

## MA 11: Bio- and Molecular Magnetism (joint session MA/CPP)

Time: Monday 15:00–17:00

Location: HSZ 101

MA 11.1 Mon 15:00 HSZ 101

**HF-EPR investigations on Co(II)- and Fe(IV)-coordination complexes** — ●LENA SPILLECKE<sup>1</sup>, CHANGHYUN KOO<sup>1</sup>, SHALINI TRIPATHI<sup>2</sup>, MAHESWARAN SHANMUGAM<sup>2</sup>, SASKIA KRIEG<sup>3</sup>, PETER COMBA<sup>3</sup>, and RÜDIGER KLINGELER<sup>1</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — <sup>2</sup>Department of Chemistry, Indian Institute of Technology, Mumbai, India — <sup>3</sup>Institute of Inorganic Chemistry, Universität Heidelberg, Heidelberg, Germany

We present high-frequency/high-field electron paramagnetic resonance (HF-EPR) studies on Co(II) and Fe(IV) coordination complexes. For Co(II) systems, we show that ligand exchange in the 2nd coordination sphere on [Co(L<sub>1</sub>)<sub>4</sub>]X<sub>2</sub>, with L<sub>1</sub> = thiourea (NH<sub>2</sub>CSNH<sub>2</sub>) and X = I (1), Br (2), SiF<sub>6</sub> (3) has significant effects on the crystal field and hence on magnetic anisotropy of the Co-ion. While the substitution of I by Br only has small impact on the axial anisotropy ( $D = -153(2)/-168(5)$  GHz, respectively), we observed strong enhancement of anisotropy in the SiF<sub>6</sub> containing sample ( $|D| > 800$  GHz). Furthermore, our data enables precise determination of weak intermolecular coupling in the range of several hundred mK which sign changes by ligand substitution. In addition, we present HF-EPR data on an octahedrally coordinated Fe(IV)-complex which was prepared under liquid N<sub>2</sub> conditions. Our results confirm the intermediate-spin state and detect axial anisotropy of  $D = 107(3)$  GHz.

MA 11.2 Mon 15:15 HSZ 101

**Magnetic field tuning of low energy spin dynamics in the single-atomic magnet Li<sub>2</sub>(Li<sub>1-x</sub>Fe<sub>x</sub>)N with  $x \ll 1$**  — ●SASCHA ALBERT BRÄUNINGER<sup>1</sup>, SIRKO KAMUSELLA<sup>1</sup>, FELIX SEEWALD<sup>1</sup>, RAJIB SARKAR<sup>1</sup>, MANUEL FIX<sup>2</sup>, STEPHAN JANTZ<sup>2</sup>, ANTON JESCHE<sup>2</sup>, ANDRE ZVYAGIN<sup>3</sup>, and HANS-HENNING KLAUSS<sup>1</sup> — <sup>1</sup>Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — <sup>2</sup>Institute of Physics, University Augsburg, D-86135 Augsburg, Germany — <sup>3</sup>Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str., 38, D-01187 Dresden, Germany

We present a systematic <sup>57</sup>Fe-Mössbauer study on highly diluted Fe centers in Li<sub>2</sub>(Li<sub>1-x</sub>Fe<sub>x</sub>)N single-crystals as a function of temperature and magnetic field applied transverse and longitudinal with respect to the single-ion anisotropy axis. Below 30 K the Fe centers exhibit a giant magnetic hyperfine field of  $\bar{B}_A = 70.25(2)$  T parallel to the axis of strongest electric field gradient  $\bar{V}_{zz} = -154.0(1)$  V/Å<sup>2</sup>. Fluctuations of the magnetic hyperfine field are observed between 50 K and 300 K and described by the Blume two-level relaxation model. An Arrhenius analysis yields a single thermal activation barrier of  $\bar{E}_A = 570(6)$  K. Mössbauer spectroscopy studies with applied transverse magnetic fields up to 5 T reveal a large increase of the fluctuation rate by more than one order of magnitude. The experimental observations are qualitatively reproduced by a single-ion effective spin Hamiltonian analysis assuming a Fe<sup>1+</sup>  $d^7$  charge state with unquenched orbital moment and a  $J = 7/2$  ground state.

MA 11.3 Mon 15:30 HSZ 101

**Intramolecular crossover from 2D diamagnetism to 3D paramagnetism** — ●CAROLIN SCHMITZ-ANTONIAK<sup>1</sup>, ALEVTINA SMEKHOVA<sup>2</sup>, DETLEF SCHMITZ<sup>2</sup>, NATALYA V. IZAROVA<sup>1</sup>, S. FATEMEH SHAMS<sup>1</sup>, MARIA STUCKART<sup>3</sup>, FRANK M. F. DE GROOT<sup>4</sup>, and PAUL KÖGERLER<sup>1,5</sup> — <sup>1</sup>Forschungszentrum Jülich (PGI-6), 52425 Jülich — <sup>2</sup>Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin — <sup>3</sup>Inst. f. Chem. Reaktionstechnik, FAU Erlangen-Nürnberg, 91058 Erlangen — <sup>4</sup>Inorganic Chemistry and Catalysis Group, Debye Inst. for Nanomaterials Science, Utrecht University, Utrecht 3584 CG — <sup>5</sup>Inst. f. Anorgan. Chemie, RWTH Aachen University, 52074 Aachen

In a 2D square-planar coordination with four surrounding oxygen anions, Pd(II) ions in polyoxopalladates are diamagnetic with a large orbital contribution to the magnetic response as revealed by XANES and XMCD. Supported by atomic multiplet calculations the dependence of electronic and magnetic properties on 4d spin-orbit coupling, bond lengths, and delocalization of 4d electrons was investigated. We found that (i) four additional out-of-plane oxygen anions around Pd(II) lead to an effective 3D symmetry causing a paramagnetic response in external magnetic fields and (ii) in the crossover region between common diamagnetism and paramagnetism, the large spin-orbit coupling of Pd facilitates an unusual diamagnetic state modified by signif-

icant mixing. Furthermore, by measuring and analysing characteristic fine structures of the diamagnetic states in the XMCD spectrum, we overcome the common limitation of XMCD to ferro/ferrimagnetic and paramagnetic materials in external magnetic fields.

MA 11.4 Mon 15:45 HSZ 101

**Chemical Doping of Individual Polynuclear Molecular Magnets on Surfaces** — ●FABIAN PASCHKE<sup>1</sup>, VIVIEN ENENKEL<sup>1</sup>, TOBIAS BIRK<sup>1</sup>, JAN DREISER<sup>2</sup>, and MIKHAIL FONIN<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — <sup>2</sup>Swiss Light Source, 5232 Villigen PSI, Switzerland

The controlled deposition, characterization and manipulation of single molecule magnets (SMMs) on surfaces is one of the crucial topics to investigate with regard to their possible implementation as units in future electronic and spintronic devices. Fe<sub>4</sub> derivatives are among the most investigated SMMs showing a giant spin and a variety of quantum mechanical phenomena. We showed that a flat derivative of this SMM is suitable for defined adsorption on decoupling monatomic layers of *h*-BN and graphene [1,2]. We proved the robust molecular magnetism to be retained on a global and single molecule scale, even on metallic substrates [2-4]. In order to manipulate electronic and magnetic properties of individual SMMs chemical doping with alkali atoms has shown to be a feasible technique [5]. Unfortunately, large polynuclear compounds like Fe<sub>4</sub> can host numerous adsorption sites for dopants. Here we present successful chemical doping with a defined adsorption configuration for the prototypical Fe<sub>4</sub> SMM and study the effect on its electronic and magnetic properties.

[1] P. Erler et al., *Nano Lett.* 15, 4546 (2015). [2] L. Gragnaniello et al., *Nano Lett.* 17, 7177 (2017). [3] F. Paschke et al., *ACS Nano* 13, 780 (2019). [4] F. Paschke et al., *submitted* (2019). [5] C. Krull et al., *Nat. Mat.* 12, 337 (2013).

MA 11.5 Mon 16:00 HSZ 101

**Numerical Challenges in Studying Families of 3d-4f Heterometallic Single-Molecule Magnets** — ●JULIUS MUTSCHLER<sup>1</sup>, HETTI M. JAYAWARDENA<sup>1</sup>, CHRISTOPHER E. ANSON<sup>2</sup>, ANNIE K. POWELL<sup>2</sup>, and OLIVER WALDMANN<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Freiburg, Germany — <sup>2</sup>Institut für anorganische Chemie, Universität Karlsruhe, KIT, Germany

The discovery of slow relaxation and quantum tunneling of the magnetization in single molecule magnets (SMMs) has inspired both physicists and chemists alike. This class of molecules has been expanded to heterometallic clusters incorporating transition metal and rare earth ions. The 4f ions are of interest because of their large angular momentum and magnetic anisotropy, but present unexpected challenges in the numerical analysis of experimental powder susceptibility and magnetization curves. For example in the case of the 3d-4f SMM Mn<sub>2</sub>Ho<sub>2</sub>-square, the dimension of the Hilbert space is 7225, and the computation time for a full exact diagonalization is only few 10 seconds. However, when fitting the powder magnetization with a 10 parameter model, which is typical for this type of molecules, ca 10<sup>7</sup> diagonalizations need to be performed, resulting in an impractical total time for completing the fit of several years. In this talk our approaches to tackle this challenge are demonstrated.

MA 11.6 Mon 16:15 HSZ 101

**Dy<sub>2</sub>O-clusterfullerenes: Strong magnetic anisotropy and fullerene-dependent single molecule magnetism** — ●GEORGIOS VELKOS<sup>1</sup>, WEI YANG<sup>2</sup>, STANISLAV AVDOSHENKO<sup>1</sup>, NING CHEN<sup>2</sup>, BERND BÜCHNER<sup>1</sup>, and ALEXEY POPOV<sup>1</sup> — <sup>1</sup>Leibniz Institute for Solid State and Materials Research, Dresden, Germany — <sup>2</sup>College of Chemistry, Soochow University, Suzhou, China

The exceptional ability of fullerenes to stabilize species which can hardly exist otherwise has been extensively used to create a number of endohedral metallofullerene families. Among them, there is a great interest in Dy-metallofullerenes, caused by their robust magnetic properties. In this work, we report on the synthesis and in-depth magnetic study of the first Dy<sub>2</sub>O-clusterfullerenes. The compact geometry of Dy<sub>2</sub>O cluster leads to both strong axial ligand field and unprecedentedly strong antiferromagnetic exchange coupling between Dy ions. We demonstrate that Dy<sub>2</sub>O-clusterfullerenes are excellent molecular magnets exhibiting broad magnetic hysteresis and the strongest

super-exchange coupling between Dy ions ever reported for non-radical bridged compounds.

MA 11.7 Mon 16:30 HSZ 101

**Dynamic magnetic response of a single Magnetite nanoparticle chain detected by Scanning Transmission X-Ray Microscopy Ferromagnetic Resonance** — •THOMAS FEGGELER<sup>1</sup>, BENJAMIN ZINGSEM<sup>1,2</sup>, RALF MECKENSTOCK<sup>1</sup>, MICHAEL WINKLHOFER<sup>3</sup>, DETLEF SPODDIG<sup>1</sup>, HENDRIK OHLDA<sup>4</sup>, MICHAEL FARLE<sup>1</sup>, HEIKO WENDE<sup>1</sup>, and KATHARINA OLLEFS<sup>1</sup> — <sup>1</sup>Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, Duisburg, Germany — <sup>2</sup>ERC and PGI, Fz. Jülich GmbH, Jülich, Germany — <sup>3</sup>School of Mathematics and Science, University of Oldenburg, Oldenburg, Germany — <sup>4</sup>Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

The dynamic magnetization of a single nanoparticle chain of 19 Magnetite particles (diameter of about 50 nm) embedded in a bacterium *Magnetospirillum Magnetotacticum* is measured using Scanning Transmission X-Ray Microscopy detected Ferromagnetic Resonance (STXM-FMR) [1]. A resonant response of the segments of the nanoparticle chain is identified and confirmed by micromagnetic simulations. STXM-FMR features the element specific detection of magnetization dynamics with a spatial resolution  $< 50$  nm and a time resolution in the ps regime. The manipulation of the genetic code of the bacteria allows to control the arrangement of the nanoparticles leading to the creation of magnonic logic devices as a future concept for magnonic computing [2]. [1] S. Bonetti, et al., Rev. Sci. Instrum. 86 (2015). [2] B. W. Zingsem, et al., Nat. Commun. 10 (2019). Financial support:

FWF Project I-3050, ORD-49, DFG Project 321560838.

MA 11.8 Mon 16:45 HSZ 101

**Biologically encoded magnonics** — •BENJAMIN ZINGSEM<sup>1</sup>, THOMAS FEGGELER<sup>1</sup>, RALF MECKENSTOCK<sup>1</sup>, MICHAEL FARLE<sup>1</sup>, and MICHAEL WINKLHOFER<sup>1,2</sup> — <sup>1</sup>University Duisburg-Essen — <sup>2</sup>Universität Oldenburg

We report on the spectral properties of spin-waves (magnons) in individual chains of dipolar coupled magnetite nanoparticles. The particle-chains are biologically produced in magnetotactic bacteria. Straight chains where obtained from wild-type, curved and looped chains form mutant bacteria. A strong link between distinct spectral properties of the chains and their geometrical arrangement is identified, paving the way towards genetically engineered spin-wave computing on the nanoscale. Each chain consists of ca. 12 nanoparticles with a diameter of about 30 nm, separated by a spacing of about 8 nm. Ferromagnetic resonance spectroscopy was employed to measure the magnonic Eigenstates of each single particle in the chain as a function of the magnitude and direction of an applied magnetic field. The measurements are supplemented with micromagnetic simulations, which reveal the origin of spectral features such as band repulsion and attraction in resonant eigenstates. The emergent topology of the spin-wave band structure exhibits functional properties such as band deflection and band deformation, which may be harnessed in energy efficient magnon computing [1] and neuro-inspired magnonic networks. Future nanomagnonic devices may be self-assembled via genetic engineering of magnetotactic bacteria.

[1] B. Zingsem, et al. Nat Commun 10, 4345 (2019)