

CPP 25: Bio- and Molecular Magnetism (joint session MA/CPP)

Time: Monday 15:00–17:00

Location: HSZ 101

CPP 25.1 Mon 15:00 HSZ 101

HF-EPR investigations on Co(II)- and Fe(IV)-coordination complexes — ●LENA SPILLECKE¹, CHANGHYUN KOO¹, SHALINI TRIPATHI², MAHESWARAN SHANMUGAM², SASKIA KRIEG³, PETER COMBA³, and RÜDIGER KLINGELER¹ — ¹Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — ²Department of Chemistry, Indian Institute of Technology, Mumbai, India — ³Institute 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(L₁)₄]X₂, with L₁ = thiourea (NH₂CSNH₂) and X = I (1), Br (2), SiF₆ (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 SiF₆ 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 N₂ conditions. Our results confirm the intermediate-spin state and detect axial anisotropy of $D = 107(3)$ GHz.

CPP 25.2 Mon 15:15 HSZ 101

Magnetic field tuning of low energy spin dynamics in the single-atomic magnet Li₂(Li_{1-x}Fe_x)N with $x \ll 1$ — ●SASCHA ALBERT BRÄUNINGER¹, SIRKO KAMUSELLA¹, FELIX SEEWALD¹, RAJIB SARKAR¹, MANUEL FIX², STEPHAN JANTZ², ANTON JESCHE², ANDRE ZVYAGIN³, and HANS-HENNING KLAUSS¹ — ¹Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — ²Institute of Physics, University Augsburg, D-86135 Augsburg, Germany — ³Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str., 38, D-01187 Dresden, Germany

We present a systematic ⁵⁷Fe-Mössbauer study on highly diluted Fe centers in Li₂(Li_{1-x}Fe_x)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/Å². 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 Fe¹⁺ d^7 charge state with unquenched orbital moment and a $J = 7/2$ ground state.

CPP 25.3 Mon 15:30 HSZ 101

Intramolecular crossover from 2D diamagnetism to 3D paramagnetism — ●CAROLIN SCHMITZ-ANTONIAK¹, ALEVTINA SMEKHOVA², DETLEF SCHMITZ², NATALYA V. IZAROVA¹, S. FATEMEH SHAMS¹, MARIA STUCKART³, FRANK M. F. DE GROOT⁴, and PAUL KÖGERLER^{1,5} — ¹Forschungszentrum Jülich (PGI-6), 52425 Jülich — ²Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin — ³Inst. f. Chem. Reaktionstechnik, FAU Erlangen-Nürnberg, 91058 Erlangen — ⁴Inorganic Chemistry and Catalysis Group, Debye Inst. for Nanomaterials Science, Utrecht University, Utrecht 3584 CG — ⁵Inst. 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.

CPP 25.4 Mon 15:45 HSZ 101

Chemical Doping of Individual Polynuclear Molecular Magnets on Surfaces — ●FABIAN PASCHKE¹, VIVIEN ENENKEL¹, TOBIAS BIRK¹, JAN DREISER², and MIKHAIL FONIN¹ — ¹Fachbereich Physik, Universitaet Konstanz, 78457 Konstanz, Germany — ²Swiss 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. Fe₄ 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 Fe₄ can host numerous adsorption sites for dopants. Here we present successful chemical doping with a defined adsorption configuration for the prototypical Fe₄ 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).

CPP 25.5 Mon 16:00 HSZ 101

Numerical Challenges in Studying Families of 3d-4f Heterometallic Single-Molecule Magnets — ●JULIUS MUTSCHLER¹, HETTI M. JAYAWARDENA¹, CHRISTOPHER E. ANSON², ANNIE K. POWELL², and OLIVER WALDMANN¹ — ¹Physikalisches Institut, Universität Karlsruhe, Germany — ²Institut 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 Mn₂Ho₂-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 10⁷ 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.

CPP 25.6 Mon 16:15 HSZ 101

Dy₂O-clusterfullerenes: Strong magnetic anisotropy and fullerene-dependent single molecule magnetism — ●GEORGIOS VELKOS¹, WEI YANG², STANISLAV AVDOSHENKO¹, NING CHEN², BERND BÜCHNER¹, and ALEXEY POPOV¹ — ¹Leibniz Institute for Solid State and Materials Research, Dresden, Germany — ²College 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 Dy₂O-clusterfullerenes. The compact geometry of Dy₂O cluster leads to both strong axial ligand field and unprecedentedly strong antiferromagnetic exchange coupling between Dy ions. We demonstrate that Dy₂O-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.

CPP 25.7 Mon 16:30 HSZ 101

Dynamic magnetic response of a single Magnetite nanoparticle chain detected by Scanning Transmission X-Ray Microscopy Ferromagnetic Resonance — •THOMAS FEGGELER¹, BENJAMIN ZINGSEM^{1,2}, RALF MECKENSTOCK¹, MICHAEL WINKLHOFER³, DETLEF SPODDIG¹, HENDRIK OHLDA⁴, MICHAEL FARLE¹, HEIKO WENDE¹, and KATHARINA OLLEFS¹ — ¹Faculty of Physics and CENIDE, University Duisburg-Essen, Lotharstr. 1, Duisburg, Germany — ²ERC and PGI, Fz. Jülich GmbH, Jülich, Germany — ³School of Mathematics and Science, University of Oldenburg, Oldenburg, Germany — ⁴Advanced 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.

CPP 25.8 Mon 16:45 HSZ 101

Biologically encoded magnonics — •BENJAMIN ZINGSEM¹, THOMAS FEGGELER¹, RALF MECKENSTOCK¹, MICHAEL FARLE¹, and MICHAEL WINKLHOFER^{1,2} — ¹University Duisburg-Essen — ²Universität 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)