TT 16.67 Sa 11:00 Poster TU C

Itinerant electron metamagnetism and weak ferromagnetism in $LaCo_9Si_4$ and YCo_9Si_4 — •H. Michor[1], S. Özcan[1], M. El-Hagary[1], E. Bauer[1], M. Reissner[1], G. Hilscher[1], S. Khmelevskyi[2], P. Mohn[2], P. Rogl[3], and H. Rosner[4] — [1]Institut für Festkörperphysik, T.U. Wien, A-1040 Wien, Austria — [2]Center for Computational Materials Science, T.U. Wien, Austria — [3]Institut für Physikalische Chemie, Universität Wien, Austria — [4]Max-Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany

$LaCo_9Si_4$ is a strongly exchange enhanced Pauli paramagnet with an instability towards weak ferromagnetism, i.e. exhibits itinerant electron metamagnetism at about 3.5 T for $H||c$ and 6 T for $H\perp c$, which is the lowest value ever found for rare earth intermetallic compounds [1]. Despite of the smaller unit cell volume isostructural and isoelectronic YCo_9Si_4 exhibits a weak itinerant ferromagnetic ground state ($T_C \simeq 25\,\mathrm{K}$) already in zero-field. The ground state properties of La- and YCo_9Si_4 are discussed on basis of magnetisation, specific heat, and resistivity measurements and via ab-initio electronic structure calculations. The band structure calculations result in a ferromagnetic groundstate for both compounds with moments substantialy larger than the experimentally observed moments. The origin of these discrepancies is briefly discussed. [1] H. Michor et al., Phys.Rev. B **69** (2004) 081404(R).

TT 16.68 Sa 11:00 Poster TU C

Magnetic Ordering in Trigonal Chain Compounds — •Christian Laschinger[1], Udo Schwingenschlögl[1], Volker Eyert[1], Thilo Kopp[1], Raymond Frésard[2], and Ulrich Eckern[1] — [1]University of Augsburg — [2]Institut des Sciences de la Matière et du Rayonnement, Caen, France

We investigate the microscopic origin of the ferromagnetic and antiferromagnetic spin exchange couplings in the quasi-one-dimensional cobalt compounds Ca_3ABO_6 with A = Fe, Co and B = Co, Rh. From electronic structure calculations we find A 3d low spin and high spin states alternating along the characteristic chains. In addition strong d-p hybridisation leads to the formation of extended localized magnetic moments centered at the high spin sites. Antiferromagnetic coupling along the chains is induced by a strong metal-metal overlap via the $d_{3z^2-r^2}$ orbitals of the low spin sites. It competes with ferromagnetic exchange, which originates in a cyclic exchange through the ligand atoms.

TT 16.69 Sa 11:00 Poster TU C

Dimerization pattern or two-dimensional spin systems with spin phonon coupling in the adiabatic limit — •Carsten Aits[1], Ute Löw[1], and Andreas Klümper[2] — [1]Universität zu Köln, Institut für Theoretische Physik, Zülpicher Str.77, D-50937 Köln — [2]Bergische Universität Wuppertal, Theoretische Physik, D-42097 Wuppertal

Little is known about the ground state phase diagram of two-dimensional spin systems with spin phonon coupling. In the adiabatic limit, however, they correspond to spin models with inhomogeneous couplings. In contrast to the one-dimensional case, where the dimerization pattern is unique, it is not clear how the two-dimensional lattice responds to a non-vanishing spin phonon coupling. As far as the S=1/2 Heisenberg model is concerned, different choices of inhomogenous patterns of couplings lead to rather different ground state properties with magnetic energy gain that may or may not compete with the energy loss of the phonon system.

We apply a loop algorithm in continuous Trotter time to clarify which distortion pattern is energetically favored. Our approach is twofold. First, we extrapolate the ground state energies and magnetizations for various patterns of alternating couplings and analyze whether a transition to a gapped state appears. Second, we consider an expansion of the free energy of the distorted models at the point of vanishing distortion. In the adiabatic limit, this corresponds to an analysis of spin layers coupled to three dimensional phonons at finite temperatures. We determine the coefficients of the leading order from the (Euclidean) dynamical dimer correlation functions, which are directly accessible within our method.

TT 16.70 Sa 11:00 Poster TU C

Incommensurate spin dynamics in underdoped cuprate perovskites — •Alexei Sherman[1] and Michael Schreiber[2] — [1]Institute of Physics, University of Tartu, Estonia — [2]Institut für Physik, Technische Universität Chemnitz

The incommensurate magnetic response observed in normal-state cuprate perovskites is interpreted based on the memory function formalism and the t-J model of Cu-O planes. In agreement with experiment the calculated dispersion of maxima in the susceptibility has the shape of two parabolas with upward and downward branches which converge at the antiferromagnetic wave vector. The maxima are located at the momenta $(\frac{1}{2}, \frac{1}{2}\pm\delta)$, $(\frac{1}{2}\pm\delta, \frac{1}{2})$ and at $(\frac{1}{2}\pm\delta, \frac{1}{2}\pm\delta)$, $(\frac{1}{2}\pm\delta, \frac{1}{2}\mp\delta)$ in the lower and upper parabolas, respectively. The upper parabola reflects the dispersion of magnetic excitations of the localized Cu spins, while the lower parabola arises due to a dip in the spin-excitation damping at the antiferromagnetic wave vector. For moderate doping this dip stems from the weakness of the interaction between the spin excitations and holes near the hot spots. The frequency dependence of the susceptibility is shown to depend strongly on the hole bandwidth and damping and varies from the shape observed in $YBa_2Cu_3O_{7-y}$ to that inherent in $La_{2-x}Sr_xCuO_4$.

TT 16.71 Sa 11:00 Poster TU C

Structural properties of $RETiO_3$ and $Y_{1-x}Ca_xTiO_3$ — •A. Komarek[1], H. Roth[1], T. Lorenz[1], W.D. Stein[1], M. Cwik[1], F. Bourée[2], A. Freimuth[1], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin

We have studied the crystal structure of the $RETiO_3$ by different diffraction techniques as function of temperature. In all compounds we find significant distortions of the TiO_6-octahedra which lead to a lifting of the t_{2g}-orbital degeneracy. A comparison with literature data on isostructural compounds with a $3d^0$ or a $4d^0$-configuration shows that such distortions not necessarily are caused by orbital physics. In the $RETiO_3$-series, however, the temperature dependence clearly points to a direct coupling. The octahedron distortions depend more sensitively on temperature than the tilt and rotation angles; and, in particular, we find strong anomalies at the Néel-temperatures in all antiferromagnetic $RETiO_3$ compounds.

Neutron diffraction on a sample of $Y_{0.62}Ca_{0.38}TiO_3$ yields strong evidence for charge ordering, which may be the key element to understand, why Ca-doped $YTiO_3$ stays non-metallic till rather high doping.

TT 16.72 Sa 11:00 Poster TU C

Orbital excitations in transition-metal compounds — •R. Rückamp[1], A. Gössling[1], M. Grüninger[1], H. Roth[1], A. Freimuth[1], L. Jongen[2], A. Möller[2], G. Meyer[2], T.T.M. Palstra[3], A. Nugroho[3], and S.-W. Cheong[4] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Anorganische Chemie, Universität zu Köln — [3]Materials Science Centre, University of Groningen — [4]Department of Physics & Astronomy, Rutgers University, New Jersey

In recent years orbital physics has attracted much interest since novel phenomena - such as an orbital liquid state or new elementary excitations in an orbitally ordered state - have been predicted. In order to observe these phenomena, one has to look for a system in which the orbital (electron-electron) coupling dominates over the coupling to the lattice (Jahn-Teller effect). We have studied orbital excitations in the optical conductivity spectra of several transition-metal compounds such as $RTiO_3$, RVO_3, TiOX or Y_2BaNiO_5 by measuring both transmittance and reflectance of single crystals. The energies of the orbital (d-d) transitions are compared with the results of a point-charge model including the hybridisation with the ligand ions. We find good agreement between experiment and theory, which suggests that the coupling to the lattice is dominant in the studied compounds.

TT 16.73 Sa 11:00 Poster TU C

Structural properties of $Ca_{2-x}Sr_xRuO_4$ — •O. Schumann[1], P. Steffens[1], R. Müller[1], G. Andre[2], P.G. Radaelli[3], P. Adelmann[4], S. Nakatsuji[5], Y. Maeno[5], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Laboratoire Léon Brillouin — [3]ISIS Facility, Rutherford Appleton Laboratory — [4]Forschungszentrum Karlsruhe, IFP — [5]Department of Physics, Kyoto University

We present our x-ray- and neutron diffraction work on $Ca_{2-x}Sr_xRuO_4$ which shows an astonishing rich phase diagram, even though the substitution of Sr^{2+} by Ca^{2+} is an isovalent one [1]. Pure Sr_2RuO_4 (x=2) exhibits no structural distortions. Upon Ca-doping a rotation of the RuO_6-octahedron sets in. This phase transition is strongly discontinuous, although a continuous one is allowed by symmetry. At rather higher Ca-content (x∼0.2) a metamagnetic transition is observed. The temperature and magnetic field dependence of small structural changes are an indication of an electron transfer between in- and out-of-plane t_{2g}-orbitals. This transfer is driven by a van-Hove singularity in one of the concerned bands [2]. At even higher Ca-content the rotational distortion changes its

stacking sequence. While for x>0.2 the octahedrons in neighboring layers rotate out of phase, for x<0.2 the rotation between neighboring layers is in-phase. This rather subtle change is in coincidence with a change of the ground state properties of the samples (metallic vs. af insulating).
[1] O.Friedt *et al.*, Phys. Rev. B **63** 174432 (2001)
[2] M.Kriener *et al.*, condmat/0408015

TT 16.74 Sa 11:00 Poster TU C

Magnetic Field Dependence of Thermodynamic Properties of $(Ca,Sr)_2RuO_4$ — •J. Baier[1], T. Zabel[1], M. Kriener[1], P. Steffens[1], O. Schumann[1], O. Heyer[1], T. Lorenz[1], A. Freimuth[1], O. Friedt[1], M. Braden[1], A. Revcolevschi[2], S. Nakatsuji[3], and Y. Maeno[3] — [1]II.Physikalisches Institut, Universität zu Köln, Germany — [2]Lab. de Physico-Chimie de l'État Solide, Université Paris-Sud, France — [3]Dep. of Physics, Kyoto University, Japan

We present a study of thermal expansion α and specific heat c_P of $Ca_{2-x}Sr_xRuO_4$ in magnetic fields. This series with the spin-triplet superconductor Sr_2RuO_4 and the antiferromagnetic Mott-insulator Ca_2RuO_4 as end members presents a rich spectrum of structural distortions accompanied by drastic changes of the magnetic and electronic properties [1]. We focus on $0.2 \leq x \leq 0.5$ where the compound is still metallic but close to localization. We find an anisotropic anomalous thermal expansion. The anomaly is suppressed by a magnetic field [2]. Below $T \simeq 20\,K$, α, c_P and the magnetization show an anisotropic field dependence. The $x = 0.2$ sample shows a metamagnetic transition (MMT) accompanied by a large magnetostriction. Furthermore, c_P/T shows a non-monotonic field dependence with a maximum at the MMT. For $x = 0.5$, c_p/T reaches an unusually large value in zero field and 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] Friedt *et al.*, Phys.Rev.B **63** (2001)
[2] Kriener *et al.*, cond-mat 0408015, submitted to Phys. Rev. Lett.
Supported by the DFG through SFB 608

TT 16.75 Sa 11:00 Poster TU C

Low temperature mixed spin state of Co^{3+} in $LaCoO_3$ evidenced from local lattice distortions — •V. Gnezdilov[1], P. Lemmens[2,3], Yu.G. Pashkevich[4], K.-Y. Choi[5], S. Shiry aev[6], G. Bychkov[6], and S. Barilo[6] — [1]B.I. Verkin Inst. for Low Temp. Physics NASU, 61164 Kharkov, Ukraine — [2]Inst. for Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany — [3]MPI-FKF, D-70569 Stuttgart, Germany — [4]A.A. Galkin Donetsk Phystech NASU, 83114 Donetsk, Ukraine — [5]Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — [6]Inst. of Physics of Solids & Semiconductors, Academy of Sciences, 220072 Minsk, Belarus

Single- and multi-phonon excitations of the single crystalline $LaCoO_3$ were studied using Raman spectroscopy in the temperature region of 5 K - 300 K. First-order Raman spectra show a larger number of phonon modes than allowed for the rhombohedral (D^6_{3d}) structure. Additional phonon modes are interpreted in terms of activated modes due to local lattice distortions arising from the Jahn-Teller (JT) activity of the intermediate-spin (IS) state of Co^{3+} ions. The temperature dependence of the breathing - and stretching-type phonon modes on cooling suggests the presence of Co^{3+} ions in the intermediate spin state, even at lowest temperatures. The anomalous temperature dependence of the second-order phonon excitations spectra is in accordance with the Franck-Condon mechanism that is characteristic for a JT orbital order.

TT 16.76 Sa 11:00 Poster TU C

Co^{3+} spin state transition detected by phonon Raman scattering in $GdBaCo_2O_{5.5}$ — •Yu.G. Pashkevich[1], V.P. Gnezdilov[2], P. Lemmens[3,4], B. Keimer[4], C. Ambrosch-D raxl[5], K.V. Lamonova[1], A.A. Gusev[1], K.-Y. Choi[6], S.N. Barilo[7], S.-V. Shiryaev[7], and G.-L. Bychkov[7] — [1]A.A. Galkin Donetsk Phystech NASU, 83114 Donetsk, Ukraine — [2]B.I. Verkin Inst. for Low Temp. Physics NASU, 61164 Kharkov, Ukraine — [3]Inst. for Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany — [4]MPI-FKF, D-70569 Stuttgart, Germany — [5]Inst. für Theoretische Physik, Universität Graz, A-8010 Graz, Austria — [6]Inst. for Materials Research, Tohoku University, Sendai 980-8577, Japan — [7]Inst. of Physics of Solids & Semiconductors, Academy of Sciences, 220072 Minsk, Belarus

The change of the spin state of Co^{3+} as function of temperature or pressure is an intriguing feature of cobalt-based perovskite compounds. In the layered cobaltites $RBaCo_2O_5O_{5.5}$ this problem is rather complicated due to the octahedral and opened square pyramidal coordinations of Co with oxygen. Raman spectroscopy can provide information about subtle changes in spin state through detecting changes of the phonon spectra, which are sensitive to the O-Co-O bonding length and angles. Raman spectra of single crystal $GdBaCo_2O_5O_{5.5}$ were measured in the temperature range 5 - 400 K and remarkable changes of frequencies and intensities were observed. Frequencies and eigenvectors of Raman active phonon modes have been defined using frozen phonon ab initio band structure calculations and structural data at 300 K in Pmmm setting.

TT 16.77 Sa 11:00 Poster TU C

Finite Temperature Properties of the 2D Kondo-Necklace — •Wolfram Brenig — Institute for Theoretical Physics, Technical University of Braunschweig, Germany

We analyze several thermodynamic properties of the two-dimensional SU(2) Kondo-necklace. Using a quantum Monte-Carlo approach based on the stochastic series expansion method we provide results for the staggered structure factor as well as the uniform and staggered susceptibilities as a function of the temperature and 'Kondo'-exchange in the vicinity of the quantum critical point, which separates long-range antiferromagnetic order from dimerization in this system. We study the local susceptibility at criticality and find evidence for a power-law temperature dependence. Finally we investigate the crossover from classical to renormalized classical behavior via the quantum critical regime. Work supported in part by the DFG through SPP 1073.

TT 16.78 Sa 11:00 Poster TU C

Orbital ordering in manganites in the band approach. — •Dmitri Efremov[1] and Daniil Khomskii[2] — [1]TU Dresden, 01062 Dresden — [2]University of Cologne, 50937 Cologne

We consider the orbital ordering in $LaMnO_3$ and similar systems, proceeding from the band picture. For the realistic magnetic structure of A-type there exist the nesting between two e_g-bands and the nesting inside the bands. We show that the interband nesting is more effective. It results in an orbital ordering – orbital density wave (ODW), the type of which coincides with those existing in $LaMnO_3$.

TT 16.79 Sa 11:00 Poster TU C

Single hole dynamics across magnetic order-disorder quantum phase transitions. — •Christian Brünger and Fakher Assaad — Universität Würzburg

We consider a bi-layer Heisenberg model with interplanar (intraplanar) exchange $J_\perp$ (J). It is known that as a function of $J_\perp/J$ the model shows an order-disorder quantum phase transition. Our aim is to understand the behavior of the single particle spectral function of a doped hole in this magnetic background. In particular, the question of the vanishing of the quasiparticle weight in the vicinity of the quantum phase transition will be addressed. Our calculations are done within a self-consistent Born approximation as well as with the quantum Monte Carlo loop algorithm.

TT 16.80 Sa 11:00 Poster TU C

The Kimball-Overhauser approach to the pair density of the 3D electron gas and Friedel-like phase-shift sum rules — •Paul Ziesche — Max-Planck-Insitut fuer Physik komplexer Systeme, D-01187 Dresden

Kimball-Overhauser geminals follow from a 2-body Schroedinger equation with an appropriately screened Coulomb repulsion. They parametrize the pair density together with geminal occupancies, which follow from the non-idempotent momentum distribution [1]. The neutrality sum rule for the pair density leads to sum rules for the geminal phase shifts, which resemble the Friedel sum rule of solid-state physics [2]. Friedel-like oscillations originate from the singularities of the geminal weight [3]. [1] P. Gori-Giorgi and P. Ziesche, Phys. Rev. B 66, 235116 (2002) [2] P. Ziesche, Phys. Rev. B 67, 233102 (2003) [3] P. Ziesche, phys. stat. sol. (b), in press.

TT 16.81 Sa 11:00 Poster TU C

Quasiparticle bands of the ionic hubbard model — •Torben Jabben and Norbert Grewe — Institut für Festkörperphysik, Tu-Darmstadt,D-64289 Darmstadt

The ionic Hubbard model on a simple cubic lattice is investigated using analytical approximations and Wilson's renormalization group for the charge excitation spectrum near the Mott insulating regime. The corresponding partial spectral weights and local densities of states show