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A new betaine complex of Cu(II) ($S = 1/2$), with the general formula 2b*3$CuCl_2$*2H_2O with b = betaine ($C_5H_{11}NO_2$), has been synthesized and characterized magnetically. The structure of this metal-organic compound consists of centrosymmetric trimer units in which the neighboring Cu(II) atoms are bridged by the carboxylate groups of two betaine molecules. All Cu(II) ions show a nearly planar quadratic environment. In the ab-plane, a two-dimensional network of hydrogen bonds connects each trimer with four other trimers in a nearly quadratic arrangement. The obtained magnetic properties of Cu-betaine complex can be satisfactorily explained by using a magnetic model of coupled spin $S = 1/2$ trimers sitting on a quadratic lattice with an intra-trimer antiferromagnetic (AF) Cu-Cu coupling of J/k_B = 14 K and weak inter-trimer AF interaction J'/k_B= 4 K.

TT 32.28 Thu 14:00 Poster B

An effective dimer-monomer model for the distorted diamond chain azurite ($Cu_3(CO_3)_2(OH)_2$) — •Sebastian Köhler[1], Bernd Wolf[1], Andreas Brühl[1], Mariano de Souza[1], Katarina Remović-Langer[1], Yeekin Tsui[1], Ulrich Tutsch[1], Jürgen Schreuer[2], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, D-60438 Frankfurt(M) — [2]Institut für Mineralogie, Ruhr-Universität Bochum, 44780 Universitätsstraße 150

The S=1/2 spins in the natural mineral azurite ($Cu_3(CO_3)_2(OH)_2$) are connected to one-dimensional structures called distorted diamond chains. Given that all three exchange constants are antiferromagnetic, the distorted diamond chain is a simple realization of a one-dimensional frustrated spin system. The theoretically examined phase diagram at $T = 0$ shows a ferrimagnetic, a dimerized and a spin-fluid phase. We present measurements of the specific heat as a function of temperature and magnetic field together with magnetic susceptibility data under hydrostatic pressure, which can be well interpreted using a simple model, where two of three spins in Azurite are connected to dimers in the singlet state ($J_{intra-dimer} \approx 50$ K), while the remaining monomer spins effectively form uniform, linear spin chains ($J_{eff} = 7$ K). Our experimental data support the description of Azurite for moderate magnetic fields in terms of the dimer-monomer model. In addition, the pressure dependence of the susceptibility directly indicates the large spin-phonon interaction in this low-dimensinal spin system.

TT 32.29 Thu 14:00 Poster B

Phase diagram close to a conductance plateau transition in a quantum wire — •Matthias Sitte[1], Julia S. Meyer[2], Achim Rosch[1], and Markus Garst[1] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln — [2]Department of Physics, The Ohio State University, Ohio 43210, USA

We consider a quantum wire of spin-polarized (spinless) electrons close to the quantum phase transition where a second sub-band becomes activated as a function of gate voltage resulting in a jump of the zero temperature conductance. The filled first sub-band is treated as a Luttinger liquid, and it exchanges pairs of electrons with the second sub-band. It was shown in Ref. [1] that the conductance plateau transition is preempted by the formation of an inter-band pairing state. In the limit of infinitely strong inter-band density-density coupling, the latter transition is of Ising type. We perform a perturbative analysis around this strong coupling limit and determine the phase diagram. We find that the critical Ising mode induces superconducting fluctuations in the Luttinger liquid of the filled band, that are reflected in a logarithmically strong attractive interaction and a corresponding reduction of its plasmon velocity. We discuss possible consequences of this strong renormalization like a fluctuation-induced first order transition to a phase separated state preempting Ising criticality.

[1] J. S. Meyer, K. A. Matveev, and A. I. Larkin, Phys. Rev. Lett. **98**, 126404 (2007).

TT 32.30 Thu 14:00 Poster B

Electric and magnetic Properties of the Kagomé Systems $YBaCo_4O_{7+\delta}$ and $YBaCo_3MO_7$ (M=Fe,Al) — •Nils Hollmann[1], Martin Valldor[1], Zhiwei Hu[1], Antoine Maignan[2], Joachim Hemberger[1], Arata Tanaka[3], Liu Hao Tjeng[1], Thomas Lorenz[1], and John Mydosh[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Labaratoire CRISMAT, Caen — [3]Department of Quantum Matter, Hiroshima University

$YBaCo_4O_{7+\delta}$, $YBaCo_3FeO_7$ and $YBaCo_3AlO_7$ are closely related systems with cobalt ions in kagomé layers. In these kagomé layers, the triangular arrangement of the cobalt ions gives rise to a high degree of magnetic frustration. $YBaCo_4O_7$ reversibly changes the oxygen content depending on temperature and oxygen pressure. We present a study of magnetization, electrical transport and X-ray absorption of these materials. The systems are insulators and the electrical resistivity shows an anisotropy. The temperature dependence of the magnetization shows signs of strong frustration and spin-glass-like behaviour. This is studied with both DC and AC magnetization measurements. With the help of polarization dependent X-ray absorption, we deduce the valency and the orbital occupation of the cobalt ions. The valencies found can be used to prove the oxygen stochiometry.

TT 32.31 Thu 14:00 Poster B

Preparation and Characterization of $BaCoO_2$ and Sr-doped $EuCoO_3$ — •Marco Reuther, Kerstin Dönecke, John Mydosh, Thomas Lorenz, and Martin Valldor — II. Physikalisches Institut, Universität zu Köln, Germany

We have prepared polycrystals of $BaCoO_2$ and (Eu,Sr)CoO_3. $BaCoO_2$ is an air sensitive material whose physical properties are hardly explored. The structure of $BaCoO_2$ is trigonal with Co^{2+} ions in tetrahedral coordination [1]. Our magnetization measurements suggest a canted antiferromagnetic order with $T_N \approx 370$ K.

$EuCoO_3$ is insulating with Co^{3+} ions in the nonmagnetic low spin state up to about 400K [2]. Already small amounts of Sr induce a ferromagnetic order with $T_C \approx 160$ K due to the presence of Co^{4+} ions. Because of Co^{3+} remains in the low spin state we can observe the pure magnetic moment of Co^{4+} by Sr-doping. The electrical resistivity decreases with Sr but remains insulating.

[1] U. Spitsbergen et al., Acta Cryst. **13**, 197 (1960).
[2] J. Baier et al., PRB **71**, 014443 (2005)

TT 32.32 Thu 14:00 Poster B

Resonant diffraction from charge and spin ordering in $La_{1.5}Sr_{0.5}CoO_4$ — •Christian Schüssler-Langeheine[1], Matthias Cwik[1], Chun Fu Chang[1], Hsueh-Hung Wu[1,2], Marcel Buchholz[1], Zhiwei Hu[1], Thomas Willers[1], Enrico Schierle[3], Ralf Feyerherm[3], Detlef Schmitz[3], Mohammed Benomar[1], Markus Braden[1], and L. Hao Tjeng[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]NSRRC, Taiwan — [3]HMI c/o BESSY

Cobalt oxides are particularly interesting materials because of the different possible spin states of the Co^{3+} ion, which can occur in the low-spin, intermediate-spin or high-spin state. This adds another degree of freedom to charge, spin and orbital occupation of other transition metal ions. For $La_{1.5}Sr_{0.5}CoO_4$ commensurate charge and spin order was reported with a very unusual suppression of static magnetic ordering.

We studied this system using resonant diffraction at the Co K and $L_{2,3}$ resonance in order to obtain information about both charge and spin ordering. We find a pronounced pattern of incommensurate charge ordering not observed by neutron diffraction. From the magnetic scattering data we are able to determine the ordered orbital momentum and find indications for a more complex magnetic ordering than discussed so far.

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TT 32.33 Thu 14:00 Poster B

Orbital degree of freedom in $La_{7/8}Sr_{1/8}MnO_3$: Temperature-dependent rearrangement of orbital states — •Michael Merz[1,2], Christian Pinta[1,3], Sebastian Prinz[2], Peter Nagel[1], Andrei Samartsev[3,1], Stefan Schuppler[1], Pascal Reutler[4], and Bernd Büchner[4] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe — [2]Institut für Kristallographie, Jägerstraße 17-19, RWTH Aachen, 52066 Aachen — [3]Fakultät für Physik, Universität Karlsruhe, 76128 Karlsruhe — [4]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01171 Dresden

One of the most unusual phases found among charge and orbital ordered systems appears for $La_{7/8}Sr_{1/8}MnO_3$ below 150 K: a *ferromagnetic insulating* (FMI) state. With O1s near-edge x-ray absorption fine structure and single-crystal x-ray diffraction we studied the temperature-dependent evolution of this FMI phase. Our results give the following picture: Above $T_{JT} \approx 275$ K, strong fluctuations prevent the orbitals from ordering. Upon cooling below T_{JT}, a first-order phase transition to a cooperative Jahn-Teller distorted phase takes

place. When decreasing the temperature below 180 K, more and more O and Mn^{3+} atoms arrange their orbitals to the orbital polaron state, and this process leads to a continuous phase transition towards the FMI state. Once established, the local orbital polarons remain stable objects upon further cooling and may well form the orbital polaron lattice below T_{CO} as suggested by resonant x-ray scattering [1].

[1] J. Geck et al. Phys. Rev. Lett. 95, 236401 (2005).

TT 32.34 Thu 14:00 Poster B

Surface topographic and spectroscopic studies of charge ordering $La_{0.5}Sr_{1.5}MnO_4$ using Scanning Tunneling Microscopy — •Paul Sass[1], Grzegorz Urbanik[1,2], Christian Hess[1], Torben Hänke[1], Bernd Büchner[1], Antoni Ciszewski[2], Pascal Reutler[3], and Alexandre Revcolevschi[3] — [1]Institute for Solid State Research, IFW-Dresden, 01171 Dresden, Germany — [2]Institute of Experimental Physics, University of Wroclaw, 50-204 Wroclaw, Poland — [3]Laboratoire de Physico-Chimie de l'Etat Solide, Université Paris Sud, Bâtiment 414, 91405 Orsay, France

We have studied the compound $La_{0.5}Sr_{1.5}MnO_4$ which can be considered as a textbook example of charge and orbital ordering by means of Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). We were able to cleave the material in-situ under Ultra High Vacuum conditions prior to the STM/STS studies. Topographic scans routinely reveal atomically resolved surfaces both above and below the charge ordering temperature $T_{CO} \approx 225$ K (down to $T \approx 205$ K). The step height analysis suggests cleaving between the (Sr,La)O-layers. We have studied the temperature dependence of the electronic structure both for $T > T_{CO}$ and $T < T_{CO}$. The STS clearly reveals finite DOS at the Fermi level for $T > T_{CO}$ and the opening of a gap $\Delta \approx 0.5$ eV just below T_{CO}. In the topographic studies we find nanometer scale modulations with various periodicity. We discuss these modulations in view of the inherent charge and orbital ordered state of this material. We compare our results with STS studies on other transition metal oxides exhibiting inhomogeneous charge distributions.

TT 32.35 Thu 14:00 Poster B

Magnetic and electrical properties of EuC_{2+x} — •Oliver Heyer[1], Derk Wandner[2], Nils Hollmann[1], Uwe Ruschewitz[2], Thomas Lorenz[1], and John A. Mydosh[1] — [1]II. Physikalisches Institut, Universiät zu Köln, D-50937 Köln — [2]Institut für Anorganische Chemie, Universität zu Köln, D-50939 Köln

We present measurements of the magnetization M, specific heat c_p and resistance ρ of EuC_{2+x} (x=0, 0.1) compounds. The magnetization data show a ferromagnetic ordering at $T_C \simeq 14$K with a saturation moment of $\simeq 7\frac{\mu_B}{FE}$. This suggests an oxidation state of Eu^{2+}. In the paramagnetic phase all compounds are semiconductors with small bandgaps ($10 - 20$meV). A very interesting feature is that the onset of the ferromagnetic order decreases the resistance ρ over a couple of orders of magnitude indicating a metal-insulator transition (MIT). Moreover, an applied magnetic field shifts the MIT temperature to higher values, resulting in a colossal magnetoresistance with changes in the resistivity up to 6 orders of magnitude. This behaviour resembles the colossal magnetorsistance of the better known system of Eu-rich EuO. Furthermore we carried out magnetization and specific heat measurements of YbC_2. The data identify this compound as a diamagnet without structural phase transitions. On this account YbC_2 is used as a non magnetic reference system.

TT 32.36 Thu 14:00 Poster B

Electronic properties of transition metal impurities in MgO thin films — •Rainald Gierth[1], Tim Haupricht[1], Chun-Fu Chang[1], Zhiwei Hu[1], Thomas Koethe[1], H. H. Hsieh[2], H.-J. Lin[3], C. T. Chen[3], and Liu Hao Tjeng[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

We have studied the electronic structure of transition metal impurities in MgO. These systems can serve as model systems for various (usually more complicated) d^n systems in octahedral symmetry. Going from bulk crystals to impurity systems the core level and valence band photoemission spectra can change significantly e.g. due to the influence of non-local screening effects. We present our core level and valence band photoemission data of Ni and Mn impurities in MgO thin films epitaxially grown on Ag(001) *in-situ*, taken at different photon energies. Changes in the shape as well as in the width of the spectra are observed. The experimental results are compared to various theoretical approaches.

TT 32.37 Thu 14:00 Poster B

Correlated band structure of $3d^2$ vanadates — •David Heilmann and Eva Pavarini — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

We study the correlated band structure and the momentum-resolved spectra for $3d^2$ vanadates, like $LaVO_3$ and YVO_3, using a combination of a first-principles technique and Dynamical Mean-Field Theory with a Monte Carlo impurity solver.

The self-energy for the effective $3d$ bands is calculated using Maximum-Entropy spectral analysis of the Monte Carlo results and a self-consistent procedure. We use this self-energy to calculate the full momentum-resolved spectrum and the correlated band structure, which we compare to available spectroscopy experimental results. We also discuss the effects of the lattice distortions and chemistry.

TT 32.38 Thu 14:00 Poster B

Quantum Monte Carlo Simulations in Continuous Time: An Application to the Hubbard Model — •Sebastian Fuchs and Thomas Pruschke — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We perform quantum Monte Carlo simulations of the Hubbard model using the Dynamical Cluster Approximation (DCA) [1]. Hereby the complexity of the full lattice problem is reduced by mapping it to a finite size cluster self-consistently embedded in a mean-field. The resulting cluster problem is solved by a Monte Carlo procedure using a weak coupling expansion in continuous imaginary time [2]. Compared to the traditional Hirsch-Fye algorithm simulations can be much more efficient and systematical errors due to a discretization of the imaginary time axis are avoided.

Our main focus is the investigation of the single-particle properties of the Hubbard model in the antiferromagnetic phase. Using analytic continuation of the Monte Carlo data the DCA permits us to calculate spectral functions with explicit k-dependence.

Our implementation of the algorithm is based on the libraries of the ALPS project [3]. ALPS is an open source effort providing libraries and simulation codes for strongly correlated quantum mechanical systems.

[1] Th. Maier *et. al.*, Rev. Mod. Phys. **77**, 1027 (2005)
[2] A. N. Rubstov *et. al.*, Phys. Rev. B **72**, 035122 (2005)
[3] `http://alps.comp-phys.org`

TT 32.39 Thu 14:00 Poster B

Mott transition in one dimension: Benchmarking dynamical cluster approaches — •Matthias Balzer[1], Werner Hanke[1], and Michael Potthoff[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]I. Institut für Theoretische Physik, Universität Hamburg

The variational cluster approach (VCA) is applied to the 1D Hubbard model at $T = 0$ using clusters (chains) of up to ten sites with full diagonalization and the Lanczos method as cluster solver. Within the framework of the self-energy-functional theory (SFT), different cluster reference systems with and without bath degrees of freedom, in different topologies and with different sets of variational parameters are considered. Static and one-particle dynamical quantities are calculated for half-filling as a function of U as well as for fixed U as a function of the chemical potential to study the interaction- and filling-dependent metal-insulator (Mott) transition. We compare the VCA results with exact results available from the Bethe ansatz, with essentially exact dynamical DMRG data, with (cellular) dynamical mean-field theory and full diagonalization of isolated Hubbard chains. Several issues are discussed including convergence of the results with cluster size, the ability of cluster approaches to access the critical regime of the Mott transition and efficiency in the optimization of correlated-site vs. bath-site parameters. We also study the role of bath sites for the description of excitation properties and as charge reservoirs for the description of filling dependencies. The VCA turns out to be a computationally cheap method which is competitive with established cluster approaches.

TT 32.40 Thu 14:00 Poster B

A new DCA scheme for calculating two-particle correlation functions of the 2D Hubbard model — •Stephan Hochkeppel, Fakher Assaad, and Werner Hanke — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Based on the Dynamical Cluster Approximation (DCA), we present a new approach to calculate two-particle Green's functions for Hubbard-