

MA 31: Bio- and Molecular Magnetism

Time: Friday 11:00–12:45

Location: H10

MA 31.1 Fri 11:00 H10

Enhanced magnetocaloric effect in frustrated magnetic molecules with icosahedral symmetry — ●JÜRGEN SCHNACK¹ and JOHANNES RICHTER² — ¹Universität Bielefeld, Fakultät für Physik, PF 100131, D-33501 Bielefeld — ²Universität Magdeburg, Institut für Theoretische Physik, PF 4120, D-39016 Magdeburg

Antiferromagnetic finite-size spin systems with icosahedral symmetry constitute very interesting frustrated materials with rather unusual magnetic properties. Among such properties are jumps to the saturation magnetization in the cuboctahedron and the icosidodecahedron as well as metamagnetic phase transitions at zero temperature for instance in the icosahedron and dodecahedron. Some of these properties, for instance the large magnetization jump to saturation, are as well present in the Kagome or other lattice antiferromagnets. In this contribution we investigate the magnetocaloric properties of certain spin clusters with icosahedral symmetry that turn out to be interesting as well. The most striking feature is that the magnetocaloric effect is largely enhanced compared to bipartite antiferromagnets.

MA 31.2 Fri 11:15 H10

A first-principles DFT study of magnetic exchange paths in a BH₄⁻-bridged dinickel(II) complex — ●CLAUDIA LOOSE — TU-Bergakademie Freiberg, Institut für Theoretical Physics, Leipziger Str. 23, 09599 Freiberg, Germany

We studied the BH₄⁻-bridged dinickel(II) complex [(L)Ni₂BH₄]⁺, with L the dinucleating hexaaza-dithiophenolate ligand by first-principles DFT as implemented in the all-electron NRLMOL code. Our calculations find in agreement with experiment a ferromagnetic coupling between the two Ni-atoms resulting in an $S = 2$ magnetic ground state of the complex. It is shown that exchange through the bridging BH₄⁻ contributes 2/3 of the total ferromagnetic exchange. This exchange proceeds through the p-states of BH₄⁻ which are energetically well aligned with the d-states of the magnetic ions. The remaining ferromagnetic exchange is partly derived from crossed interactions mediated by sulfur atoms from the ligand and partly by direct interaction of the two Ni²⁺-ions. Replacing BH₄⁻ by halides increases the ferromagnetic coupling. On the other hand in case of isoelectronic CH₄ or noble gases the magnetic exchange path vanishes completely which supports the importance of the energetic position of the p-states. This opens the possibility to control the magnetic coupling by these p-states. Further, we predict that this complex will have a negative zero field splitting parameter D , so that it should eventually behave like a single molecule magnet. We would like to thank Prof. Kersting for providing the crystal data of the complex used in our studies.

MA 31.3 Fri 11:30 H10

Growth and electronic structure of tetracyanoethylene on noble metals studied by scanning tunneling microscopy — ●DANIEL WEGNER, RYAN YAMACHIKA, YAYU WANG, and MIKE CROMMIE — Department of Physics, University of California at Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA.

Tetracyanoethylene (TCNE) is a π -electron acceptor with a very strong electron affinity that easily forms charge-transfer complexes with other organic molecules and metals. We have performed STM and STS of isolated TCNE molecules and ordered sub-monolayer coverages on noble-metal surfaces in order to study the competition between intermolecular and molecule-substrate interactions, and the impact this might have on film-growth and electronic structure. HOMO and LUMO peaks were observed for single TCNE molecules on Ag and Au substrates using STS, but not for Cu substrates which react more strongly with TCNE. The spatial distribution of the TCNE HOMO, as observed in dI/dV maps, fits well with DFT calculations and shows that TCNE is in a negatively charged state on these metal substrates. dI/dV maps of ordered TCNE arrays indicate that neighboring TCNE molecules interact strongly with each other in some cases.

MA 31.4 Fri 11:45 H10

Magnetic properties of organometallic complexes studied by XMCD — ●PAOLO IMPERIA¹, MARIA BENEDETTA CASU², MICHAEL MARTINS¹, and THOMAS CHASSÉ² — ¹Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, 22761 Hamburg

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The magnetic properties of molecular based magnets can be tuned playing with the constituent blocks and growing parameters. Strategies used to achieve high magnetic moments imply the correct positioning of electronegative atoms, like oxygen and nitrogen, leading to large occupation probability by an unpaired electron, simultaneously achieving intermolecular magnetic order without destroying the intramolecular properties. To understand their magnetic properties the knowledge of the internal magnetic structure is of paramount importance and the key question, which element in the compound shows magnetic ordering and which orbital acquires a magnetic moment, needs to be answered. Absorption spectroscopy with its elemental specificity can help in resolving such problem. Here, we present and discuss first results of x-ray magnetic circular dichroism (XMCD) measurements done at the Mn and Ni L_{2,3} edges and N K edge of a selection of organic stable compounds like manganese tricyanomethanide (Mn[C(CN)₃]₂) which due to the tridentate nature of the C(CN)₃ forms a triangular lattice and exhibits magnetic frustration, and MnNi(NO₂)₄(en)₂ (en = ethylenediamine), a bimetallic chain compound where the ferromagnetically coupled Mn and Ni ions linked by NO₂ molecules alternate.

MA 31.5 Fri 12:00 H10

Magnetic properties of high-spin tetranuclear Nickel(II) molecular complex — ●CHRISTIAN GOLZE¹, RÜDIGER KLINGELER^{1,2}, BERND BÜCHNER¹, VLADISLAV KATAEV¹, MICHEL GOIRAN², JEAN M. BROTO², HARISON RAKOTO², and BERTHOLD KERSTING³ — ¹IFW Dresden, Germany — ²LNCMP Toulouse, France — ³Institute for Anorganic Chemistry Leipzig, Germany

Electron spin resonance and magnetization data of a novel multicenter magnetic molecular complex are reported. In this compound two Ni(II) ions are coupled to a dimer via a diaminothio-bridge and a pair of dimers is coupled in a single molecule via a $\mu_{1,3}$ azide bridge. Thus a single molecule spin cluster of a quadrangular shape comprising four Ni(II) spins each with $S = 1$ is formed. Magnetization measurements in fields < 52 T evidence a high-spin ground-state with $S = 4$. ESR has been measured on the polycrystalline sample to determine the zero field splitting of the spin-levels and the g -factor of the resonating spins. Moreover, we have been able to orient the crystallites of the powder in high magnetic fields due to the magnetic anisotropy of the complex. Hence it has been possible to compare experimental quasi single-crystal and powder-averaged ESR data with the theoretical model which yields an accurate determination of the parameters of the spin-Hamiltonian.

MA 31.6 Fri 12:15 H10

Electronic structure of Mn₁₂-complexes chemically grafted on Au(111) — ●MIKHAIL FONIN¹, SÖNKE VOSS¹, MICHAEL BURGERT², YURY DEDKOV³, ULRICH GROTH², and ULRICH RÜDIGER¹ — ¹Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — ²Fachbereich Chemie, Universität Konstanz, 78457 Konstanz, Germany — ³Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany

Electronic properties of monolayers of Mn₁₂-complexes chemically grafted on the Au(111) surface have been studied in detail by means of scanning tunneling microscopy (STM) and spectroscopy (STS) as well as by x-ray absorption spectroscopy (XAS) and photoemission spectroscopy (PES). XAS measurements reveal a significant deviation of spectra obtained from molecular monolayers from those obtained from single crystals indicating a partial fragmentation of the Mn₁₂ cores on the Au(111) surface. However, a large amount of Mn₁₂-molecules seems to retain their structural integrity upon surface deposition by using an appropriate combination of Mn₁₂ cluster and substrate functionalization. The Mn 3d partial density of states for the occupied states were extracted from the resonant PES spectra of Mn₁₂-complexes whereas the unoccupied states near E_F were probed by STS. The obtained density of states within E_F shows a very good agreement with previously reported LDA+ U calculations [1].

[1] D. W. Boukhvalov *et al.*, J. Electron Spectrosc. Relat. Phenom. **137-140**, 735 (2004).

MA 31.7 Fri 12:30 H10

High field level crossing studies on spin dimers in the low dimensional quantum spin system $\text{Na}_2\text{T}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2$ with $\text{T}=\text{Ni,Co,Fe,Mn}$ — ●CHRISTOPHER MENNERICH¹, HANS-HENNING KLAUSS¹, ANJA WOLTER¹, STEFAN SÜLLOW¹, JOCHEN LITTERST¹, CHRISTIAN GOLZE¹, VLADIK KATAEV², RÜDIGER KLINGELER², VLADIK KATAEV², and DANIEL PRICE³ — ¹Institut of Condensed Matter Physics, TU Braunschweig, Mendelssohnstr.3, D-38106 Braunschweig, Germany — ²Leibniz-Institute for Solid State and Materials Research IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — ³WestCHEM, Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK

We demonstrate the application of high magnetic fields to study

the magnetic properties of low dimensional spin systems. We present a case study on the series of 2-leg spin-ladder compounds $\text{Na}_2\text{T}_2(\text{C}_2\text{O}_4)_3(\text{H}_2\text{O})_2$ with $\text{T} = \text{Ni, Co, Fe}$ and Mn . In all compounds the transition metal is in the T^{2+} high spin configuration. The localized spin varies from $S=1$ to $3/2$, 2 and $5/2$ within this series. The magnetic properties were examined experimentally by magnetic susceptibility, pulsed high field magnetization and specific heat measurements. The data are analysed using a spin hamiltonian description. Although the transition metal ions form structurally a 2-leg ladder, an isolated dimer model consistently describes the observations very well. All compounds exhibit magnetic field driven ground state changes which at very low temperatures lead to a multistep behaviour in the magnetization curves.