is observed and analyzed theoretically. This work has been supported partly by the ESF-HFM.

TT 25.17 Wed 14:30 P1

Excitation spectrum of the novel frustrated 2D s=1/2 system (CuCl)$LaNb_2O_7$ — •V. Gnezdilov[1], P. Scheib[2], P. Lemmens[2], Yu.G. Pashkevich[3], T. Kitano[4], Y. Ajiro[4], N. Oba[4], K. Yoshimura[4], and H. Kageyama[4] — [1]B.I. Verkin Inst. for Low Temp. Physics, NASU, Ukraine — [2]IPKM, TU Braunschweig, D-38106 Braunschweig, Germany — [3]A.A. Galkin Donetsk Phystech, NASU, 83144 Donetsk, Ukraine — [4]Dept. Chem., Kyoto Univ., Kyoto 606-8502, Japan

We report on the magnetic properties and Raman scattering data of the double-layered perovskite $(CuCl)LaNb_2O_7$ with a square lattice of s=1/2, prepared by topotactic ion-exchange reactions. Thermodynamic and spectroscopic experiments show a spin gap of $\approx$ 2 meV. Evidence for competing ferro- and antiferromagnetic exchange pathes connecting nearest and second-nearest-neighbors, respectively, exist. The role of the lattice system for the magnetic properties is critically discussed. This work has been supported partly by the ESF-HFM.

TT 25.18 Wed 14:30 P1

^{51}V NMR Study of Vanadium Oxide Nanotubes — •E. Vavilova[1,2], V. Kataev[1], I. Hellmann[1], R. Klingeler[1], C. Täschner[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Kazan Physical Technical Institute, RAS, 420029 Kazan, Russia

Mixed valent vanadium oxide nanotubes VO_x-NT have recently attracted much attention as they exhibit a number of unusual magnetic properties, ranging from ferromagnetism at room temperature to spin-liquid phenomena [1]. In these nanoscale magnets one finds structurally well defined V-O-V-... chains, but also isolated V-sites. In order to get an insight into the spin dynamics of this complex system we performed NMR measurements on ^{51}V nuclei in a magnetic field of 7.05 T at temperatures between 15 K and 285 K. We find a broad NMR spectrum centered at a frequency $\sim$ 78.9 MHz with a partially relsoved quadrupole structure. Measurements of transversal and longitudinal nuclear-spin relaxation times, T_2 and T_1, respectively, reveal two sites of V with distinctly different relaxation rates. These two sites are assigned to vanadium in 4+ (d^1, $S = 1/2$) and 5+ (d^0, $S = 0$) oxidation states, respectively. Though T_1 at both sites exhibit a strong temperature dependence we find no evidence for a spin gap of the order $\sim$ 700 K which possible occurrence in VO_x-NT is suggested in Ref. [1]. In addition to NMR results we present also our magnetization data and discuss possible mechanisms of vanadium nuclear spin relaxation and their interplay with the static magnetic properties.

TT 25.19 Wed 14:30 P1

Spectroscopic investigations of 2D J1-J2 quantum spin systems — •P. Scheib[1], V. Gnezdilov[2], P. Lemmens[1], S. Gonthier[3], P. Millet[3], E. Kaul[4], and Ch. Geibel[4] — [1]IPKM, TU Braunschweig, Germany — [2]B.I. Verkin Inst. for Low Temp. Physics, NASU, Ukraine — [3]CEMES, Toulouse, France — [4]MPI-CPfS, Dresden, Germany

The interest in frustrated 2D quantum spin system is increasing as novel system have been discovered that enlarge the parameter space from 2D AF to mixed AF/FM systems. We report Raman scattering results on Li_2VOSiO_4, $Pb_2VO(PO_4)_2$, and $(Sr,Ba)ZnVO(PO_4)_2$ to compare the effect of the local structure on the resulting AF and AF/FM couplings. This work has been supported partly by the ESF-HFM.

TT 25.20 Wed 14:30 P1

Spectroscopic investigation of the crossover behavior in $TeVO_4$ — •V. Gnezdilov[1], G. Caimi[2], L. Degiorgi[2], P. Lemmens[3], R.K. Kremer[4], and H. Berger[5] — [1]B.I. Verkin Inst. for Low Temp. Phys., NASU, Kharkov, Ukraine — [2]LfF, ETH Zürich, Switzerland — [3]IPKM, TU Braunschweig, Germany — [4]MPI-FKF, Stuttgart, Germany — [5]IPMC, EPFL, Lausanne, Switzerland

The magnetic susceptibility of $TeVO_4$ shows a crossover at T*=75K with different slopes of the reciprocal susceptibility. Using infrared absorption and Raman scattering we investigate the correlation of structural and electronic properties of this compound to understand the reason for this peculiar behavior. Spin-wave excitations are observed and analyzed for $T<T_c$=17K. This work has been supported by ESF-HFM.

TT 25.21 Wed 14:30 P1

Magnetic investigation on a new one-dimensional Fe(II)-triazole complex — •Katarina Remović-Langer[1], Volodymyr Pashchenko[1], Bernd Wolf[1], Michael Lang[1], Chunhua Hu[2], Jürgen Brüning[2], Kibrom Arefe[2], Jens Kühne[2], Juste E. Djanhan[2], and Martin U. Schmidt[2] — [1]Physikalisches Institut, J. W. Goethe-Universität, FOR 412, Frankfurt (M), Germany — [2]Institut für Anorganische und Analytische Chemie, J. W. Goethe-Universität, Frankfurt (M), Germany

A new one-dimensional triazole complex of Fe(II) ($S = 2$) with the general formula $\{[Fe(C_4H_7N_3O)_3](p\text{-}ClC_6H_4SO_3)_2\}_n$ has been synthesized and characterized magnetically. The structure of this polymeric compound consists of linear chains in which the neighboring Fe(II) atoms are triply bridged by pairs of bonded N atoms of the triazole ligands. Each Fe^{2+} ions have a thermodynamically stable high-spin state. The obtained magnetic properties of Fe-triazole complex can be satisfactorily explained by using a magnetic model for a one-dimensional spin $S = 2$ chain with weak antiferromagnetic Fe-Fe coupling of $J/k \approx 2.2K$.

TT 25.22 Wed 14:30 P1

Comparing the electronic structure of the quantum magnets TiOBr and TiOCl — •Michael Sing[1], Markus Hoinkis[1,2], Leonardo Pisani[3], Roser Valenti[3], Sander van Smaalen[4], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg,D-97074 — [2]Experimentalphysik II, Universität Augsburg, D-86135Augsburg, Germany — [3]Institut für Theoretische Physik, UniversitätFrankfurt, D-60054 Frankfurt, Germany — [4]Laboratory of Crystallography, University of Bayreuth,D-95440 Bayreuth, Germany

The layered Mott insulators TiOBr and TiOCl were recently interpreted as spin-Peierls compounds. They undergo two successive phase transitions with a non-magnetic spin-Peierls ground state and an intermediate state, in which an incommensurate order develops. In an extended temperature regime above the transitions the compounds display large fluctuation effects. It is still unclear how to interpret the electronic dispersions of TiOCl measured by photoelectron spectroscopy in the high temperature regime.[1] In order to elucidate the behavior of these compounds in the high temperature phase we studied the electronic structure of TiOBr and TiOCl by photoelectron spectroscopy and density-functional calculations. The experimentally and theoretically obtained density of states of both compounds are compared. Furthermore, we present momentum-resolved measurements and discuss the quasi-one-dimensional nature of the electronic dispersions. A detailed comparison of the two compounds makes the interpretation of the dispersions in a Mott-Hubbard picture appear less plausible.

[1] M. Hoinkis *et al.*, Phys. Rev. B. **72**, 125127 (2005)

TT 25.23 Wed 14:30 P1

Spatial Localization Behavior in the Two-Dimensional Inherent Conducting Polymer $\{(CH_3)_{0.92}ReO_3\}_\infty$ — •E.–W. Scheidt[1], R. Miller[1], G. Eickerling[1], Ch. Helbig[1], F. Mayr[1], R. Hermann[1], W. Scherer[1], and H.–A. Krug von Nidda[2] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]EP V, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86159 Augsburg, Germany

Polymeric methyltrioxorhenium, $(CH_3)_{0.92}ReO_3$ (*poly*-MTO), is the first member of a new class of inherent conductive organometallic hybrids and represents a prototype for a purely two-dimensional system, confirmed by X-ray- and IR-studies as well as by specific-heat and resistivity measurements. Below a characteristic temperature the resistivity changes from metallic to insulating behavior, where in the latter a positive magnetoresistance is observed. These properties are intensified by intercalation studies of *poly*-MTO with donor and acceptor molecules leading to a preliminary phase diagram. The increasing temperature range of the insulating regime is accompanied by an increasing amount of localized magnetic moments at the Re^{VI} (d^1)-ions as revealed by susceptibility and magnetization measurements and ascertained by ESR studies. Magnetic field dependent susceptibility measurements also clarify the role of the magnetic field as a tuning parameter for localization. This may be the reason for the positive magnetoresistance in these systems. This scenario is also corroborated by the magnetic field dependent electrical field gradient V_{zz} determined from the specific heat contribution of the quadrupole moments and confirmed by DFT calculations.

TT 25.24 Wed 14:30 P1

Pressure studies on the polymeric compound methyltrioxorhenium (poly-MTO) $(CH_3)_{0.9}ReO_3$ — •Valdeci Mariano de Souza[1], Michael Lang[1], Robert Miller[2], Christian Helbig[2], Ernst-Wilhelm Scheidt[2], and Wolfgang Scherer[2] — [1]Physikalisches Institut, J.W. Goethe-Univeristät, Frankfurt am Main, Germany — [2]Chemische Physik und Materialwissenschaften, Universität Augsburg, Germany

Transport measurements on the polymeric compound methyltrioxorhenium (poly-MTO) $(CH_3)_{0.9}ReO_3$ have been performed in the temperature range 2-300 K and under ^{4}He-gas pressure up to 10 kbar. The structural motive and transport properties of poly-MTO are reminiscent of those of classical perowskites in two dimensions. The metallic conductivity has been attributed to the presence of demethylated Re atoms giving rise to excess electrons which delocalize within the Re-5d bands. Upon cooling, the system remains metallic down to about 30 K, below which the resistivity starts to increase. In this non-metallic low-temperature range, the resistivity follows a log(1/T) dependence over one decade in temperature. Attempts to increase the electrical conductivity by intercalation with the organic donor molecule tetrathiafulvalene (TTF) showed that with increasing amount of TTF donors, the system becomes less conducting in the metallic high-temperature range and the low-T resistivity upturn is strongly reinforced. In contrast, the application of hydrostatic pressure results in a reduction of the resistivity over the whole T-range investigated, while the metal-to-insulator crossover around 30 K remains unaffected.

TT 25.25 Wed 14:30 P1

Thermodynamics of two-dimensional spatially anisotropic Heisenberg model — •Tatiana Antsygina, Marina Poltavskaya, Konstantin Chishko, and Igor Poltavsky — B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine

Using the formalism of two-time Green's functions and the decoupling procedure by Kondo and Yamaji we have investigated thermodynamic and magnetic properties of the 1/2-spin Heisenberg antiferromagnet on a spatially anisotropic triangular lattice with nearest neighbor exchange constant J_1 along one direction and J_2 along other two directions. The thermodynamic functions are expressed in terms of correlation functions which obey the self-consistent system of equation. At arbitrary temperatures the system can be solved only numerically, and temperature dependences of the energy, heat capacity and magnetic susceptibility at different relations between J_1 and J_2 can be calculated in the wide temperature range. We have analyzed the case $\nu = J_1/J_2 \ll 1$ and found that with the increase of ν the height of the peak on the heat capacity decreases and the peak position shifts to lower temperatures. It is shown that the temperature dependence of the magnetic susceptibility is in excellent agreement with the high temperature series expansions [1]. Possible applications of the theoretical results for the interpretation of physical properties of real low-dimensional magnets are discussed.

1. W. Zheng, R.R.P. Singh, R.H. McKenzie, R. Coldea, cond-mat/0410381.

TT 25.26 Wed 14:30 P1

Heat capacity and spin susceptibility of two-dimensional t-J model — •Marina Poltavskaya, Tatiana Antsygina, Konstantin Chishko, and Igor Poltavsky — B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine

Thermodynamic properties of the two-dimensional t-J model on square and triangular lattices near half-filling are investigated theoretically within an analytical approach based on the Kondo and Yamaji's Green function decoupling scheme. The assumption is made that in the system under study two types of elementary excitations exist: "spin wavelike"ones and those corresponding to the correlated motion of the holes. It is shown that these excitations are effectively separated if the hopping amplitude t is less than the exchange constant J. For this case the temperature dependences of the heat capacity and spin susceptibility are calculated in the wide temperature range. It was found, that with the increase of doping from the half-filling the maximum of the spin susceptibility increases and its position shifts to lower temperatures for both types of lattices. Such behavior is in agreement with the qualitative predictions made in [1]. Heat capacity demonstrates a double peak shape. The high temperature peak is associated with the "spin wavelike"excitations and shifts to lower temperatures with doping. The low

temperature peak appears due to the holes and its height and position depend on both the doping and ratio t/J.

1. E. Dagotto Rev. Mod. Phys., 66, 763 (1994).

TT 25.27 Wed 14:30 P1

Mesoscopic BCS pairing in the repulsive 1d-Hubbard model — •Andreas Osterloh[1], Luigi Amico[2], and Andrea Mastellone[2] — [1]Institut für theoretische Physik, Universität Hannover, Appelstraße 2, D-30167 Hannover, Germany. — [2]MATIS-INFM & Dipartimento di Metodologie Fisiche e Chimiche (DMFCI), Universita' di Catania, viale A. Doria 6, I-95125 Catania, Italy

We study mesoscopic pairing in the one dimensional repulsive Hubbard model and its interplay with the BCS model in the canonical ensemble. The key tool is comparing the Bethe ansatz equations of the two models in the limit of small Coulomb repulsion. For the ordinary Hubbard interaction the BCS Bethe equations with infinite pairing coupling are recovered; a finite pairing is obtained by considering a further density-dependent phase-correlation in the hopping amplitude of the Hubbard model. We find that spin degrees of freedom in the Hubbard ground state are arranged in a state of the BCS type, where the Cooper-pairs form an un-condensed liquid on a "lattice" of single particle energies provided by the Hubbard charge degrees of freedom; the condensation in the BCS ground state corresponds to Hubbard excitations constituted by a sea of spin singlets.

TT 25.28 Wed 14:30 P1

Hubbard model in a magnetic field at weak coupling — •Carsten Knecht and P.G.J. van Dongen — University of Mainz, Institut für Physik, 55099 Mainz, Germany

The phase diagram of the half-filled Hubbard model is studied at weak coupling in two spatial dimensions. A homogeneous magnetization in the z-direction and a staggered magnetization in the x-direction are assumed. We apply perturbation theory at fixed order parameter (PTFO) to this system. The results are compared with the well know Hartree-Fock solutions that usually overestimate the order parameters. This calculation is also relevant for superconductivity in the doped two-dimensional negative-U Hubbard model.

TT 25.29 Wed 14:30 P1

Collective spin excitations within the time-dependent Gutzwiller approximation for the Hubbard model — •Falk Günther and Götz Seibold — BTU Cottbus

We use a spin-rotational invariant slave-boson-formulation of the Hubbard model, in order to investigate the collective excitations of itinerant ferromagnets. The expansion of the resulting spin-rotational invariant Gutzwiller energy functional around the saddle point allows the computation of dynamic correlation functions using the random-phase approximation (RPA). We evaluate ferromagnetic and antiferromagnetic instabilities from the transverse magnetic susceptibility and compute the dispersion relation for the spin waves. Results for one- and two-dimensional systems are presented and compared with the convetional Hartree-Fock+RPA theory.

TT 25.30 Wed 14:30 P1

Doping dependence of spin excitations in the stripe phase of high-Tc superconductors — •Götz Seibold[1] and Jose Lorenzana[2] — [1]Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany — [2]SMC-INFM,ISC-CNR, Dipartimento di Fisica, Universita di Roma La Sapienza, P. Aldo Moro 2, 00185 Roma, Italy

Based on the time-dependent Gutzwiller approximation of the extended Hubbard model we calculate the energy and momentum dependence of spin excitations for striped ground states. Since our approach correctly reproduces the experimentally obtained incommensurability vs. doping behavior in La-based cuprates the present investigation allows to quantitatively predict the energy ω_{res} and intensity of the 'resonance peak' as well as the spin velocity of high energy (optical) magnons in this compound. In the underdoped regime $\delta < 1/8$ we find a linear dependence ofω_{res} on doping whereas the resonance energy significantly shifts to higher values when the charge concentration in the stripes starts to deviate from half filling for $\delta > 1/8$.

TT 25.31 Wed 14:30 P1

Spectral properties of RVB superconductor — •Bernhard Edegger[1], Claudius Gros[1], and V.N. Muthukumar[2] — [1]Institut für Theoretische Physik, Universität Frankfurt, D-60438 Frankfurt, Germany — [2]Department of Physics, City College of the City University of New York, New York, NY 10031

We use a Gutzwiller renormalized mean field theory to study properties of projected quasiparticles within the tJ model. We calculate the one-particle spectral function and discuss the relevance for tunneling and photoemmision spectroscopies in doped Mott insulators like the high T_C superconductors. Besides we consider incoherent excitations and emphasise their importance in describing the striking asymmetry seen in the tunneling experiments.

TT 25.32 Wed 14:30 P1

Competing phases of the $t-J$ model on the triangular lattice. — •Irakli Titvinidze[1] and Matthias Vojta[2] — [1]Institut fuer Theoretische Physik A, RWTH Aachen, Templergraben 55, 52056 Aachen, Germany — [2]Institut fuer Theorie der Kondensierten Materie,Universitaet Karlsruhe, Postfach 6980, 76128 Karlsruhe, Germany

Our aim is to study the $t-J$ model on a triangular lattice, employing the Sp($2N$) large-N mean-field theory used previously [1,2] for the square-lattice geometry.

Our calculations show that for low doping a spin-Peierls state is realized in the system, while for high doping s-wave superconductivity occurs. For intermediate doping two different phases with a single-site unit cell appear: For small t/J we find a symmetry-broken phase with links fields $|Q_1| = |Q_2| > |Q_3|$, whereas for large t/J a "120° phase" is realized, with $Q_1 = Q_2\, e^{2\pi i/3} = Q_3\, e^{4\pi i/3}$. This is in qualitative agreement with published results of Kumar and Shastry [3] and Ogata [4].

[1] S. Sachdev and N. Read, Int. J. Mod. Phys. B 5, 219 (2000)
[2] M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. B 62, 6721 (2000)
[3] B. Kumar and B. S. Shastry, cond-mat/0304210
[4] M. Ogata, cond-mat/0304405

TT 25.33 Wed 14:30 P1

VCA-approach to the magnetic properties of the 2-D Hubbard Model — •Sascha Brehm[1], Michael Potthoff[1], Markus Aichhorn[1,2], Enrico Arrigoni[2], and Werner Hanke[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, A-8010 Graz, Austria

A new scheme for calculating two-particle (here spin-) response functions within the Variational Cluster Approach (VCA) [1] is presented and applied to the 2D-Hubbard model. The magnetic suszebility is calculated from the normal and superconducting one-particle Green's functions extracted from the VCA for the infinite-sized system and the q- and omega-dependent 2-particle vertex obtained from a cluster calculation. It is shown that this approach reproduces some characteristic features of the neutron-scattering data for the magnetic excitations in high-Tc cuprates. [1]PRL 91,206402 (2003)

TT 25.34 Wed 14:30 P1

Competing magnetic interactions in 1D and 2D cuprates - an electronic structure study — •Ulrike Nitzsche[1], Stefan-Ludwig Drechsler[1], and Helge Rosner[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]MPI CPfS Dresden

In many copper oxygen networks, especially for Cu-O-Cu bond angles close to 90°, ferromagnetic interactions play an important role in addition to the well known superexchange $J \sim t^2/U$. We present a systematic study of the electronic structure and the exchange integrals for different types of 1D and 2D spin 1/2 cuprate systems: edge and corner shared single-chain (Li_2CuO_2, Sr_2CuO_3), double-chain ($SrCuO_2$), and planar ($CaCuO_2$, $Sr_2CuO_2Cl_2$) arrangements. Based on full potential LSDA and LSDA+U band structure calculations and subsequently derived tight-binding models we estimate sign and magnitude of the most relevant exchange integrals. We compare the results of total energy calculations with those of various tight-binding (TB) models from one-band and multi-band approaches. The ferromagnetic contributions can be estimated from the difference between the TB and the total energy results. We investigate the effect of the network configuration (edge shared vs. corner shared CuO_2 plaquettes) and of the dimensionality on the coupling strength.

TT 25.35 Wed 14:30 P1

Thermoelectric effects in layered conductors with a multisheet Fermi surface — •Olga Kirichenko and Valentin Peschansky — B.I.Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, Kharkov, Ukraine

Thermoelectric effects in layered organic conductors with the Fermi surface consisting of topologically different sheets in the form of cylinders and planes with weak corrugation of an arbitrary form, are studied theoretically. It is shown that at low enough temperatures, when account of the quantization of charge carriers orbital motion in a magnetic field is essential, the dependence of thermoelectric field upon reciprocal magnetic field takes the form of giant oscillations. Thermomagnetic coefficients of a layered conductor are shown to depend periodically upon the angle between the magnetic field direction and the normal to the layers. The presence of a group of charge carriers with a Q1D dispersion relation results in the strong anisotropy of thermoelectrical coefficients due to the existence of preferred direction for velocities of electrons belonging to this group. Experimental investigations of thermoresistanse and thermo-emf at different orientations of the magnetic field with respect to the layers allows to study in detail the energy spectrum of conduction electrons, in particular to determine electron effective masses and the distribution of their velocities at the Fermi surface.

TT 25.36 Wed 14:30 P1

Hall effect in quasi-two-dimensional conductors — •Valentin G. Peschansky[1] and Raed Hasan[2] — [1]B.I.Verkin institute for low temperature and Egineering, 61103 Kharkov, Ukraine — [2]V.N.Karazin Kharkov national university, 4 Svoboda sq., 61077 Kharkov, Ukraine

Galvanomagnetic phenomena have been studied theoretically in layered conductors with a quasi-two-dimensional electron energy spectrum of an arbitrary form in a strong magnetic field B. At low enough temperature, when the smearing of the Fermi distribution function for charge carriers is much less than the separation between quantized Landau levels the Hall field oscillates with 1/B. It is shown that in conductors with the Fermi surface consisting of topologically different elements the amplitude of quantum oscillations of the Hall field is sufficiently large and comparable to the amplitude of the Shubnikov-de Haas magnetoresistance oscillations. In the case when the Fermi surface has the form of a single corrugated cylinder there are no quantum corrections to the Hall field in the collisoinless limit. Experimental studies of the Hall field along with the B-dependence of the magnetoresistance at different orientations of the magnetic field permits one to restore the Fermi surface completely.

TT 25.37 Wed 14:30 P1

Fermionic renormalization group flow into phases with broken discrete symmetry: charge-density wave mean-field model — •Roland Gersch[1], Carsten Honerkamp[2], Daniel Rohe[3], and Walter Metzner[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Institut für Theoretische Physik, Uni Würzburg, Am Hubland, 97074 Würzburg — [3]Ecole Polytechnique - CPhT, F91128 Palaiseau Cedex, France

We generalize the application of the functional renormalization group (fRG) method for the fermionic flow into the symmetry-broken phase to finite temperatures. We apply the scheme to the case of a broken discrete symmetry: the charge-density wave (CDW) mean-field model at half filling. We show how an arbitrarily small initial CDW order parameter starts to grow at the CDW instability and how it flows to the correct final value, suppressing the divergence of the effective interaction in the fRG flow. The effective interaction peaks at the instability and saturates at low energy scales. The relation to the mean-field treatment and the prospects of the new method are discussed.

TT 25.38 Wed 14:30 P1

Analytical approach to the quantum-phase transition in the one-dimensional spinless Holstein model — •Steffen Sykora[1], Arnd Hübsch[2], and Klaus W. Becker[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Department of Physics, University of California, CA 95616, USA

We study the one-dimensional Holstein model of spinless fermions interacting with dispersion-less phonons by using a recently developed projector-based renormalization method (PRM). At half-filling the system shows a metal-insulator transition to a Peierls distorted state at a critical electron-phonon coupling where both phases are described within the same theoretical framework. The transition is accompanied by a phonon softening at the Brillouin zone boundary and a gap in the electronic spectrum. For different filling, the phonon softening appears away from the Brillouin zone boundary and thus reflects a different type of broken symmetry state.

TT 25.39 Wed 14:30 P1

Dimerization effect on Luttinger liquid behavior — •Satoshi Ejima[1], Satoshi Nishimoto[2], and Florian Gebhard[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Max-Planck-Institut für Physik Complexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

A number of organic conductors exhibit a variety of electronic phases and some of them show a Luttinger liquid behavior due to strong one-dimensionality. For instance, a description by a Luttinger liquid seems to be more appropriate to analize experimental results (optical conductivity, photoemission spectroscopy, the dc resistivity, etc.) in $(TMTCF)_2X$. However, theoretical investigation with one-dimensional extended Hubbard model at quarter filling has been more puzzling.

Very slow carrier density fluctuations have been observed by recent NMR experiments. A key factor for such fluctuations can be *dimerization* along the TMTCF stacks. We study a dimerized Hubbard chain for various band filling with density-matrix renormalization group method. We suggest that the Luttinger liquid properties are drastically affected by the dimerization especially around quarter filling.

TT 25.40 Wed 14:30 P1

Time Evolution of a Luttinger Liquid through a correlated insulator — •Salvatore R. Manmana[1,2], Alejandro Muramatsu[1], and Reinhard M. Noack[2] — [1]Institut f. Theoretische Physik III, Universität Stuttgart, Germany — [2]AG Vielteilchennumerik, Fachbereich Physik, Philipps-Universität Marburg, Germany

We investigate the time evolution of a system of spinless fermions on a one-dimensional lattice with nearest-neighbor repulsion V and nearest-neighbor hopping t at half filling. Starting from the ground state of the Luttinger liquid phase, we study the time evolution after the system is perturbed by suddenly increasing the interaction to a value associated with an insulating ground state. Using a variant of the time-dependent density-matrix renormalization group method that approximates the time-evolution operator within a Krylov subspace, we calculate the *full* time evolution of the system. In the atomic limit, $t = 0$, the density and the density-density correlation function are time-independent, while the momentum distribution $\langle n_k \rangle$ shows behavior characteristic of periodic collapse and revival of the initial Luttinger liquid state. Therefore, the density-density correlations and one-particle propagators are no longer connected by a single anomalous dimension as in the equilibrium case. For parameter values away from this classical limit, we find relaxation phenomena when the perturbed interaction is near the quantum critical point. For intermediate values new nonequilibrium states are found.

TT 25.41 Wed 14:30 P1

The spectral properties and the metal-insulator transition in the spin-fermion and s-d exchange model: equation of motion approach — •Andrey Katanin[1,2] and Valentin Irkhin[2] — [1]Max-Planck-Institut für Festkörperforschung, 70569, Stuttgart, Germany — [2]Institute of Metal Physics, 620219 Ekaterinburg, Russia

The classical s-d exchange and the spin-fermion models are studied within the equation-of-motion approach combined with the $1/N$ expansion (N is the number of spin components, $N = 3$ for physical spins). The local and magnetic splitting in the electronic spectral functions is discussed. In the $d \to \infty$ limit, where only local fluctuations are important, the s-d model yields a metal-insulator transition with increasing interaction strength, while the spin-fermion model yields nonvanishing spectral weight at the Fermi level at any finite interaction. For $d = 2$ in the presence of strong ferromagnetic fluctuations the self-energy at low temperatures T has a non-Fermi liquid form in the energy window $|\omega| < \Delta_0$ near the Fermi level, where Δ_0 is the spin splitting for magnetically ordered ground state, and $\Delta_0 \propto T^{1/2} \ln^{1/2}(v_F/T)$ in the quantum critical regime (v_F is the Fermi velocity). In the renormalized classical regime the spectral functions have a two-peak structure at finite T, which implies quasisplitting of the Fermi surface due to strong magnetic fluctuations. The role of dynamic spin fluctuations in the spin-fermion model is discussed.

TT 25.42 Wed 14:30 P1

Orbital Waves versus Vibronic Excitations — •Kai P. Schmidt[1], Markus Grüninger[2], and Götz S. Uhrig[3] — [1]Institute of Theoretical Physics, École Polytechnique Fédérale de Lausanne, CH 1015 Lausanne, Switzerland — [2]II. Physikalisches Institut der RWTH Aachen, Templergraben 55, 52056 Aachen, Germany — [3]Theoretische Physik, Geb. 38, FR 7.1, Universität des Saarlandes, D-66123 Saarbrücken, Germany

A large number of transition-metal compounds show orbital ordering at low temperatures. But the experimental observation of the corresponding elementary excitations of an orbitally ordered state, the so-called orbital waves (orbitons), turned out to be rather difficult, and a watertight experimental proof for the existence of orbitons is still lacking. It is therefore natural to ask whether other degrees of freedom are involved in transition-metal compounds which complicates the search for orbital waves. In this contribution the coupling of orbital and lattice degrees of freedom is investigated. We calculated the kinetic and the spectral properties of the orbital waves for a one-dimensional toy-model. The elementary excitations are orbital-wave-like for small orbiton-phonon coupling. In contrast, the excitations are vibronic when the coupling between orbital and lattice degrees of freedom is large. The most interesting case is the crossover regime at intermediate couplings. Here the most important spectral contribution is a continuum build by one orbiton and by one phonon. Surprisingly, the spectral density displays rather sharp resonances inside the continuum which form a shadow-like image of the one-orbiton dispersion.

TT 25.43 Wed 14:30 P1

Variational cluster approach to superconducting and antiferromagnetic phases in hole- and electron-doped cuprates — •Markus Aichhorn[1,2], Enrico Arrigoni[1], Michael Potthoff[2], and Werner Hanke[2] — [1]Institute for Theoretical and Computational Physics, Graz University of Technology — [2]Institute for Theoretical Physics, University of Würzburg

Using the recently proposed Variational Cluster Approach (VCA), we study the competition between d-wave superconductivity and antiferromagnetism in hole- and electron-doped cuprates. In both cases, our thermodynamic consistent results for the t-t'-U Hubbard model suggest the occurrence of phase separation into a mixed antiferromagnetic-superconducting phase at low doping and a pure superconducting phase at higher doping, although the energy scale for phase separation is an order of magnitude smaller on the electron-doped side. We argue that this can explain the different pseudogap and superconducting transition scales in hole- and electron-doped materials. The cluster calculations reproduce qualitatively the ground-state phase diagram of high-temperature superconductors. In particular, they include salient features such as the enhanced robustness of the anitferromagnetic phase for electron-doping, compared to the hole-doped case.

TT 25.44 Wed 14:30 P1

Kondo Shadows in Hybrid Magnetic Molecular Solids — •Mikhail Kiselev[1] and Konstantin Kikoin[2] — [1]Universität Würzburg, Germany — [2]Ben Gurion University, Beer Sheva, Israel

We discuss the properties of layered Anderson/Kondo lattices with metallic electrons confined in 2D xy planes and local spins in insulating layers forming chains in z direction. Each spin in this model possesses its own 2D Kondo cloud, so that the Nozieres' exhaustion problem does not occur. The high-temperature perturbational description is matched to exact low-T Bethe-ansatz solution. The excitation spectrum of the model is gapless both in charge and spin sectors. The disordered phases and possible experimental realizations of the model are briefly discussed.

TT 25.45 Wed 14:30 P1

DMFT/NRG Studies of the Transport Properties of Heavy Fermion Systems — •Claas Grenzebach[1], Frithjof B. Anders[1,2], and Gerd Czycholl[1] — [1]Institut für Theoretische Physik, Universität Bremen — [2]Theoretische Physik, Universität des Saarlands, Saarbrücken

Heavy fermion systems (HFS) are described by the periodic Anderson model (PAM), which is mapped onto an effective single impurity Anderson model (SIAM) by dynamical mean field theory (DMFT). The SIAM is treated with the non-perturbative method of numerical renormalization group (NRG). This has the advantage that the correct Kondo scale is obtained. We investigate the (electronic) transport properties and the characteristic low temperature scales of HFS within this DMFT/NRG approach and calculate the temperature dependence of the resistivity and the thermoelectrical power as well as the frequency and temperature dependence of the dynamical conductivity and compare our results with experimental results typical for HFS. An extension of the model and method to take into account substitutional disorder by means of the coherent potential approximation (CPA) is discussed. Furthermore, we compare our results with the corresponding results obtained by using modified perturbation theory (MPT) as impurity solver. The MPT is exact up to second order in the Coulomb correlation U and reproduces the atomic limit ($V = 0$).

TT 25.46 Wed 14:30 P1

DCA Calculations of the Kondo Lattice Model — •Lee Martin and Fakher Assaad — Universität Würzburg

We consider the two-dimensional Kondo Lattice model with exchange J and hopping t within the framework of the Dynamical Cluster Approximation. Results at different temperatures and different cluster sizes will first be compared with existing BSS results (1) at half-filling. We then move on to the doped lattice with the ultimate aim of mapping out the magnetic phase diagram as a function of doping and coupling J/t.
(1) S. Capponi, F.F. Assaad, Phys. Rev. B 63, 155114, (2001)

TT 25.47 Wed 14:30 P1

Two-particle excitations in the Dynamical Cluster Approximation — •Stephan Hochkeppel, Fakher Assaad, and Werner Hanke — Theoretische Physik, Am Hubland, D-97074 Würzburg

The two-particle properties of the two-dimensional Hubbard model in the strong-coupling regime $U = 8t$ are investigated by using the Dynamical Cluster Approximation (DCA) [1]. In the DCA approach the original lattice problem is mapped to a self-consistently embedded cluster in momentum space. The crucial approximation of the DCA approach is to use the irreducible quantities, e.g the self-energy and irreducible vertices of a cluster as a good approximation of the lattice problem. We utilize a simplified Bethe-Salpeter equation with a renormalized Coulomb coupling $U_{eff}(\vec{q}, i\omega)$ which is determined in the DCA scheme. First results are presented for the spin-excitation spectrum.
[1] M. Jarrell, Th. Maier, C. Huscroft, and S. Moukouri, Phys. Rev. B (2001).

TT 25.48 Wed 14:30 P1

Green functions for t-t' hopping on the Bethe lattice — •M. Kollar[1], M. Eckstein[1], K. Byczuk[1,2], N. Blümer[3], P. van Dongen[3], M. Radke de Cuba[4], W. Metzner[5], D. Tanaskovi ć[6], V. Dobrosavljevi ć[6], G. Kotliar[7], and D. Vollhardt[1] — [1]Theoretical Physics III, University of Augsburg — [2]Institute of Theoretical Physics, Warsaw University, Poland — [3]Institute of Physics, KOMET 337, University of Mainz — [4]Aachen — [5]MPI for Solid-State Research, Stuttgart — [6]Dept. of Physics and NHMFL, Florida State University, USA — [7]Dept. of Physics and Astronomy, Rutgers University, USA

We calculate the local Green function for a quantum-mechanical particle with hopping between nearest (t) and next-nearest neighbors (t') on the Bethe lattice, where the on-site energies may alternate on sublattices [1]. For infinite connectivity the renormalized perturbation expansion is carried out by counting all non-self-intersecting paths, leading to an implicit equation for the local Green function. By integrating out branches of the Bethe lattice the same equation is obtained from a path integral approach for the partition function. This also provides the local Green function for finite connectivity. Finally, a recently developed topological approach [1] is extended to derive an operator identity which maps the problem onto the case of only nearest-neighbor hopping. We find that t' hopping leads to an asymmetric spectrum with additional van-Hove singularities.
[1] M. Kollar *et al.*, Ann. Phys. (Leipzig) **14**, 642 (2005).
[2] M. Eckstein *et al.*, Phys. Rev. B **71**, 235119 (2005).

TT 25.49 Wed 14:30 P1

Phase diagram of the Hubbard model with t-t' hopping on the Bethe lattice — •M. Eckstein[1], M. Kollar[1], M. Potthoff[2], and D. Vollhardt[1] — [1]Theoretical Physics III, University of Augsburg — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg

Recently an efficient method for solving hopping Hamiltonians on the Bethe lattice was developed [1]. For infinite coordination number this provides the dynamical mean-field equations for the Hubbard model with

nearest-neighbor hopping t and next-nearest-neighbor hopping t'. We solve these equations using the self-energy functional approach [2] and compute the phase diagram. We find that t' hopping strongly influences the Mott-Hubbard metal-insulator transition in the paramagnetic phase. Results for the antiferromagnetic phase, which is suppressed by t' hopping, are also discussed.

[1] M. Eckstein *et al.*, Phys. Rev. B **71**, 235119 (2005); M. Kollar *et al.*, Ann. Phys. **14**, 642 (2005).
[2] M. Potthoff, Eur. Phys. J. B **32**, 429 (2003).

TT 25.50 Wed 14:30 P1

Doping an antiferromagnetic Mott insulator in two dimensions: A variational cluster approach — •Matthias Balzer, Michael Potthoff, and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

The two-dimensional single-band Hubbard model at zero temperature is studied within the variational cluster approach (VCA) [1] using clusters with up to 8 sites. A ficticious staggered magnetic field and an overall shift of the single-particle energies in the reference clusters are used as variational parameters to ensure a thermodynamically consistent determination of the staggered magnetization and the average particle number [2]. Static quantities as well as the one-particle spectral density are calculated as functions of the chemical potential. The system undergoes a transition from the antiferromagnetic Mott insulator at half-filling to a paramagnetic metal at small doping. The critical dopings on the hole- and on the electron-doped side as well as the order of the phase transition are determined. An additional next-nearest-neighbor hopping is taken into account to study a possible phase separation into macroscopically large antiferromagnetic metallic and paramagnetic metallic regions.

[1] M. Potthoff, M. Aichhorn, and C. Dahnken, PRL 91, 206402 (2003)
[2] M. Aichhorn, E. Arrigoni, M. Potthoff, and W. Hanke, preprint

TT 25.51 Wed 14:30 P1

Curie temperature in the Hubbard model with binary alloy disorder — •Krzysztof Byczuk[1], Martin Ulmke[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany — [2]FGAN-FKIE, Neuenahrer Str. 20, 53343 Wachtberg, Germany

Magnetic and electric properties of the Hubbard model with binary alloy disorder are studied within the dynamical mean-field theory. A paramagnet-ferromagnet phase transition and a Mott-Hubbard metal-insulator transition is found upon varying the alloy concentration. An enhancement of the Curie temperature due to disorder is demonstrated and is explained by the effects of band splitting and subband filling.

K. Byczuk and M. Ulmke, Eur. Phys. J. B 45, 449-454 (2005)
K. Byczuk, M. Ulmke, and D. Vollhardt, Phys. Rev. Lett. 90, 196403 (2003)

TT 25.52 Wed 14:30 P1

Energy gap in asymmetric Hubbard model — •Ihor V. Stasyuk and Orest B. Hera — Institute for Condensed Matter Physics, 1 Svientsitskii Street, 79011 Lviv, Ukraine

Energy band structure of the asymmetric Hubbard model with hopping integrals dependent on an electron spin (particle sort) is studied using an approximate analytic method within the dynamical mean-field theory. To solve the single-site problem, we use the equation of motion approach. Irreducible parts are separated by projecting on the basis of Hubbard operators, and are calculated using different-time decoupling. Our approximation is a generalization of the Hubbard-III approximation, and it includes the scattering responsible for the additional mechanism (due to the hopping of particles with different spin) of the band formation. When the single-site Coulomb repulsion U is increased, a gap appears in the spectrum. In the Falicov-Kimball limit (when particles of one sort are localized), our approach gives the exact result for the critical value of U corresponding to the alloy-analogy approximation. When a small nonzero hopping of localized particles is introduced, the spectrum is broadened and that leads to the increase of critical U.

TT 25.53 Wed 14:30 P1

Low-temperature phase diagram of the two-orbital Hubbard model — •Robert Peters and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We study the two-orbital Hubbard model by means of the dynamical mean-field theory using Wilson's numerical renormalization group to solve the effective impurity. As additional degree of freedom we include a localized spin coupled via Hund's exchange to the two orbitals, as e.g. necessary to properly describe $La_{1-x}Ca_xMnO_3$.

We investigate ferro-, antiferromagnetic and orbital order and their interplay as function of local Coulomb interaction parameters, filling and the additional localized spin degree of freedom. Comparison to generic features of the phase diagram of $La_{1-x}Ca_xMnO_3$ will be made.

TT 25.54 Wed 14:30 P1

Systematic Study of the Grüneisen-ratio near Quantum Critical Points — •Robert Küchler[1], Philipp Gegenwart[1], Niels Oeschler[1], Christoph Geibel[1], Frank Steglich[1], Karsten Heuser[2], and Ernst-Wilhelm Scheidt[2] — [1]Max-Planck Institut for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany

Recent theoretical work has shown that the Grüneisen ratio $\Gamma \propto \beta/C$ of thermal expansion , $\beta(T)$, to specific heat, $C(T)$, is a highly sensitive probe of quantum criticality. This is because Γ is divergent as T goes to zero at any quantum critical point (QCP) and the associated critical exponent can be used to distinguish between different types of QCPs. We report thermal expansion and Grüneisen ratio measurements in the temperature range 50 mK $\leq$ $T \leq$ 6 K on different Heavy-fermion systems close to magnetic QCPs. Our studies revealed the first-ever observation of a Grüneisen ratio divergence in four heavy fermion systems, which are located in the vicinity of antiferromagnetic QCPs. For $CeNi_2Ge_2$ and $Ce_xIn_{3-x}Sn_x$, $\Gamma \propto 1/T$ in accordance with the SDW scenario for three-dimensional critical spinfluctuations. By contrast, the observed singularity of Γ for $YbRh_2(Si_{0.95}Ge_{0.05})_2$ cannot be explained by the SDW theory, but is consistent with not yet published theoretical results of the locally scenario. Furthermore, the system $CeCu_{5.8}Ag_{0.2}$ has been studied, which shows a similar temperature dependence as found in $YbRh_2(Si_{0.95}Ge_{0.05})_2$ on a reduced temperature scale T/T_0, with $T_0 \approx T_K$, the Kondo temperature.

TT 25.55 Wed 14:30 P1

Hall Effect in $YbRh_2Si_2$ — •Sven Friedemann[1], Niels Oeschler[1], Silke Paschen[1,2], and Frank Steglich[1] — [1]Max-Planck-Institut for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany — [2]Vienna University of Technology, Karlsplatz 13, 1040 Wien, Austria

The heavy-fermion metal $YbRh_2Si_2$ exhibits pronounced non-Fermi liquid behaviour due to its vicinity to a quantum critical point (QCP). At zero magnetic field, the system orders antiferromagnetically at very low temperatures (T_N=70 mK). By applying a small magnetic field, $YbRh_2Si_2$ is driven through the QCP towards the paramagnetic state. Currently, two scenarios for a system at this type of QCP are discussed: The spin-density-wave scenario at which heavy electrons are expected on both sides of the QCP and the locally QCP at which the heavy electrons on the paramagnetic side disintegrate into localised magnetic moments and light conduction electrons on the magnetic side of the QCP. The field-dependent Hall effect as a measure of the Fermi volume turns out to be the appropriate method to characterize the QCP in $YbRh_2Si_2$. Low-temperature Hall-effect measurements of $YbRh_2Si_2$ show a rapid change of the Fermi volume and thus strongly hint at the existence of a locally QCP with a small Fermi surface at the magnetic side and a large one at the paramagnetic side [1]. We present similar measurements of the Hall coefficient on $YbRh_2Si_2$ and on the reference substance $LuRh_2Si_2$ in an extended temperature range.

[1] S. Paschen et al., Nature 432, 881 (2004)

TT 25.56 Wed 14:30 P1

Thermal Transport Properties of the Heavy Fermion Compound $YbRh_2Si_2$ — •Stefanie Hartmann[1], Ulrike Köhler[1], Niels Oeschler[1], Cornelius Krellner[1], Christoph Geibel[1], Samuel Maquilon[2], Zachary Fisk[2], and Frank Steglich[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, University of California, Davis, CA 95616, USA

The heavy-fermion compound $YbRh_2Si_2$ orders antiferromagnetically at T_N = 70 mK and reveals non-Fermi-liquid (NFL) behavior in the vicinity of a (magnetic field induced) quantum critical point (QCP).

Thermal conductivity κ and thermopower S measurements on high-purity single-crystalline samples of $YbRh_2Si_2$ as well as of the nonmag-

netic reference compound $LuRh_2Si_2$ in the temperature range between 30 mK and room temperature are presented and discussed within the framework of current theoretical models.

The high temperature transport properties are dominated by the transition from incoherent to coherent Kondo scattering and furthermore by the crystal electric field splitting of the Yb^{3+} ions, as the first excited doublet is situated at 200 K. The low temperature regime is governed by the strong NFL behavior due to the proximity of the antiferromagnetic instability.

TT 25.57 Wed 14:30 P1

Single crystal growth and investigation of the magnetism of the alloy $CePd_{1-x}Rh_x$ for concentrations $x \geq 0.6$ — •M. Deppe[1], P. Pedrazzini[2], N. Caroca-Canales[1], C. Geibel[1], and J.G. Sereni[3] — [1]Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]DPMC-Université de Genève, Q. Ernest - Ansermet, 1211 Genève, Switzerland — [3]Lab. Bajas Temperaturas, Centro Atómico Bariloche (CNEA), 8400 S.C. de Bariloche, Argentina

In the orthorhombic alloy $CePd_{1-x}Rh_x$ the continuous decrease of the ferromagnetic ground state $T_C(x)$ can be followed over more than a decade in T, from 6.6 K for $x = 0$ to 0.25 K at $x = 0.8$. Additional low temperature measurements suggest a smeared ferromagnetic quantum-critical point (QCP) for x_{cr} between 0.87 and 0.9.
All these results were based on $CePd_{1-x}Rh_x$ polycrystals. In order to get a more precise insight into the magnetic behaviour in the critical region we grow $CePd_{1-x}Rh_x$ single crystals in the range $x \geq 0.6$. We used the Bridgman technique with a pulling rate of 3-5 mm. Differential thermoanalysis measurements indicate a low melting point $T_m = 1090 \pm 15$ °C. The lattice parameters were defined with X-ray powder diffraction and the composition was investigated with microprobe analysis. We performed specific heat and resistivity measurements down to 0.4 K and compare our results with the previous results on polycrystalline samples. Further we studied the decrease of the magnetic anisotropy with x by susceptibility and magnetization measurements. These results will be discussed in relation to the scenario for the critical concentration.

TT 25.58 Wed 14:30 P1

Ultra-low-temperature specific heat of $CePd_{1-x}Rh_x$ – smeared ferromagnetic quantum phase transition — •Adam Pikul, Tanja Westerkamp, Robert Kuechler, Nubia Caroca-Canales, Philipp Gegenwart, Julian Sereni, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The $CePd_{1-x}Rh_x$ system exhibits a continuous evolution from ferromagnetic (FM) order in CePd ($T_C = 6.5$ K) to an intermediate–valence ground state in CeRh [1]. In the present contribution we report on results of low-temperature specific-heat measurements performed for polycrystalline samples of $CePd_{1-x}Rh_x$, with the compositions $0.8 \leq x \leq 0.95$, which are supposed to be close to a FM quantum critical point [1].

In contrast to $CePd_{0.2}Rh_{0.8}$, still demonstrating the FM phase transition at $T_C = 370$ mK, the $C(T)$ curve measured for $CePd_{0.15}Rh_{0.85}$ does not show any anomaly at least down to 70 mK. In the latter compound $C/T \sim -\ln T$, characteristic of a non-Fermi-liquid (NFL) system, and achieves a value of almost 1 J/(mol K^2) at 70 mK. Upon further increasing of the Rh-content the value of C/T decreases, but the NFL behavior is still well visible in the samples with $0.87 \leq x \leq 0.95$, for which $C/T \sim T^{-\alpha}$ ($\alpha \approx 0.5$). Upon applying magnetic fields FL behavior $C/T(T) \sim const.$ is recovered in all different samples.

The above-mentioned results indicate that the NFL behavior is observed down to mK-temperatures over an extended x-range ($0.85 \div 0.95$). This would be compatible with a smeared quantum phase transition.

A. Pikul's attendance at this conference was sponsored by the Humboldt Foundation.

[1] J. G. Sereni, R. Küchler, C. Geibel, Physica B 359–361 (2005) 41

TT 25.59 Wed 14:30 P1

Hall effect near the quantum critical point of $CeCu_{6-x}Au_x$ — •M. Röger[1], M. Uhlarz[1], S. Putselyk[1], O. Stockert[2], and H. v. Löhneysen[1,3] — [1]Physikalisches Institut, Universität Karlsruhe (TH), D-76128 Karlsruhe — [2]Max-Planck-Institut für chemische Physik fester Stoffe, D-01187 Dresden — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The heavy-fermion system $CeCu_{6-x}Au_x$ orders antiferromagnetically above $x_c = 0.1$. The quantum phase transition at x_c displays unusual features, e.g., low-dimensional spin fluctuations and locally critical slowing down of these spin fluctuations suggestive of a breakdown of the Kondo coupling between $4f$ and conduction electrons [1]. This breakdown should be reflected in the Hall effect [2]. The Hall effect of $CeCu_{6-x}Au_x$ ($0 \leq x \leq 0.2$) as measured in a finite field ($B = 0.3$ T) along the magnetically easy c axis has shown Fermi-liquid behavior at low T, i.e. a temperature-independent Hall constant R_H below ~ 0.3 K [3]. Applying the magnetic field parallel to the magnetically hard b-axis (anisotropy factor ~ 10) allows to detect the effect of magnetic order on R_H for $x = 0.2$ and of quantum criticality for $x = 0.1$.

[1] A. Schröder et al., Nature **407**, 6802 (2000)
[2] P. Coleman et al., J. Phys. Cond. Matt. **13**, R723 (2001)
[3] H. Bartolf et al., Physica B **359-363**, 86 (2005)

TT 25.60 Wed 14:30 P1

Experimental Study of the Hall Effect and Magnetoresistance in MnSi — •Andreas Neubauer, Christian Pfleiderer, Philipp Niklowitz, and Peter Böni — Physik Department E21, Technische Universität München, James-Franck-Strasse, D-85748 Garching, Germany

The itinerant-electron magnet MnSi orders magnetically at $T_c = 29.5$ K. The magnetic state is characterised by a helical modulation along the $\langle 111 \rangle$ space diagonal in the cubic B20 structure. Magnetic field suppresses the helical order above 0.6 T. The properties of MnSi are in various ways remarkable. The temperature dependence of the electrical resistivity suggests the emergences of an extended non-Fermi liquid phase above $p_c = 14.6$ kbar. Neutron scattering at ambient pressure shows an anomalous field dependence of helical fluctuations which may indicate certain similarities with the presence of partial magnetic order akin liquid crystals observed in a pocket of the NFL-phase. Here we report a detailed study of the Hall effect and the magnetoresistance of MnSi. We focus in particular on normal and anomalous contributions to the Hall effect and consider similarities and differences with conventional ferromagnets.

TT 25.61 Wed 14:30 P1

Magnetocaloric effect and Grüneisen parameter of thespin-gap system $TlCuCl_3$ — •S. Stark[1], N. Johannsen[1], T. Zabel[1], O. Heyer[1], A. Oosawa[2], H. Tanaka[3], A. Vasiliev[4], and T. Lorenz[1] — [1]II. Physikalisches Institut, Universität zuKöln, Germany — [2]Advanced Science Research Center,Japan Atomic Energy Research Institute, Japan — [3]Dep. ofPhysics, Tokyo Institute of Technology, Japan — [4]LowTemp. Physics Dep., Moscow State University, Russia

$TlCuCl_3$ is a $S = \frac{1}{2}$ quantum system with a nonmagnetic singlet ground state and a small energy gap to the excited triplet states. A magnetic field $H > 6$ T induces 3D antiferromagnetic order with a staggered magnetization perpendicular to the applied field. This transition can be described by a Bose-Einstein condensation of magnons and represents an example for a field-induced quantum phase transition. We present a study of the magnetocaloric effect, the thermal expansion α, the specific heat c_p and the magnetostriction. There exist clear predictions for the behavior of these quantities near a quantum critical point [1]. The differential magnetocaloric effect $\theta = \frac{dT}{dB}$ and the Grüneisen parameter $\Gamma = \frac{\alpha}{c_p}$ are very convenient to determine a possible quantum critical behavior of $TlCuCl_3$, since one anticipates that both Γ and $\frac{\theta}{T}$ diverge ($\sim \frac{1}{T}$) for $T \to 0$ and $B \to B_c$. Using Ehrenfest relations we also derive the uniaxial pressure dependence of the phase boundary [2]. We performed our measurements down to 0.3 K and compare our results to the existing theory.

[1] L. Zhu *et al.*, Phys. Rev. Lett. 91 (2003) 066404.
[2] N. Johannsen *et al.*, Phys. Rev. Lett. 95 (2005) 017205.

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TT 25.62 Wed 14:30 P1

Bulk and Surface Photoemission in Ytterbium Compounds — •Stefan W. Schmidt[1], Friedrich Reinert[2], and Stefan Hüfner[1] — [1]Universität des Saarlandes, 7.2 Experimentalphysik, D-66041 Saarbrücken, Germany — [2]Universität Würzburg, Experimentelle Physik II, D-97084 Würzburg, Germany

We have investigated a broad range of intermetallic intermediate-valent Yb compounds with high-resolution UPS. The results lead to interesting correlations between the binding energy ε_0 and the linewidth Γ_0 of the near-E_F spectroscopic structure and the ytterbium valence υ_{Yb} in these systems, and we discuss the influence of crystal field effects to the interpretation of our data.

From an investigation of the first order valence phase transition observed in the $4f$- and $4d$-XPS data of the prototypical compound $YbInCu_4$ [1] and a comparison to existing PE data [2,3], we conclude that a surface-near region of thickness $d \approx$ 20–40 Å with different

physical properties could be common to these materials. Therefore, the theoretical modelling of these systems on the base of UPS data has to consider the systematic differences between bulk and surface sensitive PES measurements, especially in comparison to thermodynamic measurements or bulk sensitive methods.

[1] S. Schmidt, S. Hüfner, F. Reinert and W. Assmus, Phys. Rev. B **72**, 195110 (2005).
[2] H. Sato *et al.*, Phys. Rev. Lett. **93**, 246404 (2004).
[3] H. Sato *et al.*, Phys. Rev. B **69**, 165101 (2004).

TT 25.63 Wed 14:30 P1

Spin-phonon coupling in Cr-based thiospinel systems probed by infrared spectroscopy — •Torsten Rudolf[1], Joachim Hemberger[1], Peter Lunkenheimer[1], Franz Mayr[1], Andrei Pimenov[1], Vladimir Tsurkan[1,2], and Alois Loidl[1] — [1]Center for Electronic Correlation and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, 2028 Chisinau, Republic of Moldova

We investigated several Cr-based thiospinels ACr_2S_4 with A=Mn, Fe, Zn, Cd, and Hg. In these magnetic semiconductors interesting physical features were found as e.g. relaxor ferroelectricity and colossal magnetocapacitance [1] in $CdCr_2S_4$, colossal magnetoresistance in $Fe_{1-x}Cu_xCr_2S_4$ or an orbital glass state in $FeCr_2S_4$ [2]. Beside the magnetic and thermodynamic properties we focus on the interplay between magnetism and phonon properties. We systematically studied the temperature and magnetic field dependence of the phonon spectra employing Fourier Transform Infrared Spectroscopy in a range from 5 K to 300 K and in fields of up to 7 T.

[1] J. Hemberger *et al.*, Nature **434**, 364 (2005)
[2] R. Fichtl *et al.*, Phys. Rev. Lett. **94**, 027601 (2005)

TT 25.64 Wed 14:30 P1

Detection of percolation-depercolation phase transition in silver rich Ag_xSe thin films by magneto transport measurements — •Marc von Kreutzbruck[1], Kai Allweins[1], Gertrud Lembke[1], Boris Mogwitz[2], Carsten Korte[2], and Jürgen Janek[2] — [1]Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 58, D-35392 Gießen, Germany

In this work we investigate the galvanomagnetic transport properties of polycrystalline Ag_xSe thin films with a thickness ranging from 6 nm to 200 nm and a silver excess of about $x = 2.3$. The latter is near the percolation-depercolation phase transition, where the transport is mainly mediated by silver paths and silver clusters on the nanoscale. Sample characterization by measuring the conductivity, Kohler Slope, and temperature behavior yielded no clear indication whether a sample is in the percolative regime. A more reliable characterization of the semiconductor/metal heterostructure was obtained by measuring weak localization effects. The determination of the corresponding characteristic scattering lengths, such as the spin-orbit length L_{so} and the inelastic length $L_i(T)$, divided the Ag_xSe films clearly into two groups. We interpret these findings as an indication that the weak localization approach can be used as a sound method to determine the percolative nature of a 2D-heterostructure. An analytical model with predictive power is proposed.

TT 25.65 Wed 14:30 P1

Non-equilibrium properties of quantum impurity systems from the functional renormalization group approach — •Riccardo Gezzi, Thomas Pruschke, and Volker Meden — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The functional renormalization group approach is extended to handle stationary non-equlibrium problems. As first application we study a quantum-dot system subject to a finite bias voltage. As approximations to the flow-equation scheme we employ truncation at zero and one-loop order, ignoring energy dependencies in the latter.

Since in the limit of vanishing bias voltage an analytical solution to the differential equation generated in the zero-loop approximation exists, we can discuss the analytic structure of the solution to the flow equations obtained and show that in contrast to the equilibrium formulation poles in the right hand side can lead to an ill-conditioned problem for numerical differential equation solver.

First results for non-equilibrium properties of the single-impurity Anderson model will be discussed.

TT 25.66 Wed 14:30 P1

Equilibrium dynamics of the Anderson Impurity Model from functional RG methods — •Ralf Hedden, Volker Meden, Thomas Pruschke, and Kurt Schönhammer — Institut für theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We calculate the single-particle Greens-function of quantum multi impurity systems with local correlations modelled by the Anderson Impurity Model using a functional renormalization group scheme. Systems of one, two and three impurities coupled by hopping matrix elements are studied. The influence of an Ising-like Hund's-coupling is investigated. For special parameter sets we can even treat systems with an arbitrary number of impurities. We investigate how the different parameters effect the behaviour of the local spectral function.

TT 25.67 Wed 14:30 P1

Spin-boson model dynamics for non-equilibrium initial preparation — •Andreas Hackl[1] and Stefan Kehrein[2] — [1]Theoretische Physik III, Center for Electronic Correlations and Magnetism, Department of Physics, Universitaet Augsburg — [2]Department of Physics, LMU Muenchen Theresienstr. 37, 80333 Muenchen

The spin-boson model as a paradigm for quantum dissipation is well-understood in equilibrium. [1] However, many interesting questions regarding its dynamics are still open if the spin-boson model is initially prepared in a quantum state that is not its ground state. We use infinitesimal unitary tranformations (flow equation method) [2] to eliminate the system-bath coupling in a controlled nonperturbative approximation. In this way we are able to solve the Heisenberg equations of motion for the spin operators analytically with good accuracy, which allows us to study such non-equilibrium dynamics. We discuss various correlation functions, their equilibration properties and the fluctuation-dissipation theorem for different classes of initial states.

[1] S. Kehrein und A. Mielke, Annalen der Physik (Leipzig) 6, 90 (1997)
[2] F. Wegner, Annalen der Physik (Leipzig) 3, 77 (1994)

TT 25.68 Wed 14:30 P1

Phase Diagram of the Non-Equilibrium Anisotropic Kondo Model — •Peter Fritsch and Stefan Kehrein — LMU München, Department für Physik

Using the method of infinitesimal unitary transformation (flow equations), we derive a perturbative scaling picture of the anisotropic Kondo Model in a non-equilibrium state due to an applied dc-voltage bias. The scaling picture generically contains both the equilibrium and the non-equilibrium physics of the model, thereby allowing us to study the effect of decoherence on the Kosterlitz-Thouless quantum phase transition found in the equilibrium model.

This work is a generalization of the previous flow equation analysis of the isotropic non-equilibrium Kondo Model [1].

[1] S. Kehrein, Phys. Rev. Lett. 95, 056602 (2005)

TT 25.69 Wed 14:30 P1

Kondo Effect in Bosonic Spin Liquids — •Lars Fritz, Serge Florens, and Matthias Vojta — Theorie der Kondensierten Materie, Universitaet Karlsruhe

In a metal, a magnetic impurity gets fully screened at low temperatures by the conduction electrons. In contrast, an impurity coupled to spin-1 bulk bosons, such as triplet excitations in paramagnets, is only partially screened, even at the bulk quantum critical point, where the excitations are gapless. We argue that this difference is not due to the statistics of the host particles, but instead related to the structure of the impurity-bulk coupling. We show that in frustrated quantum magnets with bosonic spinon excitations one can observe a bosonic version of the Kondo effect.

TT 25.70 Wed 14:30 P1

Nonequilibrium Transport through a Double Quantum Dot System in the Kondo Regime — •V. Koerting and P. Wölfle — Institut fuer Theorie der Kondensierten Materie, Universitaet Karlsruhe, Karlsruhe

We consider nonequilibrium electron transport through a quantum dot in the Kondo regime coupled by exchange interactions to a second quantum dot connected to a third reservoir. The current is evaluated in perturbation theory. In a magnetic field it is shown to depend on the

nonequilibrium magnetization in an essential way. The dependence of the magnetizations of both quantum dots on the exchange coupling, the magnetic field and temperature is calculated.

TT 25.71 Wed 14:30 P1

Weak Itinerant Ferromagnetism and Half-Metallicity in the New Filled Skutterudite $TlFe_4Sb_{12}$ — •Andreas Leithe-Jasper[1], Walter Schnelle[1], Helge Rosner[1], Michael Baenitz[1], Raul Cardoso-Gil[1], John A. Mydosh[2], and Yuri Grin[1] — [1]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

The chemical, structural and magnetic properties of the new filled skutterudite $TlFe_4Sb_{12}$ are described. X-ray diffraction and elemental analysis established the cubic crystal structure ($a = 9.1959(2)$ Å) without defects and disorder at the cationic site. The electronic structure is calculated by FPLO methods. Electronic structure calculations within the LDA exhibit a band ferromagnetic ground state and predict a nearly perfect half metallic state (97.5 %) similar to the isotypic compounds MFe_4Sb_{12} (M = Na, K) [1,2,3].

From experiments, $TlFe_4Sb_{12}$ is an itinerant electron ferromagnet with small magnetic moments ($M_r = 0.30\mu_B$/Fe atom) and $T_C \approx 85$ K. A Curie-Weiss behaviour with a paramagnetic moment per Fe-atom of $1.69\,\mu_B$ and $\Theta \approx T_C$ is observed above T_C, similar to MFe_4Sb_{12} (M = Na, K). The results of an NMR study are discussed.

[1] A. Leithe-Jasper *et al.,* Phys. Rev. Lett. 91, 037208 (2003).
[2] A. Leithe-Jasper *et al.,* Phys. Rev. B 70, 214418 (2004).
[3] G. Sheet *et al.,* Phys. Rev. B RC, in print (2005).

TT 25.72 Wed 14:30 P1

Magnetic order in thin films of the heavy fermion superconductor UNi_2Al_3 — •Martin Jourdan[1], Andrey Zakharov[1], Arno Hiess[2], Tim Charlton[3], Nick Bernhoeft[4], Danny Mannix[5], and Hermann Adrian[1] — [1]Institut für Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany — [2]Institut Laue Langevin, BP 156, F-38042 Grenoble, France — [3]Rutherford Appelton Laboratory, ISIS facility, UK — [4]Dépt. de Recherche Fond. sur la Matière, France — [5]XMaS UK CRG beamline, ESRF, BP 220, F-38043 Grenoble Cedex 9, France

In the case of the heavy fermion superconductor UNi_2Al_3 a strong interconnection between its superconducting and magnetic properties is expected. Thus a careful characterization of the magnetic state of thin film samples primarily prepared for the investigation of the unconventional superconducting properties of this compound is necessary.
Resonant magnetic x-ray scattering was employed to investigate the magnetic state of epitaxial a^* oriented thin films UNi_2Al_3. The observed incommensurate propagation vector as well as the Neél temperature correspond to those of bulk samples. The 1200Å film shows magnetic order with a correlation length > 800Å parallel to the growth axis. Out of the three possible magnetic domains the one with the moment direction perpendicular to the film surface is not realized.

TT 25.73 Wed 14:30 P1

Growth of heavy-fermion superconductor $CeCoIn_5$ thin films — •Oleksiy K. Soroka, Gabriele Blendin, and Michael Huth — Physikalisches Institut, Max-von-Laue-Str. 1, D-60438, Frankfurt am Main

Heavy-fermion superconductors develop superconductivity out of a normal state in which electronic correlations cause a large increase of the conduction electrons' effective mass. The superconductive state is strongly affected by the magnetic excitations in these materials and is insofar unconventional. The most direct technique to investigate the spectrum of these excitations is tunneling spectroscopy which benefits strongly from well-defined surface as presented by epitaxial thin films. $CeCoIn_5$ is a member of the heavy-fermion family with the general formula $CeMIn_5$ (M=Co, Ir, Rh). It has the highest transition temperature of all heavy-fermion superconductors discovered up to date and is close to a quantum critical point. Thin films of $CeCoIn_5$ were deposited on different substrates by using molecular beam epitaxy. The growth characteristics were studied by means of x-ray diffraction. The chemical composition of the films was examined by energy dispersive x-ray analysis.

TT 25.74 Wed 14:30 P1

Metamagnetic transition in the cubic heavy fermion compound $CeIn_{3-x}Sn_x$ — •J. Arndt[1], N. Caroca-Canales[2], M. Dörr[1], C. Geibel[2], O. Stockert[2], and M. Loewenhaupt[1] — [1]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden

We report on magnetisation measurements on single crystals of the heavy fermion alloy $CeIn_{3-x}Sn_x$ at low temperatures. $CeIn_3$ orders antiferromagnetically below $T_N = 10.2$ K. Substituting tin for indium suppresses the magnetic order until $T_N = 0$ at a critical concentration $x_c = 0.67$ [1]. In the vicinity of this quantum critical point the system shows non-Fermi liquid behaviour [2]. Magnetisation measurements on single crystals with $x \leq 0.8$ were performed in static magnetic fields up to $B = 13.5$ T and pulsed fields up to $B = 47$ T at temperatures $T > 2$ K. The susceptibility $\chi = \mathrm{d}M/\mathrm{d}B$ as a function of magnetic field displays a kink at low fields ($B < 10$ T) in the paramagnetic state of samples with $0.4 \leq x \leq 0.65$. This anomaly, observed for the first time, seems to be related to a metamagnetic transition where magnetic intersite correlations are destroyed. The critical field $B^\star$, at which the transition occurs in paramagnetic $CeIn_{3-x}Sn_x$, is lowered with increasing x, i. e. with decreasing strength of the correlations in the system. In high magnetic fields ($B > 35$ T) we observed effects ascribed to the population of the excited crystal field state.

[1] T. Rus *et al.*, Physica B, **359-361**, 62 (2005)
[2] J. Custers *et al.*, Acta Phys. Pol. B **34**, 379 (2003)

TT 25.75 Wed 14:30 P1

Crossover from Ferro- to Antiferromagnetism in the Layered Kondo Systems CeTPO (T=Ru, Os) — •Cornelius Krellner[1], Nagesh S. Kini[2], and Christoph Geibel[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Applied Chemistry, Hiroshima University, Kagamiyama 1-4-1, Higashi-Hiroshima 739-8527, Japan

Intermetallic Kondo lattice systems have attracted considerable attention in the last decades. While their exist many Ce-based compounds showing antiferromagnetical ground states, only very few systems are known with ferromagnetic order. On the way to find new Ce-based Kondo lattices close to a ferromagnetic quantum phase transition, the CeTPO (T=transition metal) compound series attracted our interest, because of the rather unusual crystal structure with alternating layers of TP_4 and OCe_4 tetrahedra. In this contribution we will present the first investigation of the physical properties of CeTPO (T=Ru, Os) crystallizing with the tetragonal ZrCuSiAs type structure (P4/nmm). Measurements of the magnetic susceptibility reveal that in both compounds Cerium is in a trivalent state. A pronounced decrease of the resistivity below 50 K indicates the coherence effects of a Kondo scale of order $T_K = 10$ K. But whereas CeRuPO shows a ferromagnetic transition at 15 K both in temperature dependent susceptibility and specific heat, the isoelectronic CeOsPO becomes antiferromagnetic below 4.4 K. The possible origin of these effects will be discussed.

TT 25.76 Wed 14:30 P1

Electronic structure, thermodynamics and transport properties of $CeRh_2Sn_4$ — •Monika Gamza[1], Walter Schnelle[2], Andrzej Slebarski[1], and Helge Rosner[2] — [1]Institute of Physics, University of Silesia, Katowice, Poland — [2]MPI CPfS Dresden

In the last years, CeRhSn was intensively investigated because it exhibits a non-Fermi-Liquid (NFL) character of the physical properties in a region of low temperatures. Recent results [1,2] confirm that CeRhSn is placed in the vicinity of an antiferromagnetic instability and indicate the significant role of atomic disorder in the formation of the NFL state.

Here, we present a study of the compound $CeRh_2Sn_4$ which has not yet been investigated so far. The Ce 3d x-ray photoelectron spectroscopy (XPS) spectrum indicates a mixed valence of Ce suggesting similarities to the above mentioned CeRhSn. We present a combined experimental and theoretical study based on thermodynamic data (heat capacity, magnetic susceptibility and resistivity) and spectroscopic data (XPS) together with ab-initio band structure calculations.
For a clear presentation of the unusual electronic properties we compare $CeRh_2Sn_4$ with the non-magnetic isostructural reference system $LaRh_2Sn_4$.

Supported by the State Commitee for Scientific Research (KBN) through Grant No. 1 P03B 052 28 and by the DFG, Emmy Noether-program.

[1] A. Ślebarski et al., Phys. Rev. B **72** (2005), 085443.
[2] H. Tou et al., Phys. Rev. B **70** (2004), 100407.

TT 25.77 Wed 14:30 P1

^{119}Sn solid state NMR as a local probe for correlations in $CeRu_4Sn_6$ — •Eva Maria Brüning[1], Michael Baenitz[1], Andrei Gippius[2], André Strydom[3], Silke Bühler-Paschen[1], and Frank Steglich[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Moscow State University, Faculty of Physics, Moscow, Russia — [3]Department of Physics APK, University of Johannesburg, South Africa

A ^{119}Sn NMR study on the tetragonal semimetal $CeRu_4Sn_6$ and the metallic structural homologue $LaRu_4Sn_6$ is presented. At low fields (1.8 T, 28.5 MHz) a broad NMR line with small (-0.33%) and nearly independent negative Knight shift $K(T)$ is observed, whereas at larger fields (up to 7.5 T) a structure in the spectra could be resolved. The NMR spectra are well represented by a superposition of two broadened anisotropic S=1/2 lines, consistent with the two different Sn sites in the tetragonal structure. The behavior of the spin-lattice relaxation rate $1/T_1$ at 28.5 MHz above approximately $T = 20$ K is consistent with a narrow-gap semiconductor ($1/T_1 \sim T\exp(-\Delta/k_BT), \Delta/k_B = 33$ K). The formation of correlations become apparent below $T^* = 10$ K where an upturn is observed in $1/T_1T$. This is consistent with the specific heat results in the framework of the Korringa model where $(T_1T)^{-1} \propto K^2 \propto N_{EF}^2 \propto (C/T)^2$ is valid. $1/T_1$ investigations at higher fields show the supression of the low-temperature upturn. In conclusion the results for $CeRu_4Sn_6$ suggest the formation of a ground state of strongly correlated quasiparticles within a low-carrier density.

TT 25.78 Wed 14:30 P1

Quantum Critical Behavior in $CeNi_{9-x}Cu_xGe_4$. — •E. –W. Scheidt[1], W. Scherer[1], G. Hilscher[2], and H. Michor[2] — [1]Chemische Physik und Materialwissenschaften, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Festkörperphysik, TU Wien, 1040

$CeNi_9Ge_4$ exhibits unusual non-Fermi liquid (nFl) behavior with the largest ever recorded value of the electronic specific heat $\Delta c/T \cong 5.5\,\mathrm{JK^{-2}mol^{-1}}$ without showing any trace of magnetic order [1]. Specific heat measurements show that the logarithmic increase of the Sommerfeld coefficient flattens off below 200 mK indicating coherent effects, whereas substitution of Ce by La in $CeNi_9Ge_4$ supports a single ion scenario as the main reason for the nFL behavior. Here we report on new substitution experiments replacing Ni by Cu. Specific heat and susceptibility results will discussed in the framework of a quantum critical phase transition scenario.

[1] U. Killer, E.-W. Scheidt, G. Eickerling, H. Michor, J. Sereni, Th. Pruschke, S. Kehrein, Phys. Rev. Lett. **92**, 27003 (2004)

TT 25.79 Wed 14:30 P1

Suppression of magnetic order in $YbNiSi_{3-x}Ge_x$ — •K. Grube[1], W. Knafo[1], C. Meingast[1], S. Drotziger[2], M. Uhlarz[2], Th. Wolf[1], P. Adelmann[1], and H. v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, Germany — [2]Physikalisches Institut, Universität Karlsruhe (TH), Germany

$YbNiSi_3$ shows moderately heavy-fermion behaviour with antiferromagnetic long-range order below $T_N = 5.1$ K. We have studied the thermodynamic and transport properties of single crystals grown using the flux method with specific heat, DC magnetization, and resistivity measurements in magnetic fields up to 14 T. The magnetic order is suppressed in a magnetic field of 8 T. On the other hand, $YbNiGe_3$ shows a very small magnetic susceptibility and no sign of magnetic order down to the lowest measured temperature of 1.9 K, indicating an intermediate-valent state. Preliminary experiments on polycrystalline $YbNiSi_2Ge$ samples exhibit signs of magnetic ordering below 3 K. We report on the magnetic phase diagram of $YbNiSi_3$ and the dependence of the specific heat on the Ge content.

TT 25.80 Wed 14:30 P1

High temperature specific heat and crystal field of the non-Fermi-Liquid system $YbRh_2Si_2$ — •J. Ferstl, C. Geibel, O. Stockert, and F. Steglich — Max-Planck-Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

The heavy fermion system $YbRh_2Si_2$ has attracted considerably interest in the last years, being located very close to a quantum critical point (QCP). Strong Kondo-like fluctuations lead to a very weak magnetic order with a transition temperature of only $T_N = 70$ mK at ambient pressure. A lot of physical investigations were done in the low temperature region, but much less investigations and analysis were devoted to the behaviour at higher temperatures. We shall present measurements of the specific heat C_p at higher temperatures. The results are analysed in view of crystal field (CEF) effects and discussed in comparison with results from inelastic neutron scattering. C_p of $YbRh_2Si_2$ and $LuRh_2Si_2$ were measured in the temperature range 2 K $\leq$ T $\leq$ 300 K. From the difference we deduced the contribution C_{4f} of the Yb-4f-electrons. We confirm the presence of a broad maximum between 40 K and 80 K in C_{4f}. This maximum can be related to the first excited CEF level which, according to neutron data, is located around 17 meV. While C_{4f} is more conclusive than neutron data for this lowest excited CEF level, $C_{4f}(T)$ is less conclusive for the higher levels, for which neutron data gave rather precise excitation energies of 25 meV and 43 meV. Thus the combination of specific heat and neutron data allows a more reliable determination of the whole CEF scheme.

TT 25.81 Wed 14:30 P1

How many Kondo-ions are seen by the electron spin resonance in $Yb_{1-x}R_xRh_2Si_2$? — •J. Wykhoff[1], J. Sichelschmidt[1], S. MaQuilon[2], L. Pham[2], Z. Fisk[2], C. Krellner[1], J. Ferstl[1], H.-A. Krug von Nidda[3], C. Geibel[1], and F. Steglich[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany — [2]Department of Physics, University of California, Davis, CA 95616 USA — [3]Experimentalphysik V, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

The heavy-fermion compound $YbRh_2Si_2$ is located very close to a magnetic field induced quantum critical point. The unexpected observation of electron spin resonance (ESR) of the Kondo-ion Yb^{3+} *below* the Kondo temperature ($T_K \simeq 25$ K) might be a direct verification of the localized moment scenario of quantum criticality [1].

We present the ESR of $Yb_{1-x}R_xRh_2Si_2$, R = La, Lu. The ESR-line observed below ≈ 30 K vanishes with increasing Lu-concentration. Taking advantage of an improved crystal growth process, we found that the crystal quality and the residual linewidth of the ESR signal are closely related. This suggests that the so-called ESR-bottleneck effect is important for the observability of the ESR-line well below the Kondo temperature. We found that the ESR signal intensity also depends on the Yb-concentration.

[1] J. Sichelschmidt et al., Phys. Rev. Lett. 91, 156401 (2003)

TT 25.82 Wed 14:30 P1

Possible critical pressure-induced valence fluctuation in $EuCu_2Ge_2$ — •Gabriel Alejandro Dionicio[1], Heribert Wilhelm[1], Zakir Hossain[2], and Christoph Geibel[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology, Kanpur-208016, India

By means of electrical resistivity measurements under pressure, we investigated the possibility of inducing a valence fluctuating regime in $EuCu_2Ge_2$ at low temperatures. The results are discussed in terms of a possible scenario for unconventional superconductivity driven by virtual exchange fluctuation of the charge density [1]. This mechanism was proposed to explain the high pressure superconducting dome in $CeCu_2(Si_{0.9}Ge_{0.1})_2$ [2]. Our porpuse is to look for further candidates where this model might be apply. Some Eu-compounds with the $ThCr_2Si_2$ structure have shown a thermal activated continuous crossover from a divalent to a trivalent state, due to the degeneracy of the f^7 and f^6 configuration. We would like to address the question whether such a degenerated state can be induced by pressure at very low temperatures in $EuCu_2Ge_2$, taking into account that this situation seems to be achieved in $EuCu_2(Si_{0.7}Ge_{0.3})_2$. The electrical resistivity measurements were performed up to 10 GPa in the temperature range 100 mK $< T <$ 300 K. A tentative phase diagram is presented and the results are compared with the studies peformed in the alloy $CeCu_2(Si_xGe_{1-x})_2$.

[1] K. Miyake, H. Maebashi; J. Phys. Soc. Jpn. 71 (2002) 1007
[2] H. Q. Yuan *et al*; Science 302 (2003) 2104

TT 25.83 Wed 14:30 P1

Fading of the magnetic order transition in $CePt_3$ Si under pressure — •Johannes Spehling[1], Olaf Zelesnik[1], Andreas Eichler[1], and Ernst Bauer[2] — [1]Inst. f. Angewandte Physik, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Inst. f. Festkörperphysik, TU Wien, A-1040 Wien, Austria

We have carried out specific heat measurements on $CePt_3$ Si at low temperatures from ambient pressure up to 1.5 GPa. A maximum of

$\frac{C}{T}$ around 2.2 K is observed which is commonly attributed to an antiferromagnetic transition. From our results it appears to consist of two superimposed anomalies separated by about 0.2 K. The pressure dependence of the lower anomaly can be described by a second order power law $T_1(p)$, which leads to a critical pressure of nearly $p_c = 2.4$ GPa. The second anomaly near the higher temperature T_2 is also weakened under pressure.

TT 25.84 Wed 14:30 P1

The quantum-functional properties of $Pr_{1-x-y}La_xPb_yTe$ — •T. Herrmannsdörfer[1], A. D. Bianchi[1], T. P. Papageorgiou[1], Y. Skourski[2], and J. Wosnitza[1] — [1]Institut Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Rossendorf, D-01314, Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, D-01069 Dresden, Germany

The intermetallic compound $Pr_{1-x-y}La_xPb_yTe$ shows a wide spectrum of physical phenomena. Depending on the metallurgical composition as function of x and y, the compound changes its behavior from nuclear magnetic order to super- or semiconductivity. In addition, there are interesting interplay effects between these ground states. In consequence, $Pr_{1-x-y}La_xPb_yTe$ may serve as an promising material for quantum-computing applications. Here we report our results of the superconducting and magnetic properties investigated in a wide temperature, 0.0001 K $\leq T \leq$ 350 K, and field range, $0 \leq B \leq 50$ T. We present data of the ac susceptibility, magnetization, and electrical conductivity of various compositions x and y, e.g. turning the system from a van Vleck paramagnet, $x = y = 0$ into either a superconductor, $x \geq 0.5$, or a doped semiconductor, $y \geq 0.999$. Recently we have measured the magnetization of $y = 0$, 0.50, and 0.90 in pulsed magnetic fields up to 50 T in order to investigate the influence of doping on the crystalline electrical-field properties.

TT 25.85 Wed 14:30 P1

Fermi Surface of the Half Heusler Compounds $Ce_{1-x}La_xBiPt$ — •A. D. Bianchi[1], J. Wosnitza[1], N. Kozlova[2], D. Eckert[2], L. Schultz[2], I. Opahle[2], S. Elgazzar[2], M. Richter[2], J. Hagel[3], M. Doerr[3], G. Goll[4], H. v. Löhneysen[4,5], G. Zwicknagl[6], T. Yoshino[7], and T. Takabatake[7] — [1]HLD, Forschungszentrum Rossendorf, Postfach 51 01 19, D-01314 Dresden — [2]IFW Dresden, D-01171 Dresden — [3]Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden — [4]Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe — [5]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe — [6]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig — [7]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

We report on the Fermi surface in the correlated half-Heusler compound $Ce_{1-x}La_xBiPt$. In CeBiPt we find a field-induced change of the electronic band structure as discovered by electrical-transport measurements in pulsed magnetic fields. For magnetic fields above ∼25 T, the charge-carrier concentration determined from Hall-effect measurements increases nearly 30%, whereas the Shubnikov–de Haas (SdH) signal disappears at the same field. In the non-$4f$ compound LaBiPt the Fermi surface remains unaffected, suggesting that these features are intimately related to the Ce $4f$ electrons. Electronic band-structure calculations point to a $4f$-polarization-induced change of the Fermi-surface topology. In order to test this hypothesis, we have measured the (SdH) signal in a $Ce_{0.95}La_{0.05}BiPt$ sample with a low La concentration.

TT 25.86 Wed 14:30 P1

Electronic structure of Fe_3O_4/MgO — •C. F. Chang[1], J. Schlappa[1], C. Schüssler-Langeheine[1], H. Ott[1], Z. Hu[1], E. Schierle[2], E. Weschke[2], G. Kaindl[2], A. Tanaka[3], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

Magnetite thin films grown on flat and stepped MgO have been studied using transport and resonant soft x-ray diffraction measurements. Down to a thickness of 38 nm a clear 1st order Verwey transition is observed. Resonant soft x-ray diffraction at the Fe $L_{2,3}$ and O-K resonances was used to study the electronic structure in the low-temperature phase. The broadening of the diffraction peaks along the surface normal in thin films allowed us not only to study the $(00\frac{1}{2})$ superstructure peak at both resonances, but also the tail of the (001) diffraction peak, which cannot be reached at the Fe-$L_{2,3}$ resonance for bulk samples. The electronic origin of both peaks turns out to be clearly different. Possible models for the ordered phase will be discussed.

TT 25.87 Wed 14:30 P1

Tb magnetism in multiferroic $TbMnO_3$ — •Jörg Voigt, Jörg Persson, Michael Prager, Yixi Su, and Thomas Brückel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Recently, there has been a debate on the origin of the ferroelectric transition in the Perowskite $TbMnO_3$ at 28 K. Some authors attribute the spontaneous polarization to a lock-in transition of the Mn^{3+} moments [1]. Kenzelmann et al. [2] observed an ordered Tb^{3+} magnetic moment at the ferroelectric phase transition by a high resolution single crystal neutron study. However, neutron scattering is not element specific and therefore his interpretation could be doubted. We report on X-ray resonance exchange scattering to probe the Tb magnetic order exclusively and time-of-flight neutron spectroscopy to derive the Tb crystal field level scheme above and below the ferroelectric transition.

[1] Kajimoto et al., PRB 70, 012401 (2004)
[2] Kenzelmann et al., PRL 95, 087206 (2005)

TT 25.88 Wed 14:30 P1

Coupling between spin and orbital order in $La_{0.5}Sr_{1.5}MnO_4$? — •C. F. Chang[1], M. Buchholz[1], C. Schüssler-Langeheine[1], M. Benomar[1], E. Schierle[2], E. Weschke[2], G. Kaindl[2], M. Braden[1], and L. H. Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

In $La_{0.5}Sr_{1.5}MnO_4$ spin, orbital and charge order occurs at low temperatures. Resonant soft x-ray diffraction data show an increase in intensity for the superstructure peak related to orbital order below T_N, when the antiferromagnetic spin order sets in [1]. While this results indicates a coupling between antiferromagnetic order and orbital order, a recent study using polarization analysis assigned the gain in intensity to a magnetic scattering contribution to the orbital order peak intensity below T_N [2]. We studied the k-space around the orbital order peak and found a broad diffuse background of magnetic origin, which has considerable intensity at the position of the orbital order peak. The relative intensity of this background varies for different positions on the sample. Sample positions without magnetic background allowed us to study the resonance behavior of the orbital order peak above and below T_N.

[1] S. B. Wilkins et al., Phys. Rev. Lett. 91, 167205 (2003)
[2] U. Staub et al., Phys. Rev. B 71, 214421 (2005)

TT 25.89 Wed 14:30 P1

Electric-field-induced insulator-metal transition in thin films of $Pr_{0.68}Ca_{0.32}MnO_3$ — •Sebastian Schramm, Peter Moschkau, and Christian Jooss — Institut für Materialphysik, Universität Göttingen

Experimental analysis and understanding of electronic phase separation in hole-doped manganites offer a fascinating research area for the fundamental properties of correlated electrons in solids. That is why those manganites are of great interest and their behaviour in electric fields should be understood. In this work $Pr_{0.68}Ca_{0.32}MnO_3$(PCMO)-thin films prepared by Pulsed Laser Deposition on $SrTiO_3$-Substrates are examined concerning their electrical transport properties. In constant-current-measurements, a resistance collapse of several orders of magnitude is observed while cooling below 175K. The resistivity exhibits a huge temperature hysteresis, which depends on the electric history of the sample. In further research explicit indications will be sought whether this abnormal resistance behaviour is due to a homogeneous or inhomogeneous resistance change in the film. There are a number of experimental evidences in favour of the inhomogeneous model, where a metallic, possibly ferromagnatic filament emerges in an insulating paramagnetic matrix.

TT 25.90 Wed 14:30 P1

Investigation of orbital ordering in $La_{7/8}Sr_{1/8}MnO_3$ by means of x-ray linear dichroism at the Mn L edge — •K. Kuepper[1,2], F. Bondino[3], K. C. Prince[3,4], M. Zangrando[3], M. Zacchigna[3], A. F. Takács[2], M. Matteucci[5], F. Parmigiani[6], A. Winiarski[7], V. R. Galakhov[8], Ya. M. Mukovskii[9], and M. Neumann[2] — [1]Forschungszentrum Rossendorf, D-01328 Dresden, Germany — [2]University of Osnabrück, Department of Physics, D-49069 Osnabrück, Germany — [3]Laboratorio TASC-INFM, I-34012 Basovizza (Trieste), Italy — [4]Sincrotrone Trieste, I-34012 Basovizza (Trieste), Italy — [5]ICGEB, I-34012 Trieste, Italy — [6]Dipartimento di Matematica e Fisica, Università Cattolica, del Sacro Cuore, Brescia, Italy — [7]Silesian Univ., A. Chelkowski Inst. Phys., PL-40007 Katowice, Poland — [8]Institute of Metal Physics, 620219 Yekaterinburg GSP-170, Russia — [9]Moscow State Steel and Alloys Institute, 117936 Moscow, Russia

We have investigated for the first time the orbital ordering in a three dimensional colossal magneto resistance manganite, namely $La_{7/8}Sr_{1/8}MnO_3$, by applying soft x-ray linear dichroism (XLD) to the Mn L edge [1]. We found that the cooperative Jahn Teller distorted orthorhombic phase, which is present at a temperature of 240 K, is probably accompanied by a predominantly cross type $(x^2-z^2)/(y^2-z^2)$ orbital ordering. This result is discussed in the light of previous results obtained by means of resonant x-ray scattering at the Mn K edge and different exchange interaction models.

[1] K. Kuepper *et al.*, J. Phys. Chem. B **109**, 15667 (2005)

TT 25.91 Wed 14:30 P1

Structural properties of Ru-codoped $La_{1-x}Sr_{1+x}MnO_4$ — •O. Schumann[1], D. Senff[1], M. Kriener[1], I. Klassen[1], N. Hollmann[1], T. Lorenz[1], A. Revcolevschi[2], G. Andre[3], F. Bouree[3] und M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]LPCES, Universite Paris Sud XI — [3]Laboratoire Léon Brillouin

We present x-ray and neutron scattering studies on ruthenium codoped $La_{1-x}Sr_{1+x}MnO_4$. This co-doping leads to a suppression of charge, orbital and magnetic order.

$La_{0.5}Sr_{1.5}MnO_4$ is the 2D-analogon of the half-doped 3D-perovskite manganites (Mn^{3+}:Mn^{4+}=1:1). While showing similar charge, orbital and spin order, a CMR effect is only observed in a very high field. As the CMR-effect in the 3D-manganites is due to a competition between antiferromagnetic (insulating) and ferromagnetic (metallic) interactions, this high field indicates a rather stable AF-order in the layered compound. To weaken this order we prepared several single crystals of Ru-codoped $La_{0.5}Sr_{1.5}MnO_4$, with Ru concentrations ranging from 2% up to 30%. Neutron diffraction, magnetization measurements and resistivity measurements shows, that Ruthenium doping rapidly suppress the charge and orbital order. Furthermore we find a ferromagnetic ground-state and an increased magnetoresistivity.

TT 25.92 Wed 14:30 P1

Magnetic excitations in charge and orbital ordered manganites — •D. Senff[1], M. Benomar[1], O. Schumann[1], F. Krüger[2], S. Scheidl[2], Y. Sidis[3], A. Revcolevschi[4] und M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany — [3]Laboratoire Léon Brillouin, France — [4]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, France

Charge and orbital ordering around half doping is a unique feature in the physics of manganite-oxides and the competition of these insulating phases with FM metallic phases seems to be the origin of the well known colossal magnetoresistance in perovskite manganites. We present the magnetic excitation spectrum within the charge and orbital ordered state of single layered $La_{0.5}Sr_{1.5}MnO_4$, a compound which exhibits a very stable CE-type AFM ordering.

Using inelastic neutron scattering techniques we determined the complete spin-wave dispersion of the CE-phase. At low temperatures the main features of the excitation spectrum is a steep dispersion along the FM exchange pathways of the CE-type structure, while the dispersion in the perpendicular directions exhibits only a very narrow bandwidth. Within linear spin-wave theory we model the observed data and conclude that the FM interaction is the most dominant magnetic energy in the AFM CE-type ordering scheme. This interpretation is confirmed by the excitation spectrum and the quasielastic diffuse magnetic scattering at temperatures well above T_N which both give clear evidence for short-range ferromagnetic correlations.

TT 25.93 Wed 14:30 P1

Anomalies in the excitation spectrum of the spinels $CdCr_2S_4$ and $FeCr_2S_4$ — •P. Scheib[1], V. Gnezdilov[2], K.Y. Choi[3], P. Lemmens[1], J. Hemberger[4], A. Loidl[4], and V. Tsurkan[4,5] — [1]IPKM, TU Braunschweig, D-38106 Braunschweig — [2]B.I. Verkin Inst. for Low Temp. Phys., NASU, 61164 Kharkov — [3]IMR, Tohoku Univ., Sendai — [4]EP V, Univ. Augsburg, 86135 Augsburg — [5]IAP, Acad. Sci. Moldova, MD-2028, Chisinau

Chalcogenide spinels show exceptional dielectric and magnetic properties, as e.g. large magnetoresistance and magnetocapacitive coupling. Using Raman scattering we study the excitations spectrum of these systems. Pronounced phonon and magnetic anomalies are observed that precede the long range ordered phases. Evidence for phase separation is observed. Work supported by ESF-HFM.

TT 25.94 Wed 14:30 P1

Metamagnetism of $(Ca,Sr)_2RuO_4$ studied by thermal expansion and magnetostriction — •J. Baier[1], M. Kriener[1], S. Stark[1], O. Heyer[1], T. Zabel[1], P. Steffens[1], O. Schumann[1], O. Friedt[1], A. Revcolevschi[2], S. Nakatsuji[3], Y. Maeno[3], T. Lorenz[1], M. Braden[1], and J. Mydosh[1] — [1]II. Phys. Institut, University of Cologne,Germany — [2]Lab. de Physico-Chimie de l'État Solide,Université Paris-Sud, France — [3]Dep. of Physics, KyotoUniversity, Japan

We present a study of the thermal expansion $\alpha(T,H)$ and the specific heat $c_P(T,H)$ down to 300 mK near the metamagnetic transition in $Ca_{2-x}Sr_xRuO_4$ with $0.2 \leq x \leq 0.5$. Isovalent substitution of Sr by the smaller Ca drives the spin-triplet superconductor Sr_2RuO_4 to the antiferromagnetic Mott-insulator Ca_2RuO_4. At $0.2 \leq x \leq 0.5$ the compounds are still metallic but close to localization. We find strong and anisotropic anomalies in $\alpha(T)$ which change sign in sufficiently high magnetic fields [1]. Striking similarities with the metamagnets $Sr_3Ru_2O_7$ and $CeRu_2Si_2$ are noticed. At $x = 0.2$, the sign change of the thermal expansion anomaly coincides with the metamagnetic transition (MMT). This MMT is accompanied by a large anisotropic magnetostriction. Furthermore, c_P/T is unusually large and shows a non-monotonic field dependence with a maximum at the MMT which turns into a minimum above 2 K. In contrast, for $x = 0.5$ we observe a strong decrease of c_p/T in a magnetic field similar to the behavior of c_p/T at $x = 0.2$ above the MMT.

[1] Kriener *et al.*, cond-mat 0408015, accepted for publication in PRL

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TT 25.95 Wed 14:30 P1

Magnetic excitations in 214-Ruthenates — •Paul Steffens[1], Olaf Schumann[1], Jörg Baier[1], Markus Krienер[1], Oliver Friedt[1], Yvan Sidis[2], Jiri Kulda[3], Satoru Nakatsuji[4], Yoshiteru Maeno[4], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin, France — [3]Institut Laue-Langevin, Grenoble, France — [4]Kyoto University, Japan

We present investigations of the magnetic excitation spectra of pure and doped Sr_2RuO_4, i.e. $Ca_{2-x}Sr_xRuO_4$ ($0 \leq x \leq 2$) and Ti-doped Sr_2RuO_4.

In the spin-triplet superconductor Sr_2RuO_4, the excitation spectrum is dominated by incommensurate fluctuations, which are caused by Fermi surface nesting. In addition, a weak ferromagnetic component is observed. Upon Ti-doping, the incommensurate component is enhanced and finally condenses into static order.

Substitution of Sr by Ca leads to a complex phase diagram with different magnetic phases. We report studies on samples with $0.2 \leq x \leq 0.6$, i.e. a region where metamagnetism is observed and where the behaviour seems to be controlled by the balance between two different types of magnetic instability: an incommensurate and a ferromagnetic one. Our results reveal how the competition between these two is influenced by temperature, magnetic field and chemical composition.

TT 25.96 Wed 14:30 P1

Valence and spin state in Ca_3FeRhO_6 and Ca_3CoRhO_6 studied by XAS — •Zhiwei Hu[1], Tobias Burnus[1], Seiji Niitaka[2], Chun-Fu Chang[1], Hua Wu[1], Júlio Criginski Ceszar[3], Nicholas B. Brookes[3], Ling-Yun Jang[4], Hong-Ji Lin[4], Hidenori Takagi[2], Keng San Liang[4], Chen Te Chen[4], and Liu Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Magnetic Material Laboratory, RIKEN (Institute of Physical and Chemical Research), Wako 351-0198, Japan — [3]European Synchrotron Radiation Facility, BP 220, Grenoble 38043, France — [4]National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan

The physical properties of triangular-lattice systems has been attracting much interest because the geometrical frustration produces novel types of phase transitions. The triangular lattice in Ca_3CoRhO_6 and Ca_3FeRhO_6 consist of one-dimensional chains with faced-sharing CoO_6 and FeO_6 trigonal prisms and of RhO_6 octahedra. Neutron diffraction experiments indicate ferromagnetic Ising-spin chains in Ca_3CoRhO_6 and a three-dimensional antiferromagnetic transition at 12 K in $CaFeRhO_6$. The valence and spin states in both compounds are a matter of controversy. The combined experimental and theoretical X-ray absorption spectroscopy (XAS) study at the Co-, Fe- and Ru-$L_{2,3}$ edges presents unambiguously Co^{2+}/Rh^{4+} and Fe^{3+}/Rh^{4+} states in Ca_3CoRhO_6 and $CaFeRhO_6$, respectively. The X-ray magnetic circular dichroism at the Co-$L_{2,3}$ edge indicates a large orbital moment of Co^{2+} in Ca_3CoRhO_6.

TT 25.97 Wed 14:30 P1

Dynamical local field corrections — •K. Morawetz — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The finite temperature dynamical response function including the dynamical local field is derived within a quasiparticle picture for interacting one-, two- and three dimensional Fermi systems. The correlations are assumed to be given by a density dependent effective mass, quasiparticle energy and a mean momentum shift as well as a relaxation time. The latter one describes disorder or collisional effects. The mean momentum ensures the zero order frequency sum rule. With a single static local field, the third order frequency sum rule can be fulfilled simultaneously with the compressibility sum rule by relating the effective mass and quasiparticle energy shift to the structure function or pair correlation function. This parameterization of correlations includes local density functionals as a special case and is therefore applicable for density functional theories though the latter ones cannot fullfill both sum rules simultaneously. The comparison to the Monte-Carlo data seems to support such quasiparticle picture.

[1] K. Morawetz, Phys. Rev. B 66 (2002) 07512

TT 25.98 Wed 14:30 P1

Metal-insulator transition in heterojunctions — •K. Morawetz[1,2], C. Olbrich[1], and M. Schreiber[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

The conductivity in quasi two-dimensional systems is calculated using the quantum kinetic equation as well as molecular dynamical simulations. The system of quasi two-dimensional electrons in hetero-junctions which interact with charged and neutral impurities and the low temperature correction to the conductivity is calculated analytically. It turns out that the dynamical screening due to charged impurities leads to a linear temperature dependence, while the scattering from neutral impurities leads to the usual Fermi-liquid behavior. The experimental metal-insulator transition at low temperatures are reproduced [1]. The effective mass of quasiparticle excitations in quasi two-dimensional systems is calculated analytically. It is shown that the effective mass increases sharply when the density approaches the critical one of metal-insulator transition. This suggests a Mott-type of transition rather than an Anderson-like transition [2].

[1] K. Morawetz, Phys. Rev. B 67 (2003) 115125
[2] K. Morawetz, Europhys. Lett. 67 (2004) 77–83

TT 25.99 Wed 14:30 P1

Domain Walls in the Hubbard model — •Rolf Helmes, Luis Craco, and Achim Rosch — Institut für Theoretische Physik, Universität zu Köln, D-50937 Cologne, Germany

Phase separation and the physics of domain walls control the properties of many correlated systems with competing ground states, ranging from the manganites to organic Mott insulators [1]. We therefore study domain walls between different phases of the Hubbard model. The interplay of domain walls and their energetics on the one hand and of long-range Coulomb interaction on the other hand, control for example the physics of phase-separation close to a first-order metal-insulator transition. We use a generalization of dynamical mean field theory (DMFT) to treat inhomogeneous correlated systems such as domain walls of Mott insulators.

[1] Sasaki et al., Phys. Rev. Lett. 92, 227001 (2004)

TT 25.100 Wed 14:30 P1

Properties of the density of states of the three dimensional Bernoulli-Anderson model — •P. Karmann, V. Cerovski, and M. Schreiber — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

The density of states of the Bernoulli-Anderson model, defined as the tight-binding Hamiltonian of non-interacting electrons with disorder introduced by the random distribution of only two on-site energies, is studied using the large scale numerical diagonalization by means of the Lanczos algorithm. In particular, we determine the band structure and the properties of characteristic features for different system sizes and disorder strength of the on-site energies and compare the results with the Anderson model of localization.

TT 25.101 Wed 14:30 P1

Coupled cluster calculation of the ground state of the J_1–J_2 model on the square lattice — •R. Darradi[1], J. Richter[1], Sven E. Krüger[2], R. Zinke[1], and D. J. J. Farnell[3] — [1]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg, P.O.B. 4120, 39016 Magdeburg, Germany — [2]IESK Kognitive Systeme, Universität Magdeburg, PF 4120, 39016 Magdeburg, Germany — [3]Unit Of Ophthalmology, Department of Medicine, University Clinical Departments, Daulby Street, University of Liverpool, Liverpool L69 3GA, United Kingdom

Using the coupled cluster method (CCM) for high orders of approximation we investigate the ground state properties of J_1–J_2 model on the square lattice. By calculation of the sublattice magnetization, the spin stiffness, and the spin gap we determine the quantum critical point J_2^c, where magnetic LRO disappears. We estimate $J_2^c \approx 0.4 J_1$ which is in good agreement with the results obtained by other approximations.

TT 25.102 Wed 14:30 P1

T=0-phase diagram of the Kondo-lattice model with quantum localized spins — •Jochen Kienert and Wolfgang Nolting — Humboldt-Universität zu Berlin*Institut für Physik*Theoretische Festkörperphysik*Newtonstraße 15*D-12489 Berlin

The ferromagnetic/non-ferromagnetic phase diagram of the Kondo-lattice model is determined at T=0 in 2D and 3D. Our approach takes into account the quantum character of the localized magnetic moments, which often are treated classically in studies of this model. Consequently, special emphasis is put on the comparison between quantum and classical spins ($S \to \infty$). The maximum region of ferromagnetic stability is reduced for small spins. We compare our findings with results based on different methods by other authors.

TT 25.103 Wed 14:30 P1

Thermodynamics of intermediate-spin Heisenberg-chains — •Simon Grossjohann and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We investigate the crossover from quantum to classical behavior in one-dimensional spin-S chains by a complementary analysis of the thermodynamic properties resulting from quantum Monte-Carlo calculations as well as from the large-S limit. Using the stochastic series expansion, results will be given for the thermodynamic limit of chains with spins ranging from S=1/2 to S=5/2 and for temperatures $0.01 \leq T/J \leq 20$. We find a tendency of the peak-positions T_m of the quantum and classical uniform susceptibilities, χ_q and χ_c, to converge as $S \to 5/2$. However for both, Haldane and non-Haldane systems, substantial quantitative and qualitative differences remain between χ_q and χ_c, regarding the low-temperature behavior even for the larger spin magnitudes. We will compare our results with Bethe-Ansatz calculations and present Padé-approximants for χ_q which improve fit-formulas previously reported in literature.

TT 25.104 Wed 14:30 P1

Series expansion analysis of a tetrahedral cluster spin chain — •Marcelo Arlego and Wolfram Brenig — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

Using series expansion by continuous unitary transformations we study the zero temperature magnetic properties of a frustrated tetrahedral spin-1/2 chain. Starting from the limit of isolated tetrahedra we analyze the evolution of the ground state energy and the elementary triplet dispersion as a function of the inter-tetrahedral coupling. The quantum phase diagram is evaluated and is shown to incorporate a singlet product, a dimer, and a Haldane phase. Comparison of our results with those from several other techniques, such as density matrix renormalization group, exact diagonalization and bond-operator mean field theory are provided and convincing agreement is found.

TT 25.105 Wed 14:30 P1

Theoretical investigation of the magnetic properties of J-alternating chains of monometallic complexes — •Sebastian Fuchs and Thomas Pruschke — Institut für Theoretische Physik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Monometallic complexes containing Ni with spin S=1 can be coupled via nitrit bridges to form chains with variable exchange coupling strengths between the Ni spins. We study the magnetic, i.e susceptibility and effective moment with and without external field, and thermodynamic properties of one particular system with three different couplings controlled through the orientation of the nitrit group. We estimate the relative strenghts of the couplings necessary to model the experimental data. Predictions for possible dynamical properties observable in Neutron scattering experiments are also made.

TT 25.106 Wed 14:30 P1

Novel mean-field theory for strongly disordered non-frustrated antiferromagnets — •Heidrun Weber and Matthias Vojta — Institut fuer Theorie der Kondensierten Materie, Universitaet Karlsruhe, 76128 Karlsruhe, Germany

Quantum paramagnets with elementary spin-1 excitations show magnetic ordering upon introducing non-magnetic impurities: the vacancies produce free spins 1/2 which order antiferromagnetically at low temperatures. We have developed a novel mean-field theory for the impurity degrees of freedom, taking into account the random distribution of coupling constants. In particular, we demonstrate that the conventional first-order spin-flop transition is split into two transitions at low temperatures, associated with seperate order parameters along and perpendicular to the easy axis. We apply our results to impurity-induced order in spin-gap magnets like $TlCuCl_3$.

TT 25.107 Wed 14:30 P1

High-order coupled cluster method calculations for the ground-state of quasi-one-dimensional spin systems — •Ronald Zinke[1], Johannes Richter[1], Jörg Schulenburg[2], and Damian J.J. Farnell[3] — [1]Institut für Theoretische Physik, Otto-von-GuerickeUniversität Magdeburg,P.O.B. 4120, 39016 Magdeburg, Germany — [2]Universitätsrechenzentrum, P.O.B. 4120, 39016 Magdeburg, Germany — [3]Unit Of Ophthalmology, Department of Medicine,University Clinical Departments, Daulby Street,University of Liverpool, Liverpool L69 3GA, United Kingdom

We consider ground-state properties of quasi-1-dimensional quantum Heisenberg antiferromagnets for spin quantum numbers $s = \frac{1}{2}$ and $s = 1$. For the investigation of the ground-state long-range order we calculate the sublattice magnetization using the high order coupled cluster method. We find that for the unfrustrated spin-$\frac{1}{2}$ system an infinitesimal inter-chain coupling $J_\perp$ is sufficient to stabilize magnetic long-range order. This result is in agreement with known results obtained by other methods. For $s = 1$ we find that a finite inter-chain coupling is necessary to stabilize magnetic long-range order, which can be interpreted as a result of the gapped ground-state of the spin-1 chain. The estimated value for the critical inter-chain coupling is: $J_\perp^c \approx 0.1$. Furthermore we consider a spin-$\frac{1}{2}$ system were a frustrating next-nearest neighbor in-chain coupling is included. We find for strong frustration that again a finite inter-chain coupling $J_\perp$ is necessary to stabilize long-range order.

TT 25.108 Wed 14:30 P1

An ab-initio correlation treatment for metals — •Beate Paulus[1], Elena Voloshina[1], Nicola Gaston[1], and Krzysztof Rosciszewski[2] — [1]MPI for the Physics of complex Systems, Dresden, Germany — [2]Institute for Physics, Jagellonian University, Krakow, Poland

Up to now wavefunction-based ab-initio correlation treatements are possible for semiconductors and insulators applying the method of increments. This method corresponds to a many-body expansion of the correlation energy of the solid in terms of localized entities. A generalization is possible for metals, where two major problems have to be faced: First, a straight-forward localization of the orbitals is not possible, localized entities have to be generated via an embedding scheme. The influence of the delocalization on the electronic correlation is treated successively with the incremental scheme [1,2] . Second, the quasi-degeneracy at the Fermi level can no longer be described with a single-reference correlation method. To solve this problem the method of increments is extended to multi-reference correlation methods [3]. First applications to the group II metals magnesium, zinc, cadmium and mercury are presented.

[1] B. Paulus and K. Rosciszewski, Chem. Phys. Lett. 394 (2004) 96.
[2] B. Paulus, K. Rosciscewski, N. Gaston, P. Schwerdtfeger and H. Stoll, Phys. Rev. B 70 (2004) 165106.
[3] B. Paulus, Chem. Phys. Lett.371 (2003) 7.

TT 25.109 Wed 14:30 P1

Electron-Phonon Coupling in $Fe_{1-x}Co_xSi$ as derived from Raman-Spectroscopy — •I. Jursic, T. Donig, A.-M. Racu, D. Menzel, and J. Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

FeSi is a paramagnetic semiconductor which is often viewed as Kondo insulator. $Fe_{1-x}Co_xSi$ becomes a ferromagnetic metal with $0.05 < x < 0.8$ whereas CoSi is a diamagnetic metal.

Raman measurements on $Fe_{1-x}Co_xSi$ with different Co content were performed to investigate the effect of Co doping on the vibrational modes. The system crystallizes in the B20 structure which according to a factor group analysis yields 9 raman-active phonons that are all observed in the experiment.

Polarisation resolved measurements allow the identification of the A-mode. For increasing Co content a change in the intensities and distribution of the vibrational modes is observed. The E- and T-modes shift to higher energies contrary to the expectations. The A-mode shifts to lower energies more than expected. The shift of the modes begins with 10% Co content which is approximately at the insulator to metal transition.

Temperature resolved measurements show that the linewidth of one particular E mode strongly depends on the Co content. This is interpretated in terms of a strong electron-phonon coupling which leads to shorter decay times with increasing Co content and a closure of the energy-gap.

TT 25.110 Wed 14:30 P1

Orbital ordering in the two-dimensional ferromagnetic semiconductor Rb_2CrCl_4 — •Udo Schwingenschlögl and Volker Eyert — Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

We present the results of electronic structure calculations for the two-dimensional ferromagnet Rb_2CrCl_4. They are obtained by the augmented spherical wave method as based on density functional theory and the local density approximation. In agreement with experimental data, Rb_2CrCl_4 is found to be semiconducting and displays long-range ferromagnetic order of the localized Cr $3d$ moments. The magnetic properties are almost independent of the structural modifications arising from a Jahn-Teller instability, which leads from the parent body-centered tetragonal K_2NiF_4 structure to a side-centered orthorhombic lattice. In contrast, our calculations give evidence for a strong response of the optical band gap to the corresponding structural changes.

TT 25.111 Wed 14:30 P1

Role of the structural distortions in the phase diagrams of $RE_{1-x}A_xTiO_3$ (A=Ca,...) — •A. C. Komarek[1], M. Cwik[1], W. D. Stein[1], H. Roth[1], H. Hartmann[1], T. Zabel[1], M. Krienер[1], N. Schittner[1], A. El-Filali[1], M. Hölzel[2], F. Bouree[3], T. Lorenz[1], A. Freimuth[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, D-50937 Köln — [2]Technische Universität Darmstadt, c/o Technische Universität München — [3]Laboratoire Leon Brillouin, CE-Saclay, F-91191 Gif-sur-Yvette, France

Having one electron in the 3d shell, the rare earth (RE) titanates $RETiO_3$ represent interesting systems to study the complex interplay of orbital and magnetic degrees of freedom as well as to investigate metal-insulator (MI) transitions enabled by hole doping due to a partial substitution of the trivalent rare earth by divalent earth alkaline ions. In the series of rare earth titanates we find an anomalous behaviour of the lattice parameter a for the samples with larger rare earth ions showing antiferromagnetic order. However, with decreasing rare-earth ionic radius the anomalous increase of the lattice constant a gets even more pronounced and sets in closer to the magnetic ordering temperature. The hole-doped system $Y_{1-x}Ca_xTiO_3$ shows a complex phase diagram of structural transitions. The structural changes are accompanied by a MI transition and anomalies in the magnetic susceptibility. We ascribe this complex behavior to the coexistence of an insulating monoclinic phase and a metallic low-temperature orthorhombic phase. Our neutron diffraction data give evidence for a charge ordering in the monoclinic phase.

TT 25.112 Wed 14:30 P1

Charge order induced pseudo gap and phonon anomalies in the superconducting cobaltate Na_xCoO_2 yH_2O — •P. Lemmens[1,2], K.-Y. Choi[3], V. Gnezdilov[4], F.C. Chou[5], C.T. Lin[1], and B. Keimer[1] — [1]MPI-FKF, D-70569 Stuttgart, Germany — [2]IPKM, TU Braunschweig, D-38106 Braunschweig — [3]IMR, Tohoku Univ., Sendai — [4]B.I. Verkin Inst. for Low Temp. Phys., NASU, 61164 Kharkov — [5]CMSE, MIT, Cambridge, MA 02139

We report on the observation of an electronic Raman scattering continuum in nonsuperconducting and superconducting cobaltates Na_xCoO_2 yH_2O. Pronounced phonon anomalies are observed in the proximity of the metal-insulator transition and the charge ordering instabilities in $Na_{0.5}CoO_2$. We analyze the scattering rates as function of composition and emphasis an anomalous non-Fermi liquid like regime for x $\geq$0.5. Work supported by DFG SPP1073, ESF-HFM and MRSEC Program of NSF under award number DMR 02-13282.

TT 25.113 Wed 14:30 P1

Probing orbital moment with resonant soft x-ray diffraction: $La_{1.5}Sr_{0.5}CoO_4$ — •C. Schüssler-Langeheine, C. F. Chang, Z. Hu, M. W. Haverkort, T. Burnus, M. Benomar, M. Braden, and L. H. Tjeng — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Magnetic circular dicroism in x-ray absorption (XMCD) is a well-established technique for the investigation of ferromagnetic materials. From the shape of the XMCD signal across resonance the z-component of the orbital and spin moments can be deduced - in many cases by means of a simple sum-rule analysis. We applied this technique to an antiferromagnetic system, which is Sr-doped La_2CoO_4. For an antiferromagnet the MCD effect cannot be observed in the x-ray absorption signal, where it cancels out, but MCD is also one of the contrast mechanisms leading to resonant magnetic x-ray scattering. For $La_{1.5}Sr_{0.5}CoO_4$ we find a vanishing magnetic diffraction signal at the Co-L_2 resonance, which indicates a large z-component of the orbital moment.

TT 25.114 Wed 14:30 P1

Charge, spin and orbital degrees of freedom in $La_{2-x}Sr_xCoO_4$ — •M. Cwik[1], M. Haider[1], M. Benomar[1], M. Reuther[1], A. Hoser[2], Y. Sidis[3], T. Lorenz[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich — [3]Laboratoire Leon Brillouin (CEA-CNRS), CEA-Saclay, 91191 Gif-Sur-Yvette Cedex, France

The layered cobaltate La_2CoO_4 is an orthorhombic distorted antiferromagnetic insulator with $T_N \sim 270$ K and Co^{2+} ($3d^7$) in the S=3/2 high spin state [1]. The substitution of La^{3+} by larger Sr^{2+} ions reduces the orthorhombic distortion, suppresses long range magnetic order and induces a nominal Co^{2+}/Co^{3+} mixed valency. For $La_{1.5}Sr_{0.5}CoO_4$ a checkerboard-like charge order ($T_c \sim 750$ K) and an antiferromagnetic order ($T_s \sim 30$ K) with the propagation vector Q=(0.25 0.25 1) have been found [2]. We present an analysis of the crystal structure, of the spin and charge order and of the magnetic correlations studied on single crystals for $0.1 \leq x \leq 1.0$. For x = 0.4 the magnetic order is incommensurate but we do not find evidence for a stripe-like ordering scheme similar to the observations in cuprates or nickelates. We interpret the different magnetic ordering , the emerging charge order and the structural anomalies in this system in terms of the Co^{3+} spin degree of freedom, several magnetic interaction parameters and geometrical frustration.

[1] K. Yamada et al., Phys. Rev. B 39, 2236 (1989)
[2] I. A. Zaliznyak et al., Phys. Rev. Lett. 85, 4353 (2000)
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TT 25.115 Wed 14:30 P1

Polarized neutron scattering study of the spin-state transition in $LaCoO_3$ — •M. Cwik[1], M. Kriener[1], M. Reuther[1], L.-P. Regnault[2], K. Schmalzl[2], T. Lorenz[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [2]Institut Laue-Langevin, F-38042 Grenoble Cedex 9, France

$LaCoO_3$ exhibits a spin state transition around 100 K which is associated with the thermal excitation of Co^{3+} ($3d^6$) ions from a nonmagnetic low-spin ($t_{2g}^6e_g^0$, S=0) to a magnetic spin state without long range order [1]. The nature of this magnetic spin state is still discussed controversially. Depending on the crystal-field splitting, the intra-atomic exchange interaction and the hybridization between Co-3d and O-2p orbitals, the so-called intermediate ($t_{2g}^5e_g^1$, S=1) or the high-spin state ($t_{2g}^4e_g^2$, S=2) could be stabilized. We present an analysis of the magnetic fluctuations in $LaCoO_3$ studied by polarized inelastic neutron scattering measurements performed on a co-mounting of six large single crystals. We find evidence for magnetic correlations in the paramagnetic phase. For a quantitative estimation of the magnetic susceptibility one needs to take these correlations into account. However, with the polarized neutrons we do not find the signal reported in reference [2] which was attributed to the LS-IS transition. In addition we present the results of inelastic neutron scattering studies on the phonon dispersion in $LaCoO_3$.
[1] C. Zobel et al., Phys. Rev. B **66**, 020402(R) (2002)
[2] Y. Kobayashi et al., cond-mat/0504351
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Thermodynamic and transport properties of doped La_2CoO_4 — •E Rose[1], N Hollmann[1], J Baier[1], M Benomar[1], K Berggold[1], M Cwik[1], M Kriener[1], D Meier[1], A Tanaka[2], T Lorenz[1], and A Freimuth[1] — [1]II.Physikalisches Institut, Universität zu Köln, Germany — [2]Department of Materials Science, Hiroshima University, Japan

Cobaltates are of special interest due to the possibility of spin-state transitions. This has been studied in detail in the insulator $LaCoO_3$. Strontium doping drives $LaCoO_3$ to a metal and induces ferromagnetic order [1,2]. Much less is known about the layered cobaltates $La_{2-x}Sr_xCoO_4$. We prepared single crystals and present a study of magnetic susceptibility, thermal and electric conductivity as well as thermal expansion and thermopower for a strontium doping range of $0.3 \leq x \leq 0.8$. All samples are insulators in the measured temperature range. The magnetic susceptibility is strongly anisotropic and deviates from Curie-Weiss-behaviour. The susceptibility was analyzed via cluster calculation [3]. Thermal transport measurements in a temperature range from 5K to 300K present a small anisotropy. In fields up to 14 Tesla a weak field dependence is found which is related to the magnetic ordering, in particular for $La_{1.5}Sr_{0.5}CoO_4$. Positive Seebeck coefficients observed at room temperature suggest p-type conduction. Furthermore we studied the effect of physical pressure due to calcium doping.
[1] Berggold *et al.*, Phys. Rev. B **72**, 155116 (2005)
[2] Kriener *et al.*, Phys. Rev. B **69**, 094417 (2004)
[3] Tanaka *et al.*, J. Phys. Soc. Jpn. **63**, 2788 (1994)
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Temperature- and doping-induced spin-state transitions of $RCoO_3$ — •K. Berggold, N. Hollmann, M. Reuther, M. Kriener, J. Baier, C. Zobel, A. Reichl, and T. Lorenz — II. Physikalisches Institut, University of Cologne, Germany

$LaCoO_3$ attracts a lot of attention, because it undergoes a temperature-induced spin-state transition. There are different ways to tune this spin-state transition, either to stabilize the low-spin state by replacing La with smaller rare earth ions R, or to suppress it by the introduction of charge-carriers[1,2]. For low doping levels so-called high-spin polarons are formed. We studied the thermal conductivity κ on $RCoO_3$ single crystals with R = La, Pr, Nd, and Eu, as well as on $La_{1-x}Sr_xCoO_3$ with $0 \leq x \leq 0.3$ and find that κ is strongly suppressed by the spin-state transition. Particularly we present magnetic-field dependent measurements for low temperatures to investigate the influence of the high-spin polarons to κ. A low thermal conductivity is one pre-condition to reach large values of the thermoelectric figure of merit ZT, which is necessary for thermoelectric applications. We observe a $ZT^{(max)} \approx 0.03$, which is rather

high for oxides[3]. We also present first measurements of $Eu_{1-x}Sr_xCoO_3$. Here, charge-carrier doping should act differently because of the stabilized low-spin state.

[1] Baier et al., PRB **72**, 155116 (2005)
[2] Kriener et al.,PRB **69**, 094417 (2004)
[3] Berggold et al.,PRB **71**, 014443 (2005)

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Quantum phase transitions in $Nb_{1-y}Fe_{2+y}$ — •Manuel Brando, Dennis Moroni-Klementowicz, Carsten Albrecht, William Duncan, and F. Malte Grosche — Dept. of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK

The C14 Laves phase $NbFe_2$ is a rare example of low temperature spin density wave order (SDW, $T_N \simeq 10$ K) among the d-metal compounds. Magnetic ordering, which is inferred from magnetic, thermodynamic and magnetoresistive signatures, as well as historic NMR and μSR data, emerges out of a nearly ferromagnetic state with a Stoner enhancement factor of about 150, and is easily suppressed by surprisingly low critical fields $\mu_0 H_c \simeq 0.2 - 0.6$ T.

The low temperature state of $NbFe_2$ can be tuned by slightly modifying the stoichiometry within the narrow Nb-Fe homogeneity range. To the Nb-rich side, a quantum critical point is approached for $y \simeq 0.008$, characterised by non-Fermi liquid temperature dependences of heat capacity and resistivity. On the Fe-rich side, however, the SDW state observed in stoichiometric $NbFe_2$ appears to transform continuously into ferromagnetic ordering for $y > 0.01$.

We present low temperature magnetic, thermodynamic and transport measurements at ambient and high hydrostatic pressure, taken on samples across the homogeneity range, in order to elucidate the unusual magnetic phase diagram of $NbFe_2$. The findings are discussed within the working hypothesis that stoichiometric $NbFe_2$ forms low-$\mathbf{Q}$, long wavelength magnetic order, which transforms continuously towards ferromagnetism ($\mathbf{Q} = 0$) on increasing Fe content.