

MA 3: Bio- and Molecular Magnetism

Time: Monday 11:00–13:00

Location: HSZ 401

MA 3.1 Mon 11:00 HSZ 401

Transition from the Quantum to the Classical Limit for the Antiferromagnetic Heisenberg Model on the Icosahedron — ●NIKOLAOS P. KONSTANTINIDIS — Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

The antiferromagnetic Heisenberg model on the icosahedron, which consists of 20 triangles and belongs to the icosahedral I_h symmetry group, presents unconventional properties at the quantum and classical level. These originate in the frustrated nature of the interactions between the spins. In the quantum limit, there are non-magnetic excitations within the singlet-triplet gap and the specific heat has a multi-peak structure as a function of temperature [1]. For classical spins, the magnetization is discontinuous as a function of an external magnetic field [2]. Here the transition from the full quantum $s_i=1/2$ to the classical limit is investigated by progressively increasing s_i and focusing on the low-energy spectrum and the magnetization in an external field. The icosahedral I_h symmetry properties of the model are fully taken into account in the characterization of the states and show how the quantum fluctuations yield to the classical properties as s_i is increased.

[1] N. P. Konstantinidis, Phys. Rev. B **72**, 064453 (2005).[2] C. Schröder *et al.*, Phys. Rev. Lett. **94**, 207203 (2005).

MA 3.2 Mon 11:15 HSZ 401

Geometrical Frustration in Molecular Spin Triangles with $S=1/2, 5/2$ — ●NICOLAS YÈCHE¹, ANDREI ZVYAGIN^{1,2}, DANIEL PLAUL³, DIRK SCHUCH³, WINFRIED PLASS³, ERIC KAMPERT⁴, TIL DELLMANN¹, CHRISTOPHER BAINES⁵, GWENDOLYNE PASCUA⁵, HANS-HENNING KLAUSS¹, and HUBERTUS LUETKENS⁵ — ¹Institut für Festkörperphysik, TU Dresden — ²Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, Kharkov — ³Institut für Anorganische Chemie, Uni Jena — ⁴Hochfeldlabor Dresden, FZ Dresden-Rossendorf — ⁵Paul Scherrer Institute, Villigen, Switzerland

In the study of finite geometrically frustrated system, the simplest problems that can be considered are paradoxically some of the hardest ones to observe experimentally. Thanks to sophisticated organic ligands, independent triangles of Cu(II) ($S = \frac{1}{2}$) and Fe(III) ($S = \frac{5}{2}$) were synthesized. Investigations carried out with macroscopic (pulsed and static field magnetization) and local probe techniques (μ SR and ^{57}Fe Mössbauer spectroscopy) show characteristic behavior of frustrated systems. Comparison of the magnetization data with theoretical calculations indicates that the antiferromagnetic coupling in the Cu system is greater than 45K: the complex shows a single magnetization plateau up to 60T at about 1/3 of the expected saturation. As for the Fe compound, several clear magnetization steps are observed in pulsed field, hinting for a coupling constant of about 10K. Slow dynamic spin fluctuations are observed in Mössbauer spectra and in the μ SR measurements down to millikelvin temperatures.

MA 3.3 Mon 11:30 HSZ 401

Inelastic Neutron Scattering Studies on the 3d-4f Heterometallic Single-Molecule Magnet Mn_2Nd_2 — ●JOSCHA NEHRKORN¹, MUHAMMAD NADEEM AKHTAR², RUGGERO MILAZZO¹, STEFAN STUIBER¹, HANNU MUTKA³, YANHUA LAN², ANNIE K. POWELL², and OLIVER WALDMANN¹ — ¹Physikalisches Institut, Universität Freiburg, Germany — ²Institut für anorganische Chemie, Universität Karlsruhe, KIT, Germany — ³Institut Laue-Langevin, Grenoble, France

The discovery of slow relaxation and quantum tunneling of the magnetization in Mn_{12}ac more than 15 years ago has inspired both physicists and chemists alike. This class of molecules, now called single-molecule magnets (SMMs), has very recently been expanded to heterometallic clusters incorporating transition metal and rare earth ions. The 4f ions were chosen because of their large angular momentum and magnetic anisotropy. Inelastic neutron scattering experiments were performed on the time-of-flight disk-chopper spectrometer IN5 at ILL on the SMM Mn_2Nd_2 . A magnetic model was developed which perfectly describes all data, including the magnetic data. It was found that neither the large anisotropy nor the large angular momentum of the Nd^{III} ions is the main reason for the SMM behavior in this molecule. Our analysis of the data indicates that it is the weak coupling of the Nd^{III} ions to the Mn^{III} ions, usually considered as a drawback of rare earth ions, which

enhances the relaxation time and therefore leads to SMM behavior.

MA 3.4 Mon 11:45 HSZ 401

Magnetic Model for Mn_2La_2 Developed from Spectroscopic Studies with Inelastic Neutron Scattering and Frequency-Domain Fourier-Transform THz EPR — ●R. MILAZZO¹, J. NEHRKORN¹, S. STUIBER¹, O. WALDMANN¹, M. N. AKHTAR², Y. LAN², A. K. POWELL², H. MUTKA³, J. DREISER⁴, A. SCHNEGG⁵, and K. HOLLDAK⁶ — ¹Physikalisches Institut, Universität Freiburg, Germany — ²Institut für Anorganische Chemie, Universität Karlsruhe, KIT, Germany — ³Institut Laue Langevin, Grenoble, France — ⁴Swiss Light Source, Paul Scherrer Institut, Switzerland — ⁵Helmholtz-Zentrum Berlin, Institut für Silizium-Photovoltaik, Germany — ⁶Helmholtz-Zentrum Berlin, Institut für Synchrotronstrahlung, Germany

Molecular nanomagnets which contain several magnetic centers with a large single-ion magnetic anisotropy are of general interest, because they could lead to interesting phenomena such as single-molecule magnet (SMM) behavior. We performed spectroscopic experiments on Mn_2La_2 using inelastic neutron scattering at the direct time-of-flight disc chopper spectrometer IN5 at ILL and the newly developed frequency-domain Fourier-transform THz EPR at BESSY. Based on the experimental results a magnetic model has been developed. It will be discussed why no SMM behavior was observed, even though Mn_2La_2 exhibits a remarkably high energy barrier of about 37 K for spin relaxation. Furthermore our results can be applied to analogous clusters, with the diamagnetic La^{III} ions replaced by magnetic rare earth ions.

MA 3.5 Mon 12:00 HSZ 401

First results obtained with the new frequency-domain Fourier-transform THz electron paramagnetic resonance technique on single-molecule magnets — ●JAN DREISER^{1,2}, KASPER S. PEDERSEN³, JOSCHA NEHRKORN², ALEXANDER SCHNEGG⁴, KARSTEN HOLLDAK⁴, MAGNUS SCHAU-MAGNUSSEN³, PHILIP TREGENNA-PIGGOTT⁵, HANNU MUTKA⁶, HOEGNI WEIHE³, JESPER BENDIX³, and OLIVER WALDMANN² — ¹Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI — ²Physikalisches Institut, Universität Freiburg, D-79104 Freiburg — ³Department of Chemistry, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen — ⁴Helmholtz-Zentrum Berlin, D-12489 Berlin — ⁵Paul Scherrer Institut, Lab. for Neutron Scattering, CH-5232 Villigen PSI — ⁶Institut Laue-Langevin, F-38042 Grenoble

Single-molecule magnets are molecular spin clusters exhibiting slow relaxation of magnetization. In order to understand the interplay of anisotropy and exchange interaction within these clusters, spectroscopic measurements are needed in addition to magnetization and susceptibility studies. Recently, a new frequency-domain Fourier-transform electron paramagnetic resonance technique working in the THz range (FD-FT THz-EPR) has been developed at the BESSY storage ring in Berlin. In this contribution we present first results obtained with this technique. We further discuss the THz-EPR spectra in the context of inelastic neutron scattering, magnetization and susceptibility measurements.

MA 3.6 Mon 12:15 HSZ 401

Quantum Coherence in Molecular Nanomagnets — ●JORIS VAN SLAGEREN — Institut für Physikalische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart

The occurrence of quantum coherence in molecular nanomagnets has recently attracted a great deal of attraction. Molecular nanomagnets are exchange coupled molecular clusters of transition metal ions, bridged by ligands and encapsulated in an organic ligand shell. They can be easily and extensively modified and tuned in terms of size, spin and anisotropy by chemical synthetic means. This makes these mesoscopic systems excellently suited to the investigation of the transition between the quantum world of single particles and the classical world that we live in.

In this presentation, we will discuss quantum coherence in molecular nanomagnets and the corresponding decoherence pathways.

MA 3.7 Mon 12:30 HSZ 401

Magnetic ground state of TM-Ni binuclear complexes studied by of x-ray circular magnetic dichroism and density functional theory — •KARSTEN KUEPPER¹, ULF WIEDWALD¹, DAVID M. BENOIT², FLORIAN MÖGELE³, BERNHARD RIEGER⁴, and PAUL ZIEMANN¹ — ¹Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm — ²Nachwuchsgruppe Theorie im SFB 569, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm — ³Institut für Materialien und Katalyse, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm — ⁴WACKER-Lehrstuhl für Makromolekulare Chemie, Technische Universität München, Lichtenbergstraße 4, 85747 Garching bei München

We investigate three planar TM-Ni-C₄₆H₆₈N₂O₆ (TM=Mn,Fe,Co) molecules [1] by low temperature XMCD revealing in this way the presence of uncompensated magnetic moments. The experiments have been performed at a temperature of 0.6K in order to probe the magnetic ground state properties. Theoretically, we address the energetic ordering of the different possible spin states of the bi-nuclear complexes using (zero-order) relativistic approximation density functional calculations and a triple-zeta quality basis set. These results show that medium-spin states are often favored over low-spin states for most metal combination, in qualitative agreement with our experimental observations.

[1] Florian Mögele et al., *Langmuir* 25, 13606 (2009).

MA 3.8 Mon 12:45 HSZ 401

Reversible chemical manipulation of the magnetic properties of Fe-porphyrin molecules on a ferromagnetic substrate — •CHRISTIAN FELIX HERMANN¹, JORGE MIGUEL², MATTHIAS BERNIEN¹, ALEXANDER KRÜGER¹, and WOLFGANG KUCH¹ — ¹Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — ²Diamond Light Source, Harwell Science Innovation Campus, OX11 0DE Chilton, Didcot, United Kingdom

Single-molecule magnets are promising building blocks for future spintronic devices. One of the key issues is to gain control over the magnetic properties of adsorbed molecules by external stimuli. We present the results of an X-ray absorption spectroscopy (XAS) study of the adsorption of NO on top of a submonolayer of Fe-octaethylporphyrin molecules adsorbed on oxygen-covered Co films grown on Cu(001). Fe *L*_{3,2} XAS spectra show that the adsorption of 24 L NO at 120 K does not cause any change of the oxidation state of the Fe ion, which remains in an Fe 3+ valence state. XMCD investigations before and after dosing NO reveal an antiparallel alignment of the Fe spins and the magnetization of the ferromagnetic substrate. Interestingly, after dosing NO, the Fe XMCD signal is reduced by a factor of two, while the spectral shape of the Fe *L*_{3,2} XMCD signal is not modified. The lower Fe magnetization at finite temperatures after dosing NO can be explained by a reduction of the magnetic coupling between the Co substrate and the molecules. Thermal desorption of NO at 350 K recovers the initial Fe XMCD signal and proves the reversibility of the process. This work is supported by the DFG (Sfb 658).