TT 5: CE: Low-dimensional Systems - Materials 1

Time: Monday 14:00–17:30 Location: H18

Invited Talk TT 5.1 Mon 14:00 H18

Field-Induced Berezinskii-Kosterlitz-Thouless Transition in a 2d Spin-Dimer System — •Michael Lang[1], Ulrich Tutsch[1], Bernd Wolf[1], Tonia Kretz[2], Hans-Wolfram Lerner[2], Matthias Wagner[2], Stefan Wessel[3], Tanusri Saha-Dasgupta[4], Harald Jeschke[5], and Roser Valenti[5] — [1]Phys. Institut, Univ. Frankfurt, SFB/TR49, D-60438 Frankfurt (M) — [2]Inst. f. Anorg. Chemie, Univ. Frankfurt SFB/TR 49, D-60438 Frankfurt(M) — [3]Inst. f. Theor. Phys. III, Univ. Stuttgart, D-70550 Stuttgart — [4]S.N. Bose National Centre f. Basic Science, 700098 Kolkata, India — [5]Inst. f. Theor. Phys., Univ. Frankfurt, SFB/TR49, D-60438 Frankfurt(M)

Weakly-coupled spin-1/2 dimer systems exposed to a sufficiently strong magnetic field offer exciting possibilities for studying critical phenomena under well-controlled conditions [1]. A prominent example is the Bose-Einstein condensation of magnetic triplet excitations in three dimensionally (3D)-coupled systems. Here we report on a chemically-constructed multilayer bulk magnet composed of molecule-based pairs of spin S = 1/2 dimers, where, by the application of a magnetic field, a gas of magnetic excitations is formed. Based on magnetic susceptibility measurements combined with Density Functional Theory and Quantum Monte Carlo calculations, we conclude that these excitations have a distinct 2D character and that the field-induced state, revealed at low temperatures of 39 mK, is a manifestation of the Berezinskii-Kosterlitz-Thouless topological order.

[1] T. Giamarchi et al., Nature Physics 4, 198 (2008).

TT 5.2 Mon 14:30 H18

Exploring the doping dependence of the Mott transition on X-ray irradiated crystals of κ-(ET)$_2$Cu[N(CN)]$_2$]Cl — •Ulrich Tutsch[1], Ammar Naji[1], Takahiko Sasaki[2], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt (M), SFB/TRR49, D-60438 Frankfurt (M) — [2]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi 980-8577, Japan

The quasi two-dimensional organic charge-transfer salt κ-(ET)$_2$Cu[N(CN)$_2$]Cl has a Mott-insulating ground state at ambient pressure, which can be transformed into a superconducting ground state ($T_c \approx 13\,\mathrm{K}$) by applying moderate pressures of $\sim 30\,\mathrm{MPa}$ (300 bar). Our objective is to study how the first-order Mott-transition line and its second-order critical end point change on doping the material away from half filling. We use X-ray irradiation in order to introduce charge carriers in this material [1] and take the shifts in the room-temperature resistivity as a measure of the amount of doping. We will present resistivity data for the temperature range $5\,\mathrm{K} \leq T \leq 60\,\mathrm{K}$ and for pressures up to 50 MPa for a κ-(ET)$_2$Cu[N(CN)]$_2$]Cl crystal at various doping levels and discuss the accompanied changes in the p-T-phase diagram.

[1] T. Sasaki *et al.*, J. Phys. Soc. Jpn. 76, 123701 (2007)

TT 5.3 Mon 14:45 H18

Finite size effects and magnetic order in the spin-1/2 honeycomb lattice compound $InCu_{2/3}V_{1/3}O_3$ — •M. Yehia[1], E. Vavilova[1,2], U. Löw[3], A. Möller[4,5], T. Taetz[5], R. Klingeler[1], V. Kataev[1], and B. Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 Dresden, Germany — [2]Zavoisky Physical Technical Institute, Russian Academy of Sciences, 420029 Kazan, Russia — [3]Technische Universität Dortmund, Theoretische Physik I, 44221 Dortmund, Germany — [4]University of Houston, Department of Chemistry and Texas Centre for Superconductivity Houston, TX 77204, USA — [5]Institut für Anorganische Chemie, Universität zu Köln, 50939 Köln, Germany

A two dimensional spin honeycomb lattice on the basis of $InCu_{2/3}V_{1/3}O_3$ was studied by means of high field electron spin resonance, nuclear magnetic resonance and magnetic susceptibility. Previous structural studies suggest the occurrence of uncorrelated finite size in-plane domains, which is expected to inhibit long range magnetic order. Surprisingly, ESR data reveal the development of two collinear AFM sublattices below $\sim$ 20 K whereas NMR results show the presence of the staggered internal field. This is consistent with the magnetization data which implies a reorientation of the spin sublattices at $\sim$ 5.7 T. Quantum Monte-Carlo calculations of spin clusters of the coupled honeycomb spin planes indicate the development of the staggered magnetization at a finite temperature. This may explain the occurrence of the AFM state in $InCu_{2/3}V_{1/3}O_3$ despite unfavorable for magnetic order structural effects.

TT 5.4 Mon 15:00 H18

Low temperature magnetic response of CePt surface alloy — •Annemarie Köhl, Christian Praetorius, Sebastian Brück, and Kai Fauth — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We have used X-ray magnetic circular dichroism (XMCD) at Cerium edges to determine the low temperature paramagnetic local moment response of a CePt intermetallic surface alloy. The ultrathin alloy film is prepared in situ by evaporation of few atomic layers of Ce onto Pt(111) and subsequent annealing. LEED patterns of the resulting alloy hint at a (1.85×1.85) superstructure. The temperature dependent susceptibility is partially compatible with the response of the crystal field split Ce $4f^1$ state with a crystal field splitting of ≈ 60 K. Below 20 K our data are indicative of a magnetic phase transition at a critical temperature of ≈ 9 K. We discuss our results in view of the recent findings of Kondo lattice physics in the related $CePt_5$ surface alloy.

TT 5.5 Mon 15:15 H18

Magnetism in Azurite Studied by Muon Spin Rotation — Mathias Kraken[1], Josefin Engelke[1], Stefan Süllow[1], •Jochen Litterst[1], Anja Wolter[2], Bernd Wolf[3], Michael Lang[3], Chris Baines[4], and Hubertus Luetkens[4] — [1]IPKM, Technische Universität Braunschweig, Braunschweig, Germany — [2]IFW , Dresden, Germany — [3]Physikalisches Institut, Universität Frankfurt, Frankfurt am Main, Germany — [4]LEM, PSI, Villigen, Switzerland

The natural mineral azurite $Cu_3(CO_3)_2(OH)_2$ represents a new type of low-dimensional frustrated quantum spin system with a diamond spin chain as basis. From specific heat [1] there is evidence for a phase transition at ca. 1.8 K which however is magnetically still ill-defined. Earlier muon spin rotation experiments [2] have indicated a magnetic transition yet no systematic study has been reported. We have performed zero field and transverse field muon spin rotation experiments at Paul Scherrer Institut Villigen (Switzerland) in the temperature range from 0.02 K to 6 K on polycrystalline powder and a single crystal. We could corroborate the appearance of magnetic order below 1.9 K from spontaneous muon spin rotation with a frequency following a magnetization curve. The rotation profile is indicative of a modulated spin structure. In addition we find a pre-cursor phase between 1.9 K and about 3 K which we relate to the onset of magnetic correlations between Cu monomers via dimers.

[1] H. Kikuchi, et al., Phys. Rev. Lett. 94 (2005) 227201.

[2] H. Kikuchi, et al., Progress of Theoretical Physics Supplement. 159 (2005)1 2005

TT 5.6 Mon 15:30 H18

Neutron scattering investigations of the magnetic properties of azurite $Cu_3(CO_3)_2(OH)_2$ — •Kirrily Rule[1], Clare Gibson[1,2], Manfred Reehuis[1], Bachir Ouladiaff[3], Matthias Gutmann[4], Jens-Uwe Hoffmann[1], Sebastian Gerischer[1], Alan Tennant[1,2], Stefan Süllow[5], and Michael Lang[6] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]ISIS Facility, Rutherford Appleton Laboratory, Didcot UK — [5]Institut für Physik der Kondensierten Materie, TU Braunschweig, Braunschweig, Germany — [6]Physikalisches Institut, J.W. Goethe-Universität Frankfurt, Germany

Azurite, $Cu_3(CO_3)_2(OH)_2$, has been considered an ideal example of a one-dimensional (1D) diamond chain antiferromagnet. Early studies of this material imply the presence of an ordered antiferromagnetic phase below TN 1.9 K while magnetization measurements have revealed a 1/3 magnetization plateau. Until now, no corroborating neutron scattering results have been published to confirm the ordered magnetic moment structure. In this talk, we will present neutron diffraction data which reveal the presence of a commensurate magnetic order in azurite. The results of magnetic structural refinement from single crystal diffraction will also be discussed. Finally we will show some recent inelastic neutron scattering results which reveal new information about the dynamics in this material.

15 min. break

TT 5.7 Mon 16:00 H18

Consequence of the intra-chain dimer-monomer spin frustration and the inter-chain dimer-monomer spin exchange in the diamond-chain compound Azurite $Cu_3(CO_3)_2(OH)_2$ — •R. K. Kremer[1], J. Kang[2], C. Lee[2], and M.-H. Whangbo[2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Department of Chemistry, North Carolina State University, Raleigh, North Carolina 27695-8204

The spin lattice appropriate for Azurite $Cu_3(CO_3)_2(OH)_2$ was determined by evaluating its spin exchange interactions on the basis of first principles density functional calculations. It is found that Azurite cannot be described by an isolated diamond chain with no spin frustration, but by a two-dimensional spin lattice in which diamond chains with spin frustration interact through the interchain spin exchange in the *ab*-plane.[1] Our analysis indicates that the magnetic properties of Azurite at low temperatures can be approximated by two independent contributions, i.e., an isolated dimer and an effective uniform chain contributions. This prediction was verified by analyzing the magnetic susceptibility and specific heat data of Azurite.

[1] J. Kang, *et al.* J. Phys. Cond. Matter **21** 392201 (2009).

TT 5.8 Mon 16:15 H18

Effective spin-chain model for azurite: derivation from ab-initio computations (exchanged with TT 5.9) — Ingo Opahle[1], Hem C. Kandpal[2], Niels Jackson[1], Hena Das[3], Tanusri Saha-Dasgupta[3], Andreas Honecker[4], •Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [2]IFW Dresden — [3]Bose Institute, Kolkata, India — [4]Institut für Theoretische Physik, Universität Göttingen

The observation of complex spin dynamics and a 1/3 magnetization plateau has revived the interest in the famous pigment azurite $Cu_3(CO_3)_2(OH)_2$. We revisit the question of the underlying microscopic Hamiltonian using a combination of first principles methods. As a guiding tool, we employ NMTO downfolding which yields the relative importance at low energies of the many possible hybridization paths between the copper centers. In order to obtain the corresponding exchange coupling strengths we perform total energy calculations for many spin configurations and several supercells. We employ FPLAPW and FPLO basis sets with LDA+U functionals, and we investigate the dependence of the exchange couplings on the correlation strength U. We find that the low-energy Hamiltonian of azurite is a diamond chain with a monomer-monomer coupling and some nonzero interchain couplings. We show that the neglect of interchain couplings effectively leads to a less symmetric diamond chain.

TT 5.9 Mon 16:30 H18

Effective spin-chain model for azurite: comparison with experimental results (exchanged with TT 5.8) — •Andreas Honecker[1], Robert Peters[1], Thomas Pruschke[1], Roser Valentí[2], Harald Jeschke[2], Ingo Opahle[2], Hem Kandpal[2], Tanusri Saha-Dasgupta[3], Hena Das[3], Johannes Richter[4], Helge Rosner[5], Oleg Janson[5], Shijie Hu[6], Xiaoqun Wang[6], Bernd Wolf[2], and Michael Lang[2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen — [2]Johann Wolfgang Goethe-Universität Frankfurt am Main — [3]Bose National Centre for Basic Sciences, Kolkata — [4]Institut für Theoretische Physik, Otto-von-Guericke Universität Magdeburg — [5]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [6]Department of Physics, Renmin University of China, Beijing

We analyze a spin-1/2 Heisenberg model with a generalized diamond chain exchange geometry which has been derived from ab-initio computations for the mineral azurite $Cu_3(CO_3)_2(OH)_2$. Using numerical results, we demonstrate that a consistent description can be obtained for various physical properties of azurite: (i) the low-temperature magnetization curve, (ii) inelastic neutron scattering on the 1/3 magnetization plateau, (iii) nuclear magnetic resonance measurements on the 1/3 magnetization plateau, and (iv) the magnetic susceptibility as well as the specific heat. Our results resolve previous controversies on the modeling of azurite. Furthermore, we explain why a one-dimensional model can be used in many situations although interchain exchange in azurite is actually non-negligible at a microscopic level.

TT 5.10 Mon 16:45 H18

The low-temperature structure of azurite — •Clare Gibson[1,2], Kirrily Rule[1], Manfred Reehuis[1], Bachir Ouladdiaf[3], Alan Tennant[1,2], Stefan Suellow[4], and Michael Lang[5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, D-14109 Berlin, Germany — [2]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [5]Phys. Inst., J.W. Goethe-Universität Frankfurt, Germany

The low-dimensional quantum magnet and natural mineral azurite, $Cu_3(CO_3)_2(OH)_2$, is considered to be a model of the distorted diamond chain lattice. Recently, much study has been devoted to determining the magnetic exchange parameters in this frustrated magnetic material. However, results have been contradictory [1,2,3] and the validity of the one-dimensional model has been called into question [4]. An accurate structural determination of azurite below the Nèel temperature may prove useful for the purpose of exchange parameter calculation in terms of precise knowledge of the magnetic superexchange pathways. We report on single crystal and powder neutron diffraction data taken over the temperature range 200 mK - 5 K to determine the low temperature lattice parameters and space group. Analysis reveals strain in the material which coincides with the magnetic ordering transition at 1.86 K.

[1] H. Kikuchi et al., Phys. Rev. Lett. 94, 227201 (2005)
[2] K.C. Rule et al., Phys. Rev. Lett. 100, 117202 (2008)
[3] G. Bo and G. Su, Phys. Rev. Lett. 97, 089701 (2006)
[4] J. Kang et al., J. Phys.: Condens. Matter 21, 392201 (2009)

TT 5.11 Mon 17:00 H18

Analyzing the complex spin-coupling structure in the single-molecule magnet Mn_{12}wheel by inelastic neutron scattering — •Joscha Nehrkorn[1], Oliver Waldmann[1], Taketo Tagushi[2], George Christou[2], Thierry Strässle[3], Philip L. W. Tregenna-Pigott[3], and Hannu Mutka[4] — [1]Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany — [2]Department of Chemistry, University of Florida, Gainesville, Florida 32611-7200, USA — [3]LNS, ETH Zürich & Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [4]Institut Laue-Langevin, 38042 Grenoble, France

Recently the single-molecule magnet (SMM) $[Mn_{12}(O_2CMe)_{14}(R\text{-}mda)_8]$, or Mn_{12}wheel in short, has attracted interest because of its unusual quantum tunneling transitions in the magnetization, which were explained by describing it as a dimer of two magnetically coupled SMM subunits [1,2]. In order to analyze the underlying complicated spin structure we performed inelastic neutron scattering experiments. They show that the model of two coupled SMMs has to be refused. A microscopic model was devised which reproduces the data and provides values for the exchange coupling and magnetic anisotropy parameters. By using basic principles for bipartite lattices the low-energy sector can be reduced again to that of two coupled subunits, which, however, are substantially different than the two subunits in the originally proposed dimer model. The new model resolves some controversies as regarding the magnetic tunneling transitions.

[1] C. Ramsey *et al.*, Nature Physics **4**, 277 (2008)
[2] W. Wernsdorfer *et al.*, Phys. Rev. Lett **101**, 237204 (2008)

TT 5.12 Mon 17:15 H18

Molecular Magnets Confined in the Nanocage of a Globular Protein — •Peter Lemmens[1,4], Dirk Wulferding[1,4], Dirk Menzel[1], Tamoghna Mitra[2], Achim Müller[2], Rajib Kumar Mitra[3], Pramod Kumar Verma[3], and Samir Kumar Pal[3] — [1]IPKM, TU-BS, Braunschweig — [2]FC, Univ. Bielefeld — [3]SNBC, Kolkata, India — [4]IGSM, TU-BS, Braunschweig

We investigate the effect of confinement and energy transfer on the dynamics of a molecular magnet known as a model system to study quantum coherence. The polyoxovanadate V_{15} is incorporated into a protein cavity and the energy transfer probed by time resolved experiments. Work supported by DFG and B-IGSM.