TT 16: Correlated Electrons: Low-dimensional Systems - Materials 1

Time: Tuesday 9:30–13:00 Location: HSZ 304

TT 16.1 Tue 9:30 HSZ 304

High field ESR study of the new low dimensional S=1/2 system: $Cu(NO_3)_2{\cdot}H_2O$ — •M. Yehia[1], E. Vavilova[1,2], V. Kataev[1], R. Klingeler[1], O. Volkova[3,4], E. Lapsheva[4], V. Shutov[4], O. Savelieva[4], A.N. Vasiliev[4], and B. Büchner[1] — [1]Institute for Solid State Physics, IFW Dresden, 01171 Dresden, Germany. — [2]Kazan Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia. — [3]Institute of Radiotechnics and Electronics, 125009 Moscow, Russia. — [4]Moscow State University, 119991 Moscow, Russia.

$Cu(NO_3)_2{\cdot}H_2O$ is a new low dimensional spin system based on transition metal nitrates. It contains two-dimensional $Cu^{2+}(S = 1/2)$ layers separated by water molecules. ESR, magnetic susceptibility, specific heat and NMR have been measured on single crystalline samples of $Cu(NO_3)_2{\cdot}H_2O$. Specific heat and magnetic susceptibility data imply a phase transition possibly of antiferromagnetic (AFM) nature at $T_N \sim 3.4$ K. However, no long range order is observed in the temperature dependence of ESR measurables. The temperature dependence of the electron spin dynamics has been investigated by NMR. Various spin gap excitations have been observed using high field ESR. We discuss these features by considering the ground state and magnetic excitations of the orthogonal spin-dimers network which is realized in the Cu-layers of this material.

TT 16.2 Tue 9:45 HSZ 304

Electron Spin Resonance in GdI_2H_x — •Georg Andreas Hilscher[1], Joachim Deisenhofer[1], Hans-Albrecht Krug von Nidda[1], Alois Loidl[1], Mikhail Ryazanov[2], Arndt Simon[2], and Reinhard K. Kremer[2] — [1]Experimentalphysik V, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany — [2]Max-Planck Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

The spin dynamics of hydrogen-doped GdI_2H_x ($0 \leq x \leq 1$) have been investigated by electron spin resonance (ESR) spectroscopy. With rising hydrogen concentration the lattice constants of the hexagonal layered structure change: a decreases and c increases [1]. Furthermore, the ferromagnetic Curie temperature T_C, which for pristine GdI_2 lies at approximately 290 K, decreases and the system exhibits a spin-glass-like state for $x > 0.33$. For higher H concentrations the system remains paramagnetic down to 4 K [1]. From the ESR intensity we can estimate the dominant exchange coupling constant within the Gd layers for $x < 0.33$ using the model for the spin susceptibility proposed by Eremin *et al.* [2].

[1] M. Ryazanov, A. Simon, R. K. Kremer, H. Mattausch, Sol. State Chem. **178**, 2339 (2005).

[2] I. Eremin, P. Thalmeier, P. Fulde, R. K. Kremer, K. Ahn, A. Simon, Phys. Rev. B **64**, 064425 (2001).

TT 16.3 Tue 10:00 HSZ 304

Magnetic field-induced ordering in a metal-organic spin-1/2 dimer system – a candidate for a Kosterlitz-Thouless transition — •U. Tutsch[1], B. Wolf[1], M. Lang[1], T. Kretz[2], H.-W. Lerner[2], M. Wagner[2], S. Wessel[3], T. Saha-Dasgupta[4], H. Jeschke[5], and R. Valenti[5] — [1]Phys. Inst., Goethe-Universität, SFB/TRR49, D-60438 Frankfurt (M), Germany — [2]Inst. f. Anorg. Chemie, Goethe-Universität, SFB/TRR49, D-60438 Frankfurt (M), Germany — [3]Inst. f. Theor. Phys. III, Universität Stuttgart, D-70550 Stuttgart, Germany — [4]S.N. Bose National Centre for Basic Sciences, Salt Lake City, Kolkata 700098, India — [5]Inst. f. Theor. Phys., Goethe-Universität, SFB/TRR49, D-60438 Frankfurt (M), Germany

We have investigated the spin-1/2 metal-organic dimer system $C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$ (TK91) by means of high-resolution susceptibility measurements at very low temperatures ($0.04\ \mathrm{K} \leq T \leq 0.5\ \mathrm{K}$) and magnetic fields up to $B = 7.5$ T. The spins, located on the Cu^{2+} ions, are coupled into dimers by a hydroquinone-derived linker, giving rise to an *intra*-dimer exchange interaction of $J_1/k_B \approx 10$ K. As suggested by *ab initio* calculations, the *inter*-dimer couplings J_i have a quasi-two-dimensional (quasi-2d) character with a very weak interlayer coupling. Quantum Monte Carlo simulations for 2d and various strongly anisotropic 3d coupling schemes are used to model our susceptiblity data yielding clear signatures of a B-induced ordering phenomenon. A very good agreement is obtained for the 2d scenario, making TK91 a good candidate for the very rare phenomenon of a magnetic Kosterlitz-Thouless transition.

TT 16.4 Tue 10:15 HSZ 304

Crystal water induced switching of magnetic active orbitals in $CuCl_2$ — •Miriam Schmitt[1], Oleg Janson[1], Marcus Schmidt[1], Stefan Hoffmann[1], Walter Schnelle[1], Stefan-Ludwig Drechsler[2], and Helge Rosner[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW Dresden, Germany

Low dimensional transition metal compounds show an intimate interplay between the crystal structure and their magnetism. Nevertheless, it is a widespread belief that crystal water has just a moderate, renormalizing influence on the magnetic properties due to a modification of interactomic distances. In contrast, the dehydration of $CuCl_2{\cdot}2H_2O$ to $CuCl_2$ leads to a dramatic change in magnetic behavior and ground state – driving a classical example of a 3D antiferromagnet (T_N=4.3 K) to a quasi 1D system with long range order below T∼23 K. Combining electronic structure calculations based on DFT, model calculations and thermodynamical measurements we reveal the microscopic origin of this surprising behavior. Regarding our calculations $CuCl_2$ can be well described as a frustrated J_1–J_2 Heisenberg chain with ferromagnetic exchange J_1 and $J_2/J_1 \sim$ -1.5 predicting a helical ground state. The hydration of $CuCl_2$ flips the magnetically active orbitals, resulting in a fundamental change of the coupling regime. As $CuCl_2$ consists edge-shared Cu-Cl_4 plaquettes with the magnetically active orbital in the chain plane, $CuCl_2{\cdot}2H_2O$ forms its magnetically active orbitals out of the former chain plane resulting in isolated plaquettes arranged back to back. This new arrangement strongly reduces the former in-chain interactions yielding an almost isotropic 3D coupling.

TT 16.5 Tue 10:30 HSZ 304

Magnetocaloric effect near a B induced quantum critical point in an S = 1/2 antiferromagnetic Heisenberg chain — •Deepshikha Jaiswal-Nagar[1], Georg Hofmann[1], Yeekin Tsui[1], Katarina Remović-Langer[1], Ulrich Tutsch[1], Bernd Wolf[1], Andrey Profofiev[1,2], Wolf Assmus[1], Andreas Honecker[3], and Michael Lang[1] — [1]Phys. Institut, Goethe-Universität, D-60438 Frankfurt(M), SFB/TR49, Germany — [2]Inst. f. Festkörperphys., TU Wien, 1040-Wien, Austria — [3]2 Inst. f. Theor. Physik, Georg-August-Universität at Göttingen, 37077, Göttimgen, Germany

The magnetocaloric effect (MCE), i.e., heating or cooling of a system under adiabatic conditions in response to an external magnetic field, is an important tool for exploring quantum critical points (QCP's), as it is expected to diverge at the QCP. The competition between different ground states at a QCP leads to an accumulation of entropy at the QCP at finite temperature and hence to a variety of interesting properties in thermodynamic quantities like the MCE. A one-dimensional spin S = 1/2 antiferromagnetic Heisenberg chain (AfHC) is quantum critical in magnetic fields up to the saturation field Bs, above which it undergoes a transition to a ferromagnetically polarized state. In this talk, we present MCE data on a metal-organic polymer system built from Cu2+ (S = 1/2) ions, which is shown to be a very good realization of an AfHC. We obtain field-induced temperature changes which are an order of magnitude larger than those of paramagnetic salts! Our data compare favorably with theoretical results based on exact diagonalization of finite systems.

TT 16.6 Tue 10:45 HSZ 304

Magnetic properties of a novel quasi-2D Cu(II)-trimer system — •Bernd Wolf[1], Katarina Removic-Langer[1], Eiken Haussühl[2], Leonore Wiehl[2], Francesca Sauli[3], Nils Hasselmann[3], Peter Kopietz[3], and Michael Lang[1] — [1]Physikalisches Institut, Universität Frankfurt, SFB/TR 49, D-60438 Frankfurt — [2]Institut für Geowissenschaften, Universität Frankfurt, D-60438 Frankfurt — [3]Institut für Theoretische Physik, Universität Frankfurt, SFB/TR 49, D-60438 Frankfurt

The rational design of low-dimensional quantum spin systems with novel exchange coupling topologies is of interest since it allows the testing of fundamental concepts in theoretical solid state physics. Up to now, only a few examples for 2D coupled-trimer systems are known. We have managed to synthesize a new magnetic Cu(II)-trimer system 2b*3$CuCl_2$*2H_2O (b = betaine), where the trimers form a quasi-2D

quantum spin system with an unusual intralayer exchange coupling topology, which in principle supports ring-exchange processes. We discuss the structural aspects together with magnetic susceptibility and magnetization data. In addition, a theoretical model, enabling us to describe the magnetic properties over a wide temperature and field range is presented. The low-energy description and effective parameters are obtained from numerical calculations based on four coupled trimers. The model calculations indicate that for certain ranges of the inter-trimer coupling constants, which might be experimentally accessible, the low-energy properties of 2b*3$CuCl_2$*2H_2O will be dominated by non-trivial four-spin exchange processes.

TT 16.7 Tue 11:00 HSZ 304

Electronic structure and exchange coupling of a frustrated S=1/2 pyrochlore $Hg_2Cu_2F_6S$ — •Deepa Kasinathan[1], Klaus Koepernik[2], and Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Spin systems with geometric frustration have a macroscopic number of degenerate low lying states. An interesting question to answer for such kind of systems is: "Which state is chosen as the ground state at low T?"Our talk will focus on the pyrochlore compound $Hg_2Cu_2F_6S$ which exibits a perfectly cubic CuF_6 octahedral environment.[1] This is quite unusual for a Cu^{2+} ion which is normally in the 4+2 coordination. The lack of distortion for the CuF_6 octahedron leads to a 2-fold degenerate e_g band complex at the Fermi level. Since the system is insulating due to the presence of strong Coulomb repulsion, this 2-fold degeneracy is strongly disfavoured because it would lead to metallicity. Orbital or charge ordering can lift this degeneracy. Strong magnetic frustrations will also play a role in determining the ground state of this system due to the presence of 3D linkages of corner sharing Cu_4 tetrahedra. We will present results from density functional theory (DFT) calculations within the LDA and LDA+U methodology. We will discuss the role of total energies, hoppings and possible orbital ordering (visible in the spin density) in this compound.

[1]. S. Kawabata et al., J. Phys. Soc. Japan Vol 76, No.8, 084705 (2007).

15 min. break.

Invited Talk TT 16.8 Tue 11:30 HSZ 304

Two Dimensional Electron Gases at Oxide Interfaces — •Jochen Mannhart — Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Two-dimensional electron gases based on conventional semiconductors such as Si or GaAs have played a pivotal role in fundamental science and technology. The high mobilities achieved enabled the discovery of the integer and fractional quantum Hall effects and are exploited in high electron mobility transistors. Recent work has shown that 2-DEGs can also exist at oxide interfaces. These electron gases typically result from reconstruction of the complex electronic structure of the oxides, so that the electronic behavior of the interfaces may differ from the behavior of the bulk.

In the presentation I will provide an overview of our studies of the properties of these unusual electronic systems and explore whether electron gases at oxide interfaces have the potential to be used in nanoscale electronic devices.

TT 16.9 Tue 12:00 HSZ 304

The Two-Dimensional Electron Gas between $LaAlO_3$ and $SrTiO_3$: A Fascinating System for Electronic Devices — •Christoph Richter, Rainer Jany, Stefan Thiel, Christof Schneider, German Hammerl, and Jochen Mannhart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany

The conducting, two-dimensional electron gas that is formed at the interface between the band insulators $LaAlO_3$ and $SrTiO_3$ is characterized by remarkable fundamental properties and has therefore generated intense scientific interest. In the presentation we will demonstrate that this apparently fragile, ultrathin electronic system can be used to fabricate robust electronic devices.

We will report on field effect transistors that use the two- dimensional electron gas as drain source channel as well as on diodes with unique properties.

TT 16.10 Tue 12:15 HSZ 304

Profiling the interface electron gas of $LaAlO_3/SrTiO_3$ heterostructures by hard X-ray photoelectron spectroscopy — •G. Berner[1], M. Sing[1], K. Goss[1], A. Wetscherek[1], A. Müller[1], A. Ruff[1], S. Thiel[2], J. Mannhart[2], S.A. Pauli[3], C.W. Schneider[3], P.R. Willmott[3], and R. Claessen[1] — [1]Experimentelle Physik IV, Universität Würzburg — [2]Experimentelle Physik VI, Universität Augsburg — [3]Paul Scherrer Institut, CH-5232 Villingen, Switzerland

Oxide heterostructures are of special interest due to unexpected new physics occurring at the interface. One heavily discussed topic is the quasi-two-dimensional electron gas (2DEG), which emerges at the interface of the two band insulators $LaAlO_3/SrTiO_3$, if at least 4 unit cells of $LaAlO_3$ are grown on TiO_2-terminated $SrTiO_3$. Moreover, both a magnetic and a superconducting phase at low temperatures have been reported for the ground state of the 2DEG. We have studied this buried interface by angle dependent hard x-ray photoemission spectroscopy (HAXPES), which is a powerful tool to get insight in both change in chemical state and vertical distribution of the additional charge at the interface. The distinct angle-dependence of the intensity ratio of the Ti^{3+} 2p and Ti^{4+} 2p core lines indicates that the thickness of the 2DEG is much smaller than the HAXPES probing depth of 4 nm. It is observed that the carrier density varies between differently prepared heterostructures and increases with increasing numbers of $LaAlO_3$ overlayers. Our results point to electronic reconstruction in the overlayer as driving mechanism for the 2DEG formation and is supportive for the recently observed 2D superconductivity.

TT 16.11 Tue 12:30 HSZ 304

Resonant soft x-ray scattering studies of buried interfaces — •Jochen Geck[1,2], Hiroki Wadati[2], Enrico Schierle[3], P. Kommissinskiy[4], L. Alff[4], D.G. Hawthorn[5], T. Higuchi[6], Y. Hikita[6], H.Y. Hwang[6], S.-W. Huang[7], D.J. Huang[7], H.-J. Lin[7], L.H. Tjeng[8], H.-H. Wu[7,8], E. Weschke[3], C. Schüssler-Langeheine[8], and G.A. Sawatzky[2] — [1]IFW Dresden, Germany — [2]University of British Columbia, Canada — [3]Helmholtz-Zentrum Berlin, Germany — [4]University of Technology Darmstadt, Germany — [5]University of Waterloo, Canada — [6]University of Tokyo, Japan — [7]National Synchrotron Radiation Research Center, Taiwan — [8]University of Cologne, Germany

Resonant soft x-ray scattering (RSXS) is a unique experimental tool to access the electronic properties of buried interfaces in heterostructures that contain transition metal oxides. In this contribution, studies of $SrTiO_3/LaAlO_3$, $SrTiO_3/(La,Ca)MnO_3$ and $NdGaO_3/(La,Ca)MnO_3$ interfaces are presented. Specifically, RSXS was employed to examine the electronic reconstruction of Ti 3d and O 2p valence states at the interfaces of $SrTiO_3/LaAlO_3$ superlattices. Similarly, we used resonant soft x-ray reflectivity to investigate the electronic structure at the interfaces of $SrTiO_3/(La,Ca)MnO_3$ and $NdGaO_3/(La,Ca)MnO_3$ thin film systems.

TT 16.12 Tue 12:45 HSZ 304

Ab initio Quantum Monte Carlo study of interlayer binding in graphitic nanostructures — •Norbert Nemec and Richard Needs — Dept. of Physics, University of Cambridge, UK

The electronic structure of graphitic systems is studied using ab initio quantum Monte Carlo methods implemented in the CASINO code. The diffusion Monte Carlo method allows the exact handling the long-ranged correlations responsible for the London dispersion forces that dominate the interlayer binding. The finite size errors caused by the limited volume of the simulation cell are reduced by a careful extrapolation to infinite size giving a reliable theoretical prediction of the interlayer binding of graphite and related nanostructures.