

TT 33: Low-Dimensional Systems: Other Materials

Time: Tuesday 9:30–12:15

Location: H 3010

TT 33.1 Tue 9:30 H 3010

NMR on the Antiferromagnetic $S=1/2$ Heisenberg Spin Chain Sr_2CuO_3 under the Impact of Ni Impurities — ●YANNIC UTZ¹, FRANZISKA HAMMERATH¹, SATOSHI NISHIMOTO¹, STEFAN-LUDWIG DRECHSLER¹, NEELA SEKHAR BEESETTY², ROMUALD SAINT-MARTIN², ALEXANDRE REVCOLEVSCHI², CHRISTIAN HESS¹, BERND BÜCHNER¹, and HANS-JOACHIM GRAFE¹ — ¹IFW Dresden, Germany — ²SP2M-ICMMO UMR-CNRS, Université Paris-Sud, France

We present ⁶³Cu NMR measurements on single crystals of Sr_2CuO_3 doped with different amounts of nickel and compare them to numerical DMRG results. The parent compound contains copper-oxygen chains with $S=1/2$ on the copper site coupled by a large antiferromagnetic exchange coupling $J \approx 2000$ K and is known to be a good realization of the 1D Heisenberg model. The measurements show that replacing only a few of the $S=1/2$ Cu ions with $S=1$ Ni has a major impact on the magnetic properties of the spin chain system. An unusual line broadening in the low temperature NMR spectra reveals the existence of an impurity-induced local alternating magnetization (LAM), and exponentially decaying spin-lattice relaxation rates T_1^{-1} towards low temperatures indicate the opening of a spin gap similar to Ca-doped Sr_2CuO_3 [1]. While the T_1^{-1} measurements could be explained by pure chain segmentation, as expected for a $S=0$ impurity, the spectra can only be understood by taking the nickel.

[1] F. Hammerath et al., Phys. Rev. B 89, 184410 (2014).

TT 33.2 Tue 9:45 H 3010

Thermodynamic investigations of the quasi-2d triangular Heisenberg antiferromagnet $\text{Cs}_2\text{CuCl}_2\text{Br}_2$ — ●ULRICH TUTSCH, LARS POSTULKA, BERND WOLF, MICHAEL LANG, NATALIJA VAN WELL, FRANZ RITTER, CORNELIUS KRELLNER, and WOLF ASSMUS — Physikalisches Institut, Goethe-University Frankfurt (M), SFB/TR 49

The system $\text{Cs}_2\text{CuCl}_{4-x}\text{Br}_x$ ($0 \leq x \leq 4$) is a quasi-two-dimensional Heisenberg antiferromagnet with a triangular in-plane arrangement of the spin-spin couplings. The ratio J'/J of the corresponding coupling constants determines the degree of frustration in the system and has been found to be 0.34 ($x=0$) and 0.74 ($x=4$) [1] for the border compounds. One may ask whether for some intermediate Br concentration an even higher degree of frustration can be reached. Indeed, some indications have been reported by Ono *et al.* [1]. Here, we present specific heat C and susceptibility χ measurements below 1 K in magnetic fields B up to 13.5 T for the intermediate compound $\text{Cs}_2\text{CuCl}_2\text{Br}_2$, which, due to site-selective substitution, shows a well-ordered halide sublattice. Indications for an antiferromagnetic transition are observed around 90 mK for $B=0$. A small field of $B=0.14$ T is sufficient to fully suppress this anomaly. Taking into account the high saturation field of about 20 T, extrapolated from $\chi(T=\text{const}, B)$ scans at low temperatures, this small ordered region in the B - T plane clearly indicates a high degree of frustration in $\text{Cs}_2\text{CuCl}_2\text{Br}_2$.

[1] T. Ono *et al.*, J. Phys. Soc. Jpn. 74 (2005) Suppl. pp. 135-144.

TT 33.3 Tue 10:00 H 3010

Weakly coupled spin-dimer systems based on stable organic biradicals — ●BERND WOLF¹, LARS POSTULKA¹, ULRICH TUTSCH¹, MARTIN BAUMGARTEN², YULIA BORODINA² und MICHAEL LANG¹ — ¹Physics Institute, Goethe-University Frankfurt (M), SFB/TR 49, D-60438 Frankfurt (M), Germany — ²Max-Planck-Institute for Polymer Research, SFB/TR 49, D-55128 Mainz, Germany

We present low-temperature susceptibility data of newly synthesized $S=1/2$ spin-dimer systems consisting of stable organic biradicals, formed by bridging nitronyl-nitroxides (NN) and imono-nitroxides (IN) via tolane molecules. The choice of this bridging molecule ensures a moderately strong intra-dimer coupling constant J_{intra}/k_B around 9.0 K (NN) and 4.3 K (IN). In addition, a weak coupling between the spin dimers of the order of 1 K can be inferred from high-temperature susceptibility data. The crystal structure suggests a 2D arrangement of the dimer units. To determine potential field-induced ordered phases, highest-resolution AC-susceptibility measurements have been performed down to a temperature of $T=27$ mK and magnetic fields up to $B=10.5$ T. We observed for both materials double-peak structures in the susceptibility below the saturation field. For a detailed understanding, especially with regard to the dimensionality of the magne-

tic interactions and the nature of the field-induced magnetic order, we compare the experimental results with measurements on metal-organic coupled dimer compound $\text{C}_{36}\text{H}_{48}\text{Cu}_2\text{F}_6\text{N}_8\text{O}_{12}\text{S}_2$, which shows clear signatures of 2D physics [1].

[1] Tutsch et al., Nat. Commun. 5, 5169 (2014).

TT 33.4 Tue 10:15 H 3010

Low-energy effective interactions beyond cRPA by the functional renormalization group — ●MICHAEL KINZA and CARSTEN HONERKAMP — Institut für theoretische Festkörperphysik, RWTH Aachen University

In the derivation of low-energy effective models for solids targeting the bands near the Fermi level, the constrained random phase approximation (cRPA) has become an appreciated tool to compute the effective interactions. Here we present applications of a constrained functional renormalization group (cFRG) scheme to two simple multi-band systems and compare the resulting effective interactions to the cRPA. The employed wick-ordered fRG scheme generalizes the cRPA approach by including all interaction channels in an unbiased way. First we consider a multiband model for graphene, where we integrate out the σ -bands to get an effective theory for π -bands. It turns out that terms beyond cRPA are strongly suppressed by xy -plane reflection-symmetry of the bands and that in our model, the cRPA stays qualitatively correct even if one breaks this symmetry slightly. The second example is a model for a Cu-O-chain, where we consider an effective theory for the Cu 3d-orbital. Here the fRG data points to relevant corrections compared to the cRPA results.

15 min. break.

TT 33.5 Tue 10:45 H 3010

Ultrafast optical spectroscopy of quasi one dimensional Ta_2NiSe_5 — ●SELENE MOR, MARC HERZOG, CLAUDE MONNEY, JULIA STÄHLER, and MARTIN WOLF — Fritz-Haber-Institut der MPG, Dep. of Phys. Chem., Berlin, Germany

Ta_2NiSe_5 is a layered compound in which atomic chains are aligned in the layers, forming a quasi one dimensional crystal structure. At 328 K, the system shows a structural change, which is accompanied by an electronic phase transition from a semiconductor to an excitonic insulator, with an estimated energy gap of about few hundreds millielectronvolts. Our aim is to unveil the microscopic mechanisms underlying the phase transition in Ta_2NiSe_5 . The system is excited with a femtosecond Ti:sapphire fundamental laser pulse and the mid-infrared (MIR) transient optical response is monitored by ultrafast optical spectroscopy. We observe a fast rise of transient reflectivity, which decays exponentially. This incoherent response is superimposed by a coherent phonon oscillation. A preliminary study with white light (WL) probe beam shows that low repetition rate is mandatory to study the response of the photoexcited system. The analysis unveils the presence of two phonons at 3 and 4 THz, that dominate at high (HT) and low (LT) temperature, respectively. We study the time evolution of the two phonons in the LT phase. We reveal a finite lifetime for the LT phase phonon, whose amplitude decays within few picoseconds, while the HT phase phonon amplitude remains almost constant. The picture is supported by temperature-dependent Raman spectroscopy.

TT 33.6 Tue 11:00 H 3010

Structural effects on charge order in single-layered manganites $R_{1-x}A_{1+x}\text{MnO}_4$ — ●JOHANNES ENGELMAYER, HOLGER ULBRICH, LISA WEBER, MARKUS BRADEN, and THOMAS LORENZ — II. Physikalisches Institut, Universität zu Köln, Germany

Single-layered manganites show a complex interplay between charge, orbital, and magnetic degrees of freedom. For half-doped ($x=1/2$) $R_{1-x}A_{1+x}\text{MnO}_4$ ($R=\text{Pr, La}$; $A=\text{Ca, Sr}$) the so-called Goodenough model is well established. This model proposes a site-centered charge order with a checkerboard pattern of Mn^{3+} and Mn^{4+} ions accompanied by an orbital order. Furthermore a magnetic order develops with ferromagnetic three-spin zig-zag chains and antiferromagnetic inter-chain coupling. For $x=2/3$ the charge order appears as stripe pattern with two adjacent stripes of Mn^{4+} ions alternating with a single stripe of Mn^{3+} ions, while in the magnetically ordered state four-spin zig-zag chains arise [1]. For a deeper understanding of the emergence of

charge order, it is appropriate to vary on the one hand the elements R and A while keeping the doping level x constant—involving structural changes at fixed charge carrier density—and on the other hand change the doping level with the same R and A . Therefore various single crystals of $R_{1-x}A_{1+x}\text{MnO}_4$ with $R = (\text{Pr}, \text{Nd}, \text{Sm}, \text{Tb})$, $A = (\text{Ca}, \text{Sr})$ and $0.5 \leq x \leq 0.7$ were grown and their structural parameters were determined by x-ray diffraction. Based on measurements of resistivity, magnetization, specific heat, and crystal structure we discuss the influence of structural variations on the ordering temperature.

[1] H. Ulbrich, M. Braden, *Physica C* **481**, 31 (2012)

TT 33.7 Tue 11:15 H 3010

Effect of Cu Doping on the Phonon Softening in TiSe_2 — •ROLAND HOTT, ROLF HEID, and FRANK WEBER — Karlsruhe Institute of Technology, Institute of Solid State Physics, P.O.B. 3640, D-76021 Karlsruhe, Germany

We investigated the effect of Cu doping on the soft-mode behaviour of phonons in the Charge Density Wave (CDW) system TiSe_2 both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) and theoretically in Density Functional Theory (DFT) based ab-initio phonon calculations. Within this theoretical framework the experimentally observed hardening of the soft phonons can not be explained in terms of a simple charge doping effect but it is due to a substantial change of the ionic displacement forces due to the additional Cu ion potentials.

[1] F. Weber et al., *Phys. Rev. Lett.* **107** (2011) 266401.

TT 33.8 Tue 11:30 H 3010

Electron Energy-Loss Spectroscopy on the Dichalcogenide 2H-MoS_2 — •CARSTEN HABENICHT, MARTIN KNUPFER, and BERND BÜCHNER — Institute for Solid State Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Two-dimensional transition metal dichalcogenides may complement graphene in future applications. This requires a detailed knowledge of their electronic properties. We have investigated the electronic excitations in 2H-MoS_2 using electron energy-loss spectroscopy (EELS). The electron energy-loss spectra of 2H-MoS_2 in the (100) and (110) directions were measured for various momentum transfer values. The results allow the identification of the A and B exciton peaks and, in particular, their energy-momentum dispersion. The dispersions exhibit approximately quadratic upward trends and slight anisotropies in the (100) and (110) directions. The dispersions allow the estimation of the effective masses of the excitons which are in close proximity to predicted values.

TT 33.9 Tue 11:45 H 3010

Doping dependence of the plasmon dispersion in 2H-TaSe_2 and related systems — •ERIC MÜLLER, CARSTEN HABENICHT, MARTIN KNUPFER, and BERND BÜCHNER — IFW-Dresden, P.O.Box 270116, DE-01171 Dresden, Germany

The electronic excitations of 2H-TaSe_2 and related single crystalline systems have been investigated using electron energy-loss spectroscopy. These systems consist of hexagonal layers with weak interlayer van-der-Waals bonding. We show the influence of alkali metal intercalation on the energy position and the dispersion of the charge-carrier plasmon. Further we demonstrate how the slope of dispersion is affected by the additional charge and the change of charge-carrier density in consequence. Our results indicate a universal evolution of the plasmon dispersion independent of the intercalant (Na, K) and the dichalcogenide (TaSe_2 , TaS_2 , NbSe_2).

TT 33.10 Tue 12:00 H 3010

ARPES and NMTO Wannier Orbital Theory of $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ — •L. DUDY¹, J.W. ALLEN², J.D. DENLINGER³, J. HE⁴, M. GREENBLATT⁵, M.W. HAVERKORT⁶, O.K. ANDERSEN⁷, and Y. NOHARA⁷ — ¹Physikalisches Institut, Universität Würzburg, D- 97074 Würzburg, Germany — ²University of Michigan, Ann Arbor, MI, USA — ³Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — ⁴Clemson University, Clemson, SC, USA — ⁵Rutgers University, Piscataway, NJ, USA — ⁶Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — ⁷Max-Planck-Institut für Festkörperphysik, Stuttgart, Germany

$\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$ displays theoretically interesting [1] metallic quasi-one dimensional (1D) behavior that is unusually robust against 3D crossover with decreasing temperature, and is characterized by a large value of anomalous exponent $\alpha \approx 0.6$ [2]. We present very high resolution, low temperature ($T=6\text{K}-30\text{K}$) angle resolved photoemission spectroscopy (ARPES) of its band structure and Fermi surface (FS), analyzed with N-th order muffin tin orbital (NMTO) Wannier function band theory. We confirm a previous conclusion [3] that LDA band theory is unusually successful, implying a small Hubbard U , and find in ARPES the dispersion and FS warping and splitting expected for predicted small and long range hoppings ($t_{\perp} \approx 10-15$ meV) between chains.

[1] P. Chudzinski, T. Jarlborg and T. Giamarchi, *Phys. Rev. B* **86**, 075147 (2013).

[2] L. Dudy et al., *J. Phys. Cond. Matter* **25**, 014007 (2013).

[3] M. Nuss and M. Aichhorn, *Phys. Rev. B* **89**, 045125 (2014).