

for a 2D field-induced phase transition.

TT 13.9 Tue 11:45 H 2053

Magnetic properties of the spin-1/2 chain material (6MAP)CuCl₃ — ●M. OZEROV¹, E. ČIŽMÁR¹, S. ZVYAGIN¹, C. LANDEE², M. TURNBULL², and J. WOSNITZA¹ — ¹Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden - Rossendorf, Germany — ²Clark University, Worcester, MA, USA

Recently, low-dimensional spin systems have received a considerable amount of attention due to their relevance to numerous quantum phenomena such as quantum criticality problems, spin-Peierls transitions, etc. Here we report on magnetization, electron paramagnetic resonance (EPR) and specific-heat measurements of the spin-1/2 Heisenberg antiferromagnetic chain material (6MAP)CuCl₃. Magnetization data measured at 0.1 T exhibit a maximum at about 70 K, indicating the low-dimensional character of the magnetic interactions. The data are in a good agreement with the temperature dependence of the resonance peak intensity measured at 73 GHz. At low temperatures ($T < 25$ K) the EPR linewidth drastically increases, indicating a possible enhancement of 3D short-range-order correlations. Such behavior is consistent with a broad maximum in the specific heat observed at about 1.5 K, which can be interpreted in terms of 3D magnetic ordering. In addition, we present results of room-temperature X-band EPR measurements of (6MAP)CuCl₃, including angular dependence of the g -factor and of the resonance linewidth.

The work was supported in part by the DFG through Grant No. ZV 6/1-1.

TT 13.10 Tue 12:00 H 2053

Magnetic properties of the Haldane-gap material NENB — ●ERIK ČIŽMÁR¹, MIKHAYLO OZEROV¹, OLEG IGNATCHIK¹, THOMAS P. PAPAGEORGIOU¹, J. WOSNITZA¹, S. A. ZVYAGIN¹, JUREK KRZYSZEK², ZHIXIAN ZHOU³, CHRISTOPHER P. LANDEE⁴, BRIAN R. LANDRY⁴, MARK M. TURNBULL⁴, and JAN L. WIKAIRA⁵ — ¹Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf, 01314 Dresden, Germany — ²National High Magnetic Field Laboratory, Tallahassee, USA — ³Department of Physics and Astronomy, Wayne State University, Detroit, USA — ⁴Department of Physics and Carlson School of Chemistry, Clark University, Worcester, USA — ⁵Department of Chemistry, University of Canterbury, Christchurch, New Zealand

Results of magnetization and high-field ESR studies of the new spin-1 Haldane-chain material $[\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2](\text{BF}_4)$ (NENB) are reported. A definite signature of the Haldane state in NENB was obtained. From the analysis of the frequency-field dependence of magnetic excitations in NENB, the spin-Hamiltonian parameters were calculated, yielding $\Delta/k_B = 17.4$ K, $g_{\parallel} = 2.14$, $D/k_B = 7.5$ K, and $|E/k_B| = 0.7$ K for the Haldane gap, g factor, and the crystal-field anisotropy, respectively. The presence of fractional $S = 1/2$ chain-end states, revealed by ESR and magnetization measurements, is found to be responsible for spin-glass-freezing effects. In addition, extra states in the excitation spectrum of NENB have been observed in the vicinity of the Haldane gap, whose origin is discussed.

The work was supported in part by the DFG through Grant No. ZV 6/1-1.

TT 13.11 Tue 12:15 H 2053

New natural spin-1/2 kagomé systems — kapellasite Cu₃Zn(OH)₆Cl₂ and haydeeite Cu₃Mg(OH)₆Cl₂ — ●OLEG JANSON and HELGE ROSNER — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer str. 40, 01187 Dresden

New natural spin-1/2 systems with kagomé layers — kapellasite Cu₃Zn(OH)₆Cl₂ and haydeeite Cu₃Mg(OH)₆Cl₂ — are studied by full

potential density functional calculations using the fplo6.00-24 code. The band structure, obtained by a paramagnetic calculation, was used to solve a tight-binding model. The transfer integrals were mapped subsequently to a Hubbard model and to a Heisenberg model, giving an estimate for the antiferromagnetic (AF) exchange. The total exchange, containing AF and ferromagnetic (FM) parts, was derived from LSDA + U supercell calculations. As the main result, we find that in both compounds only two exchange integrals are relevant: the nearest neighbour exchange J_1 and the interaction J_d along the diagonals of the Cu²⁺ hexagons. Surprisingly, the size of these integrals depends strongly on the O—H bond length which was therefore optimized with respect to the total energy, resulting in about 1 Å for both compounds. Using the optimized O—H bond length, we find $J_1 > J_d$ in kapellasite and $J_1 \sim J_d$ in haydeeite. According to our results, kapellasite can be described as a modified kagomé lattice, while interpenetrating chains should be considered for haydeeite. Our results should encourage new experimental studies of these interesting materials.

TT 13.12 Tue 12:30 H 2053

Charge excitations and local magnetism: Li₂CuO₂ — ●STEFAN-LUDWIG DRECHSLER¹, JIRŔI MÁLEK^{1,2}, MARTIN KNUPFER¹, ULRIKE NITZSCHE¹, HELGE ROSNER³, and HELMUT ESCHRIG¹ — ¹IFW-Dresden, D-01171 Dresden — ²Institute of Physics, ASCR, Prague — ³Max-Planck-Inst. f. Chem. Phys. Fester Stoffe

Electron energy loss spectroscopy and optical conductivity data of the frustrated edge-shared chain cuprate Li₂CuO₂ are reanalyzed within exact diagonalizations of multiband Hubbard models for CuO₂ chains taking into account Cu $3d_{xy}$, $4s$ and/or $4p_{x,y}$ and O $2p_{x,y}$ orbitals. We show that Zhang-Rice (ZR) singlet charge excitations which are generic for most cuprates are strongly suppressed in favor of ZR triplets as a consequence of substantial ferromagnetic correlations at $T=0$. A significant suppression also at $T=300$ K is obtained approximately. The frequency region above 6eV is dominated by O $2p$ to Cu $4p_y$, $4s$ and $4p_x$ transitions. The cluster mapping of these multiband Hubbard models on the Heisenberg J_1 - J_2 model is in accord with a total energy analysis of various magnetic structures within LSDA+ U FPLO calculations. According to all these theoretical results the observed ferromagnetic ordering of Li₂CuO₂ is caused already by a strong nearest-neighbor (CuO₄ plaquette) ferromagnetic in-chain interaction $J_1 \approx -200$ K compared with the next-nearest neighbor exchange $J_2 \approx 35$ K and it is only a bit further stabilized by a specific frustrating weak antiferromagnetic interchain exchange in contrast with previous studies [1].

[1] Y. Mizuno *et al.*, Phys. Rev. B **57**, 5326 (1998).

TT 13.13 Tue 12:45 H 2053

Competing exchange interactions in the one-dimensional spin-1/2 system Li₂CuO₂ — ●ULRIKE NITZSCHE¹, STEFAN-LUDWIG DRECHSLER¹, and HELGE ROSNER² — ¹IFW Dresden, P.O. Box 270116, D-01171 Dresden — ²MPI CPDS Dresden, Nöthnitzer Straße 40, D-01187 Dresden

The spin 1/2 chain-cuprate Li₂CuO₂ is the archetype for competing nearest-neighbor and next-nearest-neighbor exchange interaction J_1 and J_2 along the CuO₂ chains. The magnitude of J_1 and J_2 , especially their ratio α is crucial for the understanding of the magnetic ground state and is controversially disputed since a decade. Here, we report a density functional based electronic structure study to evaluate the leading in-chain and inter-chain exchange constants. We combine an LDA+ U total energy approach for different spin configurations with the results from a tight-binding fit mapped onto a Heisenberg model. Our results yield a ferromagnetic ground state with a ferromagnetic J_1 and an antiferromagnetic J_2 and an α value well inside the region of the ferromagnetically ordered phase. A brief comparison with results from literature is given.

TT 14: Transport: Nanoelectronics III - Molecular Electronics

Time: Tuesday 9:30–13:00

Location: H 3010

TT 14.1 Tue 9:30 H 3010

Conduction Properties of Bipyridinium Functionalized Molecular Wires — ●ALEXEI BAGRETS^{1,2}, ANDREAS ARNOLD², and FERDINAND EVERS^{1,2} — ¹Institute of Nanotechnology, Research Center Karlsruhe, PO Box 3640, D-76021, Germany — ²Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, D-76128 Karl-

sruhe, Germany

For functionality of organic molecules it is of primary importance to understand how they can operate as current switches. On the way to this goal, we examine possible mechanisms of the reported experimentally "conductance switching" behavior in alkyldithiol molecular wires modified with a viologen (bipyridinium) moiety, which oxidation state

can be controlled by *electrochemical gating* [1,2]. Based on density functional theory calculations, we show that molecules under study behave as weakly coupled quantum dots, where the current is carried by a redox-active LUMO-(lowest unoccupied molecular) level [3]. We calculate how the conductance decays with increasing the wire length and thereby recover quantitatively the experimental tunneling exponent [4]. Our calculations imply, that the charging induced conformational change in the bipyridinium unit is not a main switching agent, rather than the phonon-assisted inelastic electron transport through the viologen redox-level explains the observed switching behavior [3].

[1] W. Haiss *et al.*, *J. Am. Chem. Soc.* **125**, 15294 (2003). [2] Zh. Li *et al.*, *Nanotechnology*, **18**, 044018 (2007). [3] A. Bagrets, A. Arnold, and F. Evers, arXiv:0711.XXXXv1. [4] Ch. Li, I. Pobelov, Th. Wandlowski, A. Bagrets, A. Arnold, and F. Evers, to appear in *J. Am. Chem. Soc.*

TT 14.2 Tue 9:45 H 3010

Effects of polaron hopping on the transport through DNA — ●BENJAMIN B. SCHMIDT^{1,2}, MATTHIAS H. HETTLER², and GERD SCHÖN^{1,2} — ¹Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — ²Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Postfach 3640, 76021 Karlsruhe, Germany

Experiments probing the equilibrium transport in DNA [1] have led to the consensus that polaron hopping is the dominant transport mechanism of charge carriers in DNA. On the other hand in non-equilibrium experiments where short DNA molecules are connected to two biased leads various types of behaviour is seen (reaching from ballistic transport to insulating behaviour). The reason for this discrepancy is not resolved. We suggest that polaron hopping plays an important role in the non-equilibrium transport through DNA. Our theory is based on work by Böttger and Bryksin [2] on small polaron transport in bulk materials, which we extend to nanostructures where we also account for coupling of the DNA to the leads. It describes the polaron hopping quantum mechanically by expanding the time evolution of the occupation number on the different bases along the Keldysh contour. We observe non-symmetric current-voltage characteristics which we relate to partial charge redistribution on the DNA due to the applied bias.

[1] P.Henderson *et al.*, *PNAS USA*, **96**, 8353 (1999)

[2] H. Böttger and V. V. Bryksin, 'Hopping conduction in Solids', Akademie Verlag Berlin, (1985)

TT 14.3 Tue 10:00 H 3010

Dynamical effects in the conductance properties of short DNA molecular wire: a combined study using molecular dynamics and model Hamiltonians — ●RODRIGO CAETANO¹, RAFAEL GUTIERREZ¹, BEN WOICZIKOWSKI², TOMAS KUBAR², MARCUS ELSTNER², and GIANAURELIO CUNIBERTI¹ — ¹Institute for Materials Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, D-01062 Dresden, Germany — ²Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany

The potential applications of DNA either as template or as molecular wires make of crucial importance to understand the microscopic mechanism leading supporting (or hindering) charge migration through this molecule. The experimental studies give very striking results, which range from insulating up to superconducting behavior. Theoretically, it is very important to include dynamical effects, since DNA is known to be a very flexible molecule. The dynamical effects of the solvent should be taken into account. In this work, we study charge transport through short Poly(G)-Poly(C) DNA within a minimal tight binding model. The model parameters are extracted from snapshots along QM/MM trajectories via DFTB approximation and thus include internal and solvent dynamical effects. We perform a statistical analysis of the time-dependent onsite and electronic hopping and show a broad non symmetric distribution. Green function formalism is used to calculate the transport characteristics and demonstrate how the average quantities depend on the relation between system time scales.

TT 14.4 Tue 10:15 H 3010

Switching response of DNA conduction under stretching — ●BO SONG¹, MARCUS ELSTNER², and GIANAURELIO CUNIBERTI¹ — ¹Institute for Materials Science, Dresden University of Technology, D-01062 Dresden, Germany — ²Institute for Physical and Theoretical Chemistry, Braunschweig University of Technology, D-38106 Braunschweig, Germany

By merging DFTB calculations and model-Hamiltonian approaches, we study the stretching-twisting process of poly(GC) DNA oligomers. A local maximum for the transfer integral t between two nearest-neighbor GC pairs is found in the stretching process, which arises from the competition between stretching and twisting. This results in a local maximum for the current in the case that the electrode-DNA coupling Γ is greater than t . Reducing Γ to the values smaller than t gives rise to plateaus in the current. The heights of such plateaus are almost equal to each other.

TT 14.5 Tue 10:30 H 3010

Modeling of tunneling through single endohedral N@C₆₀ molecules — ●CARSTEN TIMM¹, JACOB E. GROSE², WOLFGANG HARNEIT³, and DANIEL C. RALPH² — ¹University of Kansas, Lawrence, USA — ²Cornell University, Ithaca, USA — ³Freie Universität Berlin, Germany

We report on recent experimental and theoretical results for single-molecule transistors involving endohedral N@C₆₀ fullerene molecules. In this talk, we will focus on the theoretical modeling. The observed differential conductance shows strong evidence for the exchange interaction between electrons in the fullerene LUMO and the nitrogen p-electrons, favoring an antiferromagnetic interaction. In addition, soft vibrational modes are seen, which are attributed to oscillations of the molecule as a whole. We discuss a model Hamiltonian that reproduces the main features of the experimental conductance.

TT 14.6 Tue 10:45 H 3010

Silicon based nanogap devices for transport studies on molecule-nanoparticle junctions — ●SEBASTIAN STROBEL¹, ROCIO MURCIA¹, ALLAN HANSEN², and MARC TORNOW² — ¹Walter Schottky Institut, TU München, Germany — ²Institut für Halbleitertechnik, TU Braunschweig, Germany

One possible realization of future nanoelectronics may be a hybrid combination of existing silicon circuitry with functional molecular units. Such approach requires a silicon based technology that allows for the parallel fabrication of contact structures for molecules, as well as the fundamental characterization of such hybrids.

We have fabricated arrays of individually addressable nanogap electrodes with a predefined separation down to ~20 nm using silicon on insulator (SOI) as substrate material. The samples were processed using standard optical lithography, dry and wet chemical etching, and metal thin film deposition, only.

We realized hybrid molecular junctions using such nanogap electrode devices by self-assembling a monolayer of mercaptohexanol onto the metal contacts, and trapping 30 nm diameter Au nanoparticles between the functionalized electrodes, subsequently. Transport measurements at 4.2 K revealed pronounced Coulomb staircase behaviour, characteristic for asymmetric double-barrier tunnelling junctions. We analyse our data by means of model calculations.

TT 14.7 Tue 11:00 H 3010

Length-dependent conductance and thermopower in metal-molecule-metal junctions — ●JANNE VILJAS^{1,2}, FABIAN PAULY¹, and JUAN CARLOS CUEVAS^{3,1,2} — ¹Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures, Universität Karlsruhe, D-76128 Karlsruhe — ²Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — ³Departamento de Física Teórica de la Materia Condensada C-V, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Using a method based on density-functional theory, we investigate the conductance and the thermopower in metal-molecule-metal junctions made of dithiolated oligophenylenes contacted to gold electrodes [1]. We find that while the conductance decays exponentially with increasing molecular length, the thermopower increases linearly in good quantitative agreement with recent experiments [2]. We also analyze how these transport properties can be tuned with methyl side groups. The characteristic substituent effects in our ab-initio calculations are explained using a π -electron tight-binding model, which we have studied in detail.

[1] F. Pauly, J. K. Viljas, and J. C. Cuevas, arXiv:0709.3588.

[2] P. Reddy *et al.*, *Science* **315**, 1568 (2007).

15 min. break

TT 14.8 Tue 11:30 H 3010

Current switching in single molecule transport and con-