

## MA 2: Bio- and Molecular Magnetism

Time: Monday 10:45–13:15

Location: H10

## MA 2.1 Mon 10:45 H10

**Quantum control and entanglement in an avian chemical compass** — •JIANMING CAI<sup>1,2</sup>, GIAN GIACOMO GUERRESCHI<sup>1,2</sup>, and HANS BRIEGEL<sup>1,2</sup> — <sup>1</sup>University of Innsbruck, Innsbruck, Austria — <sup>2</sup>Institut für Quantenoptik und Quanteninformation, Innsbruck, Austria

The contribution has been withdrawn.

## MA 2.2 Mon 11:00 H10

**Electric quantum control of spins in molecular magnets** — •MIRCEA TRIF<sup>1</sup>, DIMITRIJE STEPANENKO<sup>1</sup>, FILIPPO TROIANI<sup>2</sup>, and DANIEL LOSS<sup>1</sup> — <sup>1</sup>Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — <sup>2</sup>CNR-INFM National Research Center S3 c/o Dipartimento di Fisica via G. Campi 213/A, 41100, Modena, Italy

Single molecule magnets show clear signatures of coherent behavior. The control of the spins can allow for the quantum information processing and study of quantum dynamics. Electric fields are good for quantum control at the nanoscale. There are many SMMs and it is hard to predict which ones are suitable for control. Here, we provide two tools for the search for suitable SMMs. We analyze the form and mechanisms that lead to spin-electric coupling in the molecules with the shape of regular polygons. We find that the SEC in triangles is governed by the modification of the exchange interaction, while in pentagon the spin-electric coupling proceeds via spin-orbit interaction. The symmetry analysis leaves the coupling constant undetermined, and we apply a Hubbard model to single-molecule magnet to find a connection between the spin-electric coupling and the properties of the chemical bonds in a molecule. We study the experimental signatures of spin-electric coupling in the standard experiments, NMR, ESR, and thermodynamics.

## MA 2.3 Mon 11:15 H10

**Ultra-low temperature x-ray magnetic circular dichroism of TM-Ni binuclear molecular magnets.** — •KARSTEN KUEPPER<sup>1</sup>, ULF WIEDWALD<sup>1</sup>, FLORIAN MÖGELE<sup>2</sup>, BERNHARD RIEGER<sup>3</sup>, and PAUL ZIEMANN<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm — <sup>2</sup>Institut für Materialien und Katalyse, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm — <sup>3</sup>WACKER-Lehrstuhl für Makromolekulare Chemie, Technische Universität München, Lichtenbergstraße 4, 85747 Garching bei München

Molecular magnets display a large variety of new and complex chemical and physical properties. We have investigated three planar TM-Ni-C<sub>46</sub>H<sub>68</sub>N<sub>2</sub>O<sub>6</sub> (TM=Mn,Fe,Co) molecules, which show uncompensated magnetic moments [1] by means of ultra-low temperature XMCD. The experiments have been performed at a temperature of 0.6K in order to probe the magnetic ground state properties. For all three complexes we find Ni to be divalent, also Mn and Co are in a 2+ valence state, whereas mainly Fe<sup>3+</sup> ions are present in the Fe-Ni molecule. We find different internal magnetic structures. In the Co-Ni molecule the Ni appears to be in a low spin state, thus no dichroic signal is present, whereas Co shows a strong MCD. A similar result is observed for the Mn-Ni complex, only a very small dichroic Ni signal is present. However, for the Fe-Ni complex both, the Fe and Ni spectra are dichroic, revealing a ferromagnetic alignment of the Ni and Fe ions in this molecule.

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

## MA 2.4 Mon 11:30 H10

**Approximate eigenvalue determination of geometrically frustrated magnetic molecules** — •ROMAN SCHNALLE — Universität Bielefeld, Fakultät für Physik, Universitätsstraße 25, D-33615 Bielefeld

Geometrically frustrated magnetic molecules have attracted a lot of interest in recent years. Interesting physical phenomena related to frustration that have been observed in zero-dimensional systems directly link the research fields of molecular and highly frustrated magnetism. In order to further investigate frustration effects in finite-size systems like magnetic molecules numerical exact diagonalization would be the method of choice. Having calculated the full energy spectra of such systems all thermodynamic and spectroscopic properties can be deduced.

Unfortunately, although not affected by conceptual problems arising from geometrical frustration, the application of numerical exact diagonalization is limited to rather small molecular systems. Especially, the magnetic behavior of the zero-dimensional representation of the Kagomé lattice – one of the most investigated extended antiferromagnetic systems – cannot be resolved by a numerical exact diagonalization. Nevertheless, an approximate numerical method that is based on a diagonalization within a reduced but carefully chosen set of basis states can be used to get insight into the physics of rather large frustrated systems [1].

[1] R. Schnalle, A. Läuchli, J. Schnack, *Cond. Mat. Phys.* **12**, 331 (2009).

## MA 2.5 Mon 11:45 H10

**Magnetic response of magnetic molecules with non-collinear local d-tensors** — •JÜRGEN SCHNACK — Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld

Investigations of molecular magnets are driven both by prospective applications in future storage technology or quantum computing as well as by fundamental questions. Nowadays numerical simulation techniques and computer capabilities make it possible to investigate spin Hamiltonians with realistic arrangements of local anisotropy tensors. In this contribution I will discuss several recently synthesized molecules and their magnetic properties [1-3].

[1] Ian S. Tidmarsh, Luke J. Batchelor, Emma Scales, Rebecca H. Laye, Lorenzo Sorace, Andrea Caneschi, Jürgen Schnack and Eric J. L. McInnes, *Dalton Trans.* (2009) 9402-9409

[2] J. Schnack, *Condens. Matter Phys.* **12** (2009) 323-330

[3] Thorsten Glaser, Maik Heidemeier, Hubert Theil, Anja Stammler, Hartmut Bögge and Jürgen Schnack, *Dalton Trans.* (2010) in print

## MA 2.6 Mon 12:00 H10

**Magnetization measurements of a novel family of heteronuclear Mn<sub>2</sub>Ni<sub>3</sub> SMM clusters** — •KLAUS GIEB<sup>1</sup>, ANIMESH DAS<sup>2</sup>, YULIA KRUPSKAYA<sup>3</sup>, WOLFGANG KROENER<sup>1</sup>, SERHIY DEMESHKO<sup>2</sup>, RÜDIGER KLINGELER<sup>3</sup>, VLADISLAV KATAEV<sup>3</sup>, BERND BÜCHNER<sup>3</sup>, FRANC MEYER<sup>2</sup>, and PAUL MÜLLER<sup>1</sup> — <sup>1</sup>Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany — <sup>2</sup>Institut für Anorganische Chemie, Georg-August-Universität Göttingen, Germany — <sup>3</sup>Leibniz-Institute for Solid State and Materials Research IFW Dresden, Germany

We report on magnetic measurements of two heterometallic Mn<sub>2</sub><sup>II</sup>Ni<sub>3</sub><sup>II</sup>X<sub>2</sub>L<sub>4</sub>(LH)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> (X = Cl, Br) complexes. These compounds have a ground state spin of  $S = 7$  and show an easy-axis type of anisotropy. DC and AC susceptibility measurements were performed with a commercial SQUID magnetometer. A home-made micro-Hall-probe magnetometer was used to perform the characterization at mK temperatures. We found an uniaxial anisotropy parameter of  $D \simeq -0.5$  K. Magnetic hysteresis and quantum tunneling of magnetization was observed at temperatures below a blocking temperature  $T_B \simeq 1.5$  K. The shape of the hysteresis loop is influenced by intermolecular interactions. The signature of these interactions can be modified by the variation of the Mn coordination partner X.

## MA 2.7 Mon 12:15 H10

**High-field ESR on the Mn<sub>2</sub>Ni<sub>3</sub> single molecular magnet** — •Y. KRUPSKAYA<sup>1</sup>, A. DAS<sup>2</sup>, K. GIEB<sup>3</sup>, W. KROENER<sup>3</sup>, S. DEMESHKO<sup>2</sup>, S. DECHERT<sup>2</sup>, R. KLINGELER<sup>1</sup>, V. KATAEV<sup>1</sup>, P. MÜLLER<sup>3</sup>, F. MEYER<sup>2</sup>, and B. BÜCHNER<sup>1</sup> — <sup>1</sup>Leibniz Institute for Solid State and Materials Research (IFW) Dresden, D-01171 Dresden, Germany — <sup>2</sup>Institut für Anorganische Chemie, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — <sup>3</sup>Lehrstuhl für Experimentalphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Magnetic properties of a novel metal-organic molecular complex with [Mn(III)<sub>2</sub>Ni(II)<sub>3</sub>(μ-O)<sub>8</sub>] core have been studied by means of high-field electron spin resonance (HF-ESR) spectroscopy and magnetization measurements. We observe a ferromagnetic coupling between three Ni(II) and two Mn(III) ions which yields a high spin magnetic ground state with  $S_{\text{tot}} = 7$ . Frequency-tunable HF-ESR spectroscopy reveals a substantial magnetic anisotropy gap with a negative axial anisotropy  $D = -0.55$  K which gives evidence for a bistable (easy axis) magnetic

ground state of the molecule. The analysis of the ESR data by means of a minimal effective spin Hamiltonian enables an accurate description of the energy level scheme and the spin states of the complex. The observed high spin ground state and the negative axial anisotropy ensure necessary prerequisites for the realization of a single molecular magnet. Indeed, at low temperatures ( $T < 1$  K) magnetization measurements reveal a single molecular magnet behavior such as hysteresis and tunnelling of the magnetization.

MA 2.8 Mon 12:30 H10

**Magnetic coupling between Fe phthalocyanine molecules and ferromagnets** — •CLAUDIA WEIS, BERNHARD KRUMME, FRANK STROMBERG, ANNE WARLAND, CAROLIN ANTONIAK, WERNER KEUNE, and HEIKO WENDE — Fakultät für Physik and CeNIDE, Universität Duisburg-Essen

On the road towards molecular spintronic devices magnetic organic molecules on ferromagnetic surfaces play an important role. Going beyond earlier investigations on Fe porphyrin (FeOEP) molecules [1-2] the present work aims to study the influence of changes in the ligand field on the magnetic coupling. From Mössbauer spectra of bulk-like samples, it is obvious that a considerable difference occurs between Fe phthalocyanine (FePc) and FeOEP. We investigate sub-monolayer coverages of magnetic FePc molecules on ultrathin ferromagnetic films of Ni and Co on Cu(100) by X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD). We find that also the FePc molecules couple to ferromagnets similar to the FeOEP molecules [1-2]. The magnetic coupling between the molecules and the magnetic substrate turns from ferromagnetic to antiferromagnetic if an interlayer of oxygen is introduced by oxygen surfactant-assisted growth of the ferromagnetic film. Similarities and differences in the fine structure of the spectra will be discussed in detail.

[1] H. Wende et al., Nature Materials **6**, 516 (2007).

[2] M. Bernien et al., Phys. Rev. Lett. **102**, 047202 (2009).

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MA 2.9 Mon 12:45 H10

**Preparation and characterization of Mn<sub>6</sub>Cr single-molecule-magnets on surfaces** — •MARC SACHER<sup>1</sup>, ANDREAS HELMSTEDT<sup>1</sup>, AARON GRYZIA<sup>1</sup>, PETER KOOP<sup>1</sup>, SEBASTIAN STEPPLE<sup>1</sup>, NORBERT MÜLLER<sup>1</sup>, ARMIN BRECHLING<sup>1</sup>, ULRICH HEINZMANN<sup>1</sup>, VERONIKA HÖKE<sup>2</sup>, THORSTEN GLASER<sup>2</sup>, MIKHAIL FONIN<sup>3</sup>, and ULRICH RÜDIGER<sup>3</sup> — <sup>1</sup>Fak. f. Physik, Uni Bielefeld — <sup>2</sup>Fak. f. Chemie, Uni Bielefeld — <sup>3</sup>Fak. f. Physik, Uni Konstanz

The single-molecule-magnet (SMM) Mn<sub>6</sub>Cr consists of two bowl-

shaped Mn<sub>3</sub>-salen complexes, bridged by a complex containing a Cr atom. Three counterions are coupled to the SMM to ensure charge neutrality. To study the influence of the molecule-substrate-interaction on the electronic and the magnetic properties a homogeneous preparation of the SMM on the substrate is necessary. The preparation is done by dropping SMM, dissolved in methanol with certain concentration. Depending on the choice of the substrate, the Mn<sub>6</sub>Cr concentration, the substrate inclination and the droplet size the arrangement of the SMM strongly varies. This will be visualized in videos of the drying process obtained by optical microscopy with a magnification of up to 1000. The electronic properties of the deposited SMM are investigated by X-ray absorption spectroscopy. These properties change with exposure time due to a low stability of the SMM against X-rays. These changes can be accelerated or slowed down via the choice of the counterions and the SMM concentration on the substrate. Possible reasons will be discussed.

MA 2.10 Mon 13:00 H10

**Understanding the Composition of the Ground-State Spin - Subtle Structural Differences lead to Spin Maximization in Mn<sub>7</sub> Disks** — •JOSCHA NEHRKORN<sup>1</sup>, OLIVER WALDMANN<sup>1</sup>, SHREYA MUKHERJEE<sup>2</sup>, GEORGE CHRISTOU<sup>2</sup>, THIERRY STRÄSSLE<sup>3</sup>, and HANNU MUTKA<sup>4</sup> — <sup>1</sup>Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany — <sup>2</sup>Department of Chemistry, University of Florida, Gainesville, Florida 32611-7200, USA — <sup>3</sup>LNS, ETH Zürich & Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — <sup>4</sup>Institut Laue-Langevin, 38042 Grenoble, France

The magnetic properties of molecular nanomagnets depend strongly on the ground-state spin  $S$  of the molecule. For instance, a large value of  $S$  can give rise to quantum tunneling of the magnetization, while systems with small  $S$  can show quantum tunneling of the Néel vector.  $S$  depends on the magnetic exchange couplings between the spin centers in the molecule. Small differences in the ligands should only have a small effect, however, for two related Mn<sub>7</sub> disks a big effect on  $S$  was observed: in Mn<sub>7</sub>11 the ground-state spin is  $S = 11$  while in Mn<sub>7</sub>16 it has the maximal value  $S = 16$ . To understand the spin maximization we studied the magnetic interactions in the two Mn<sub>7</sub> disks by inelastic neutron scattering, which allowed us to determine the magnetic exchange couplings and weak magnetic anisotropy. The small perturbation in the ligand shell leads to slightly different exchange coupling constants, which, however, due to the frustrating nature of some of these couplings, leads to very different energy schemes and ground states.