

MA 40: Molecular Magnetism

Time: Thursday 15:00–17:15

Location: H23

MA 40.1 Thu 15:00 H23

Single molecule magnets from magnetic building blocks — ●WOLFGANG KROENER¹, ALEXA PARETZKI^{2,3}, CHRISTIAN CERVETTI^{2,4}, STEPHAN HOHLOCH³, STEPHAN RAUSCHENBACH⁴, KLAUS KERN⁴, MARTIN DRESSEL², LAPO BOGANI², and PAUL MÜLLER¹ — ¹Lehrstuhl für Experimentalphysik, Universität Erlangen — ²1. Physikalisches Institut, Universität Stuttgart — ³Institut für Anorganische Chemie, Universität Stuttgart — ⁴Max Planck Institut für Festkörperforschung, Stuttgart

We present measurements of a basic set of magnetic building blocks that were rationally assembled, similar to magnetic LEGO bricks, in order to create a huge variety of magnetic behavior¹. Using rare-earth centers and multipyridine ligands, fine-tuning of intra and intermolecular exchange interaction was demonstrated. We have investigated a series of molecules with monomeric, dimeric and trimeric lanthanide centers using SQUID susceptometry and Hall bar magnetometry. A home-made micro-Hall-probe magnetometer was used to measure magnetic hysteresis loops at mK temperatures and fields up to 17 T. All compounds show hysteresis below blocking temperatures of 3 to 4 K. The correlation of the assembly of the building blocks with the magnetic properties will be discussed.

¹A. Paretzki et al. Nature Chemistry, submitted

MA 40.2 Thu 15:15 H23

Substrate Dependent Thermal Deposition of NdPc₂ Single Molecules — ●SARAH FAHRENDORF^{1,2}, FRANK MATTHES^{1,2}, CLAIRE BESSON^{1,2,3}, PAUL KÖGERLER^{1,2,3}, DANIEL E. BÜRGLER^{1,2}, and CLAUS M. SCHNEIDER^{1,2} — ¹Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — ²Jülich-Aachen Research Alliance (JARA-FIT), Forschungszentrum Jülich, 52425 Jülich, Germany — ³Institute of Inorganic Chemistry, RWTH Aachen, D-52074 Aachen, Germany

Single molecule magnets play an important role in the field of molecular spintronics. A relevant class of molecules are the lanthanide double-decker phthalocyanines (LaPc₂) with only one metal atom in the center of the two organic phthalocyanine ligands. For envisaged spintronics applications it is important to understand the interaction between the substrate and the molecules and its influence on the electronic properties. Here, we study the substrate dependent deposition characteristics of neodymium double-decker phthalocyanines (NdPc₂) by means of low temperature scanning tunneling microscopy and spectroscopy (STM and STS). The NdPc₂ molecules were in-situ evaporated from a Knudsen cell on clean metallic surfaces such as Au(111), Cu(100), and Fe(110). It is observed that a significant fraction of the double-decker phthalocyanines decompose into two single-decker phthalocyanine molecules. The decomposition probability is found to be strongly substrate dependent. By means of STS-spectra we find that stronger substrate molecule interaction leads to enhanced charge transfer which strengthens the intramolecular electrostatic bonding.

MA 40.3 Thu 15:30 H23

Exchange-based and single-ion based relaxation of the magnetization in Ni₂Dy — ●ALEXANDER SUNDT¹, AMIN KHAN², PASCAL WENDLER¹, YANHUA LAN², ANNIE K. POWELL², and OLIVER WALDMANN¹ — ¹Physikalisches Institut, Universität Freiburg, Germany — ²Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Germany

Ever since the discovery of slow relaxation of the magnetization at the molecular scale in Mn₁₂ac scientists focused on increasing the energy barrier for magnetization reversal U_{eff} in order to lift the single molecule magnet (SMM) behaviour from cryogenic to easier accessible temperatures for possible applications. A promising road to increase U_{eff} is the incorporation of highly anisotropic magnetic ions such as rare earth ions in heterometallic SMMs. However, using these ions presents novel challenges such as complicated relaxation pathways.

In this talk we present an experimental study by means of AC and DC susceptibility as well as single crystal magnetization measurements on the 3d4f heterometallic SMM Ni₂Dy. The data show that the blocking mechanism for magnetization reversal undergoes as function of temperature a crossover from an exchange-based to a single-ion based relaxation mechanism. In contrast to the situation in Co₂Dy₂, where we could identify the phenomenon for the first time [1], some significant

differences are observed, which will be discussed.

[1] K. C. Mondal, A. Sundt, *et. al.*, Angew. Chem. 124, 7668 (2012)

MA 40.4 Thu 15:45 H23

The role of dysprosium in single-molecule magnets based on mixed metal nitride cluster fullerenes — ●RASMUS WESTERSTRÖM^{1,2}, JAN DREISER², CINTHIA PIAMONTEZE², ROLAND STANIA^{1,2}, FUMIHIKO MATSUI^{1,3}, STEPHEN WEYENETH¹, VEACHE-SLAV VIERU⁴, LIVIU UNGUR⁴, LIVIU CHIBOTARU⁴, STEFANO RUSPONI⁵, HARALD BRUNE⁵, SHANGFENG YANG^{6,7}, ALEXEY POPOV⁶, MATTHIAS MUNTWILER², LOTHAR DUNSCH⁶, and THOMAS GREBER¹ — ¹Physik-Institut, Universität Zürich, Switzerland — ²Swiss Light Source, Paul Scherrer Institut, Switzerland — ³NAIST Ikoma, Nara, Japan — ⁴Division of Quantum and Physical Chemistry, Katholieke Universiteit Leuven, Belgium — ⁵Institute of Condensed Matter Physics, EPFL, Lausanne, Switzerland — ⁶Hefei National Laboratory for Physical Sciences at Microscale, Department of Materials Science and Engineering, USTC, China — ⁷Department of Electrochemistry and Conducting Polymers, Leibniz Institute of Solid State and Materials Research, Dresden, Germany

So far it was known that the metal nitride cluster fullerenes Ln₃N@C₈₀ (Ln = Tb, Ho) are paramagnetic above 1.8 K [1]. Here we report on the first fullerene exhibiting single-molecule magnet behaviour [2]. The magnetism of DySc₂N@C₈₀ was studied using x-ray magnetic circular dichroism (XMCD), SQUID, and *ab initio* calculations. SQUID show hysteresis and thermal and nonthermal spin relaxation. In a next step endofullerenes containing more than one Dy ion were investigated.

[1] M. Wolf *et al.*, Angew. Chem. Int. Ed. 44, 3306 (2005).

[2] R. Westerström *et al.*, J. Am. Chem. Soc. 134, 9840 (2012).

15 min. break

MA 40.5 Thu 16:15 H23

Large-scale numerical investigations of the antiferromagnetic Heisenberg icosidodecahedron — JÖRG UMMETHUM¹, ANDREAS LÄUCHLI², and ●JÜRGEN SCHNACK¹ — ¹Bielefeld University, P.O. box 100131, D-33501 Bielefeld — ²Innsbruck University, Technikerstr. 25, A-6020 Innsbruck

We present up to date investigations of the antiferromagnetic Heisenberg icosidodecahedron by means of the Density Matrix Renormalization Group method. We compare our results with modern Correlator Product State as well as Lanczos calculations.

J. Ummethum, J. Schnack, A.M. Laeuchli, J. Magn. Magn. Mater. 327 (2013) 103-109

MA 40.6 Thu 16:30 H23

Unconventional Magnetic Properties of the Antiferromagnetic Heisenberg Model on Two Linked Dodecahedra — ●NIKOLAOS P. KONSTANTINIDIS — Fachbereich Physik und Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

The antiferromagnetic Heisenberg model has been shown to possess a non-trivial magnetic response in an external field for spins located on the vertices of a dodecahedron [1,2]. Here a first step towards a lattice of dodecahedra is taken by considering two dodecahedra linked along one of their faces with varying exchange coupling. The competition between intramolecular frustration, intermolecular coupling and magnetic field leads to a richer phase diagram compared to the single dodecahedron case. In the case of classical spins, the magnetization response may contain up to six magnetization discontinuities. In the full quantum case $s_i = 1/2$ the states are characterized by the full symmetry of the Hamiltonian, and for weak intermolecular couplings there can be up to two magnetization discontinuities in a field. These discontinuities are unexpected for the antiferromagnetic Heisenberg model, which lacks magnetic anisotropy, and are a direct consequence of the exchange coupling geometry and its competition with the field. These results show the potential for non-trivial magnetic properties in structures build up from dodecahedra.

[1] N. P. Konstantinidis, Phys. Rev. B 72, 064453 (2005).

[2] N. P. Konstantinidis, Phys. Rev. B 76, 104434 (2007).

MA 40.7 Thu 16:45 H23

Huge magnetically coupled orbital moments of Co porphyrin molecules and their control by CO adsorption —

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We report on a combined experimental-theoretical study of physisorbed Co-porphyrin molecules on a graphene-protected Ni film. By using X-ray magnetic circular dichroism, we show that an antiferromagnetic coupling between the Co and Ni spins is established across graphene. According to density functional theory calculations the coupling is mediated via the π electronic system of graphene. The Co ions, despite their four-fold coordination, reveal a huge measured in-plane orbital moment m_l , even comparable in size to the spin moment. Carbon monoxide adsorption on top of the molecules reduces the Co orbital moment by $(77 \pm 6)\%$ and the entire magnetic moment by $(37 \pm 3)\%$, without modifying the spin state $S=1/2$. This is attributed to the change of the crystal field by the chemical stimulus, which determines m_l together with the spin-orbit coupling.

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MA 40.8 Thu 17:00 H23

Quenching the quantum tunneling of magnetization in

Mn₆Cr single-molecule magnets — •KLAUS GIEB¹, VERONIKA HOEKE², WOLFGANG KROENER¹, THORSTEN GLASER², and PAUL MÜLLER¹ — ¹Department für Physik, Universität Erlangen — ²Department Chemie und Pharmazie, Universität Bielefeld

We report on low-temperature magnetic measurements of Mn₆Cr³⁺ single molecule magnets with different counter ions and crystal structures [1]. From SQUID susceptibility measurements it can be concluded that the ground state spin for these molecules is $S_t = 21/2$. Ac susceptibility measurements reveal a D parameter of around $D = -0.23$ K. By variation of the counter ions and solvent molecules, the molecular C_3 symmetry can be slightly changed. This results in a tuning of the transversal anisotropy parameter that can be directly observed in low temperature single crystal Hall probe measurements: No tunneling steps were present in these measurements. Based on ac and dc relaxation measurements we show, that the transversal anisotropy is completely quenched in some cases. For the first time it is proved that a true C_3 molecular symmetry can lead to a vanishing E term and therefore to stable magnetized state over month without an external field.

1. Hoeke, V., K. Gieb, P. Muller, L. Ungur, L.F. Chibotaru, M. Heidemeier, E. Krickemeyer, A. Stammler, H. Bogge, C. Schroder, J. Schnack, T. Glaser, Chemical Science, **3**, 2868 (2012).