

MA 18: Posters Magnetism V

Topics: Magnetic Particles / Clusters (18.1-18.8), Magnetic Instrumentation and Characterization (18.9-18.18), Magnetic Imaging Techniques (18.19-18.21), Computational Magnetism (18.22-18.27), Electron Theory of Magnetism and Correlations (18.28-18.31), Bio- and Molecular Magnetism, Biomedical Applications (18.32-18.38), Magnetic Information Technology, Recording, Sensing (18.39-18.42)

Time: Friday 10:00–13:00

Location: P

MA 18.1 Fri 10:00 P

Influence of surface water on adhesive forces in chondritic material — ●CYNTHIA PILLICH¹, TABELA BOGDAN², JOACHIM LANDERS¹, GERHARD WURM², and HEIKO WENDE¹ — ¹University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Faculty of Physics, Lotharstr. 1, 47057 Duisburg, Germany — ²University of Duisburg-Essen, Faculty of Physics, Lotharstr. 1, 47057 Duisburg, Germany

The growth of planetesimals at the so called "bouncing barrier" is still not fully understood. Evaporation of surface water on protoplanetary dust grains induced by high temperatures in the vicinity of the young star might explain improved sticking at the mm-range. As meteorites contain primordial phases representing the material in our young solar system, they offer an insight into the mechanics of planetary formation. A fragment of the iron-rich meteorite "Sayh al Uhaymir" was ground and subsequently heated in vacuum at temperatures up to 1400 K and adhesive forces were determined by Brazilian tests after cooling down to room temperature. We compare changes in adhesive forces upon exposure to high temperatures of meteoritic matter holding surface water and dried material. Compositional and concomitant structural transformations induced by tempering were investigated by ⁵⁷Fe-Mössbauer spectroscopy, probing the abundance of iron bearing phases. Funding by the DFG (projects WE 2623/19-1 and WU 321/18-1) is gratefully acknowledged.

MA 18.2 Fri 10:00 P

Exploring the dynamical behaviour of spherical exchange-biased Janus particles as a new tool for microfluidic biointeraction screening — ●RICO HUHNSTOCK, CLAUDIA JAUREGUI CABALLERO, MEIKE REGINKA, MICHAEL VOGEL, and ARNO EHRESMANN — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSA-T), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Janus particles (JPs) with engineered magnetic properties show significant potential for controlled motion in fluids by external dynamic magnetic fields [1]. In this work, we introduce an exchange bias (EB) thin film system on spherical non-magnetic particles as functionalized JPs and investigate their motion behaviour when being manipulated by dynamically varying artificial magnetic field landscapes above a topographically flat substrate. Due to the EB an Onion magnetization texture is stabilized within the magnetic cap of the JP [2], which is usually not accessible for micron-sized particles and allows for comparably high transport velocities. Probing the dynamics of the JPs in a microfluidic environment resulted in a superposition of controlled translational and rotational movements, emphasizing their potential use for biomolecular interaction analysis. This holds true not only for one-dimensional, but also two-dimensional translational motion. In addition, we highlight experimental possibilities to address and separate each motion domain (translation and rotation) individually.

[1] Baraban *et al.* (2012), *ACS Nano*, 6(4):3383-3389.

[2] Tomita *et al.* (2021), *J. Appl. Phys.*, 129:015305.

MA 18.3 Fri 10:00 P

Study of nanoparticle dynamics in binary solutions across phase transitions — ●JURI KOPP¹, JOACHIM LANDERS¹, SAMIRA WEBERS¹, SOMA SALAMON¹, JULIAN SEIFERT², KARIN KOCH², ANNETTE M. SCHMIDT², and HEIKO WENDE¹ — ¹Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — ²Institute for Physical Chemistry, University of Cologne

In previous magnetorheological measurements of cobalt ferrite nanoparticles in aqueous polymer solutions, Webers *et al.* [1] studied the thermomagnetic behavior across phase transitions showing a distinct change in magnetization. To prepare pre-aligned hybrid materials, it is important to know their stability and magnetic behavior under the influence of phase transitions such as crystallization. Here,

we study the dynamics of hematite nanospindles and cobalt ferrite nanoparticles in sucrose solutions of different concentration via temperature dependent Mössbauer spectroscopy and AC-susceptometry (ACS). These methods enable us to analyze the particle mobility and particle orientation across phase transitions. ACS data obtained upon decreasing temperature reveal a supercooled state and spontaneous crystallization whereas during the heating process a mixed-fluid phase is observed, which has also been shown in the Mössbauer spectroscopy results of the sample with the smallest amount of sucrose. This work is supported by the DFG, priority programme SPP1681 (WE 2623/7-3). [1] S. Webers *et al.*, *ACS Appl. Polym. Mater.* 2020, 2, 7, 2676-2685

MA 18.4 Fri 10:00 P

High throughput analysis of surface-functionalized superparamagnetic particles in dynamic magnetic field landscapes — ●YAHYA SHUBBAK^{1,2}, RICO HUHNSTOCK^{1,2}, KRISTINA DINGEL^{2,3}, KATHARINA GETTFERT^{1,2}, BERNHARD SICK^{2,3}, ARNO EHRESMANN^{1,2}, and MICHAEL VOGEL^{1,2} — ¹Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSA-T), University of Kassel, D-Kassel — ²AIM-ED - Joint Lab Helmholtzzentrum für Materialien & Energie, D-Berlin — ³Intelligent Embedded Systems, University of Kassel, D-Kassel

The precise manipulation of micro- and nano-particles in microfluidic environments opens new avenues for investigations of biomolecular analyte detection and interactions.[1] Motion control schemes based on a combination of static magnetic field landscapes superposed with external magnetic field pulses enable translatory motion control of magnetic particles at the nanoscale over macroscopic distances.[3] Here we demonstrate a novel method harnessing AI-enhanced fully-automated optical recognition algorithms [4] to analyze changes in the motion behavior of such particles due to liquid mediated surface to surface (particle to substrate) interaction.

[1] Lim, B. *et al.* *J. Phys. D: Appl. Phys.* 50, 33002 (2017) [2]*Lin, G. *et al.* *Lab on a chip* 17, 1884*1912 (2017) [3]*Issadore, D. *et al.* *Lab on a chip* 14, 2385*2397 (2014) [4] Dingel, K. *et al.* *Computer Physics Communications*, 262, 107859 (2021)

MA 18.5 Fri 10:00 P

Structure and magnetism of Fe/Fe₃C/Carbon nanocomposites: Influence of the pyrolysis conditions — ●ELISAVET PAPADOPOULOU¹, NIKOLAOS TETOS¹, ARAM MANUKYAN², HARUTYUN GYULASARYAN², GAYANE CHILINGARYAN², MICHAEL FARLE¹, and MARINA SPASOVA¹ — ¹Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany — ²Institute for Physical Research of National Academy of Sciences (IPR-NAS), Ashtarak, 0203 Armenia

Carbon-encapsulated iron-cementite (Fe/Fe₃C) magnetic nanoparticles were synthesized by an up-scalable solid-state pyrolysis method using iron phthalocyanine as metal precursor. The dependence of the magnetic, structural and morphological parameters on the pyrolysis conditions are presented. The nanocomposites contain α -Fe, cementite (Fe₃C) and pure carbon with an average particle size of 12.5 * 2 nm. The saturation magnetization of Fe M=102 Am²/kg measured at room temperature increases by 30 % for higher synthesis temperature (973 K < T < 1173 K), indicating an increase in Fe content. This is in good agreement with the increasing volume fraction of iron from 0.5% to 8.6% in the same synthesis temperature range from the XRD. The effective magnetic anisotropy constant obtained from an analysis of approach to saturation magnetization (LAS) is 4.9 * 0.72 x 10⁴ J/m³ at room temperature.

This work was supported by the EC project H2020-EU.4.b. - Twinning of research institutions no. 857502 (MaNaCa).

MA 18.6 Fri 10:00 P

Magnetic structure of Fe chains on Rh(111) substrate — ●BALÁZS NAGYFALUSI¹, LÁSZLÓ UDVARDI^{1,2}, and LÁSZLÓ SZUNYOGH^{1,2} — ¹Budapest University of Technology and Eco-

nomics, Budapest Hungary — ²MTA-BME Condensed Matter Research Group, Budapest, Hungary

As the size of the functional elements of spintronics devices approaches the scale of a few hundreds of atoms, the role of first principles simulations designed to model the magnetic properties of such systems becomes more pronounced. We present a method developed in the framework of the embedded cluster Green's function method aimed at minimizing the overall torque on the magnetic moments. In order to find the local minima of the energy landscape we use the gradient descent method combined with Newton-Raphson iterations where the torque and the Hessian matrix are calculated directly from first principles instead of relying on an effective spin Hamiltonian.

This procedure is applied to Fe chains deposited on Rh(111) substrate in different stacking positions. The stability of the ground state spin configurations is tested against a small vertical relaxation of the layers. The symmetry of the magnetic configurations is explained in terms of exchange interactions appearing in a suitable spin model. The comparison of the magnetic ground states obtained from ab initio and spin model calculations indicates the limits of spin models.

MA 18.7 Fri 10:00 P

Element-specific characterization of catalytic ferrite nanoparticles via Mössbauer spectroscopy — ●SOMA SALAMON¹, JOACHIM LANDERS¹, GEORG BENDT², SASCHA SADDELER², ANNA RABE², SWEN ZEREBECKI³, MALTE BEHRENS², STEPHAN SCHULZ³, STEPHAN BARCIKOWSKI³, and HEIKO WENDE¹ — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen — ²Institute of Inorganic Chemistry and CENIDE, University of Duisburg-Essen — ³Institute of Technical Chemistry I and CENIDE, University of Duisburg-Essen

Mössbauer spectroscopy is utilized as an element-specific, non-destructive measurement method to probe hyperfine interactions in ferrite materials, which are promising candidates for electrocatalysis applications. Evaluation of low temperature spectra recorded at high magnetic fields allows us to determine the degree of inversion in spinel systems, providing important clues on the distribution of Fe-ions on different crystallographic sites, while the isomer shift makes it possible to draw conclusions on the valency states. This enables us to correlate changes in ion distribution in the lattice with improvements in catalytic activity, which can be achieved by a number of methods. Several examples of nanoparticulate systems will be shown: The modification of particle composition during and after synthesis, as well as laser treatment of nanoparticles. In all cases, our measurement method offers valuable insights into which parameters are modified by the respective sample treatment, facilitating a more effective search for the best method to increase catalytic efficiency. Funding by the DFG via the CRC/TRR 247 (ID 388390466, Project B2) is acknowledged.

MA 18.8 Fri 10:00 P

Electronic and magnetic properties of building blocks of Mn and Fe atomic chains on Nb(110) — ●ANDRÁS LÁSZLÓFFY¹, KRISZTIÁN PALOTÁS¹, LEVENTE RÓZSA², and LÁSZLÓ SZUNYOGH³ — ¹Wigner RCP, ELKH, Budapest, Hungary — ²Department of Physics, University of Konstanz — ³Budapest University of Technology and Economics, Budapest, Hungary

We present results for the electronic and magnetic structure of Mn and Fe clusters on Nb(110) surface, focusing on building blocks of atomic chains as possible realizations of topological superconductivity. The magnetic ground states of the atomic dimers and most of the monatomic chains are determined by the nearest-neighbor isotropic interaction. To gain physical insight, the dependence on the crystallographic direction as well as on the atomic coordination number is analyzed via an orbital decomposition of this isotropic interaction based on the spin-cluster expansion and the difference in the local density of states between ferromagnetic and antiferromagnetic configurations. A spin-spiral ground state is obtained for Fe chains along the [110] direction as a consequence of the frustration of the isotropic interactions. Here, a flat spin-spiral dispersion relation is identified, which can stabilize spin spirals with various wave vectors together with the magnetic anisotropy. This may lead to the observation of spin spirals of different wave vectors and chiralities in longer chains instead of a unique ground state.

MA 18.9 Fri 10:00 P

Magnetic field dependent power loss of surface acoustic waves in thin nickel layers — ●JAN PHILIPP KRESS, SEBASTIAN KÖLSCH, ALFONS SCHUCK, and MICHAEL HUTH — Physikalisches Institut, Goethe Universität, Frankfurt am Main, Germany

Though mostly applied in mobile communication devices for high-frequency filtering in the GHz regime, surface acoustic wave (SAW) technology is also a promising approach in magnonics by employing the coupling of spin degrees of freedom with time-dependent elastic deformations. We present a simple setup for ferromagnetic resonance excitation by a surface acoustic wave with a rotatable electromagnet operating at room temperature. We tested our setup with an interdigital-transducer structure made from Cr/Au by UV lithography on YZ-cut LiNbO₃ and excited a Rayleigh-type SAW at a fundamental frequency of 290 MHz and measured its attenuation for various higher harmonics after passing a polycrystalline Ni thin film. By varying the magnetic field direction within the Ni thin film plane we measured the angle-dependent attenuation which can be related to the magneto-elastic coupling coefficient of Ni.

MA 18.10 Fri 10:00 P

Analysis of the magnetization profile of 3D printed shape programmable magnetic elastomer actuators — ●KILIAN SCHÄFER, MARTIN LEHMANN, ILIYA RADULOV, and OLIVER GUTFLEISCH — Institute of Materials Science, Technical University Darmstadt, Germany

Magnetically responsive materials can be used as sensors and actuators. The advantages of magnetic actuation mechanisms are fast response, wireless operation and the possibility to operate in enclosed confined spaces. Mechanically soft sensors and actuators are beneficial when compliant and safe interaction with the human body is needed. In addition to that, they can easily adapt to changing environments and can have a simpler design, which potentially results in greater durability and lower cost.

One example of magneto responsive soft materials are composites of polymers and hard magnetic particles, like NdFeB. Recently it was shown that the shape of these composites can be controlled with a magnetic field if the material was magnetized in a specific way beforehand. The material has to be folded in the same way as the desired deformation. Here we realized a programmable magnetic elastomer actuator based on polyurethane and NdFeB particles and present a method to characterize the imprinted magnetization profile in these composites with a custom build 3D Hall Mapper. The device measures all components of the stray field with a spatial resolution of 150 μm. The detailed information will help to improve the design and magnetization strategies of magneto-active composites. Based on this, we evaluate the actuation performance of a 3D printed composite.

MA 18.11 Fri 10:00 P

Kompaktes membranbasiertes Faraday-Magnetometer für tiefe Temperaturen — ●LUKAS WORCH, MARKUS KLEINHANS, MARC A. WILDE and CHRISTIAN PFLEIDERER — Technische Universität München, Garching, Deutschland

Auf Basis von metallisierten SiN-Membranen wurde ein kompaktes, kapazitiv ausgelesenes Faradaymagnetometer konstruiert, welches in einem ³He-Einsatz und einem supraleitenden 15 T Magneten betrieben wird. Mithilfe einer unabhängigen supraleitenden Gradientenspule können die Kraft- und Drehmomentbeiträge zur Kapazitätsänderung voneinander getrennt werden. Eine elektrostatische Kalibrationsroutine erlaubt die quantitative Bestimmung der Magnetisierung. Die kommerziell verfügbaren Membranen erlauben ein einfaches und schnelles Tauschen der Probe. Durch eine drehbare Probenbühne können zudem winkelabhängige Messungen durchgeführt werden. Erste Messergebnisse an Gadolinium Gallium Granat zeigen Signaturen des komplexen Phasendiagramms in der Magnetisierung.

MA 18.12 Fri 10:00 P

Quadratic and third-order magneto-optic Kerr effect in Ni(111) thin films with and without twinning — ●MAIK GAERNER¹, ROBIN SILBER², TOBIAS PETERS¹, JAROSLAV HAMRLE³, and TIMO KUSCHEL¹ — ¹Bielefeld University, Germany — ²IT4Innovations, VŠB - Technical University of Ostrava, Czech Republic — ³Charles University, Prague, Czech Republic

To separate and study the dependencies of the linear magneto-optic Kerr effect (MOKE) and quadratic MOKE on the crystallographic direction, the so-called eight-directional method can be used [1]. So far, this method or similar ones have been utilized to characterize (001)- and (011)-oriented thin films of cubic crystal structure [2,3]. Here, we apply the eight-directional method to Ni(111) thin films and report on a strong three-fold anisotropy in longitudinal MOKE (LMOKE). This anisotropy can be explained by theory as an optical interplay of elements in the permittivity tensors of first and second order in M, effectively creating cubic MOKE contributions, i.e., MOKE of third

order in M. Furthermore, we observe that in a Ni(111) thin film with twinning (two structural (111) phases with 60 deg. in-plane rotation), those oscillations are substantially reduced compared to a thin film with almost no twinning. This indicates that the LMOKE anisotropy truly is of crystallographic origin in the ferromagnetic layer and is not due to other, e.g., interface effects.

- [1] K. Postava et al., J. Appl. Phys. 91, 7293 (2002)
 [2] R. Silber et al., Phys. Rev. B 100, 064403 (2019)
 [3] J. H. Liang et al., Appl. Phys. Lett. 108, 082404 (2016)

MA 18.13 Fri 10:00 P

Exploring the phase diagram of GdTe₃ using thermal expansion and magnetostriction — ●THOM OTTENBROS¹, CLAUDIUS MÜLLER¹, SHIMING LEI², RATNADWIP SHINGHA², LESLIE SCHOOP², NIGEL HUSSEY^{1,3}, and STEFFEN WIEDMANN¹ — ¹HFML-EMFL, Nijmegen, Netherlands — ²Princeton University, USA — ³University of Bristol, UK

Thermal expansion and magnetostriction are powerful tools to explore phase transitions and ultimately determine the phase diagram of correlated electron systems.

We present the mapping of the phase diagram of GdTe₃, a van der Waals layered antiferromagnetic metal with high carrier mobility [1]. At zero magnetic field, we find three magnetic transitions in the thermal expansion: a Néel transition at 12.0 K, and two others at 7.0 and 10.0 K. In magnetostriction experiments up to 30 T and at 1.3 K, another transition occurs around 20 T before the onset of quantum oscillations.

Furthermore, we give an overview of capacitive dilatometry at the HFML-EMFL in Nijmegen and discuss new high field experiments using a uniaxial stress dilatometer [2].

- [1] S. Lei et al., Science Advances 6, eaay6407 (2020). [2] R. Kuechler et al., Rev. Sci. Instr. 87, 073903 (2016).

MA 18.14 Fri 10:00 P

Single-crystal growth and magnetic characterization of rare-earth-doped yttrium orthosilicate — ●TIM HOFMANN, ANDREAS BAUER, FABIAN KESSLER, and CHRISTIAN PFLEIDERER — Chair for the Topology of Correlated Systems, Department of Physics, Technical University of Munich, Germany

The monoclinic Yttrium orthosilicate Y₂SiO₅ doped with several ten ppm of rare-earth atoms, such as Er³⁺, Yb³⁺, or Nd³⁺, is a candidate material for optical applications in quantum information technology. The amount of dopants decisively influences key properties, such as the linewidth or the coherence time, and in turn precise control on the doping levels is essential. Here, we report the preparation of polycrystalline material using a sol-gel process, followed by single-crystal growth by means of the optical floating zone technique. The quantitative determination of doping on ppm level is challenging when using conventional characterization techniques. Instead, we infer information from magnetization measurements at low temperature for magnetic fields up to 14 T applied along the optical axes *b*, *D1*, and *D2*. We find paramagnetic contributions characteristic of rare-earth ions. Distinct anisotropy hints towards the importance of crystal electric field effects for both the fundamental characterization and potential applications in quantum information technology.

MA 18.15 Fri 10:00 P

2.6 Tesla Cryogen Free Mu3e System — ●DR. ROGER MITCHELL — Cryogenic Ltd, London, UK

Cryogenic Ltd has manufactured a large bore cryogen-free magnet system to enable investigations of the lepton-flavour violating decay of muons into an electron and two positrons. The magnet is installed at the Paul Scherrer Institute in Villigen, Switzerland. The cryostat has a 1 metre room temperature bore and houses a 2.6T magnet with a base homogeneity of <0.12% over a 1.3m central region. The NbTi magnet comprises four separately powered windings. Varying the current in the windings permits subtle changes to the field profile as well as establishing a shallow gradient field along the bore. The magnetic stray field is limited to 5mT at 1m by encasing the cryostat in a 27 tonne passive shield with overall dimensions of 2.1m diameter x 3.4m long. Access to 1m bore tube is via semicircular swing doors each weighing 0.5 tonnes. The magnet cold mass is 1.5 tonnes and is cooled to 3.5K using four 1.5W Gifford McMahon two-stage cryocoolers. The magnet operated to full field without training. To ensure safety in operation the magnet is magnetically balanced within the iron shield using a series of load cells to monitor relative displacements between the cryostat and the shield. The overall system footprint was subject to severe

spatial restrictions imposed by the beamline architecture. Careful optimisation was necessary to achieve the critical specifications within the dimensional constraints. The room temperature bore will house a purpose-built detector developed at PSI which is inserted via a rail system attached to the bore wall.

MA 18.16 Fri 10:00 P

Measurement of de Haas-van Alphen effect by means of temperature modulation — ●MICHELLE HOLLRICHER, MARC A. WILDE, and CHRISTIAN PFLEIDERER — Department of Physics, Technical University of Munich, D-85748 Garching, Germany

Measurements of the quantum oscillations of the magnetization *M* as a function of magnetic field *B*, i.e. the de Haas-van Alphen effect, are a powerful tool for mapping the Fermi surfaces of metals. The most established methods for measuring *M*(*B*) or other quantities utilize either the magnetic torque or inductively pick up the response to a large-amplitude modulation of *B*. Here we report the development and characterization of a temperature modulation technique (TMT) for measuring quantum oscillations in *M*, combining a thermally linked sample-heater-thermometer arrangement with an inductive pick-up. Advantages of the method are the absence of dissipation due to a modulated field and the ability to separate signals arising from orbits with different effective masses. It was found that TMT may prove to be especially advantageous for detecting oscillations related to orbits with heavy effective masses. The TMT was employed on Bi single crystals at temperatures down to 1.9K and in magnetic fields up to 9 T. Pronounced quantum oscillations well into the quantum limit of the electron pockets were observed.

MA 18.17 Fri 10:00 P

Meissner flux repulsion and trapped flux in sub-millimeter size superconductors observed with enhanced neutron depolarization — ●JORBA PAU¹, SCHULZ MICHAEL², SEIFERT MARC^{1,2}, TSURKAN VLADIMIR^{3,4}, BÖNI PETER¹, and PFLEIDERER CHRISTIAN¹ — ¹Physik-Department, Technische Universität München, Garching, Germany — ²Heinz-Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — ³Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — ⁴Institute of Applied Physics, Chisinau, Republic of Moldova

Neutron depolarization is a unique probe which can quantify the level of magnetic inhomogeneity at a mesoscopic scale in the bulk of a sample. We report the construction of a focusing neutron guide module increasing the neutron flux at the focal spot by a factor of 20. This module was used to enhance ND measurements, demonstrating an increase of an order of magnitude in the signal to noise ratio while maintaining the exposure time. The construction and utilization details are addressed. Additionally, a proof of principle experiment on superconducting niobium and lead was conducted. We demonstrate that, with the enhanced ND technique, the Meissner flux repulsion and trapped magnetic flux of very small superconducting samples can be observed. This opens the possibility of using ND to investigate superconductors, ferromagnets, or even spin glasses under very high pressures.

MA 18.18 Fri 10:00 P

MIASANS at the longitudinal neutron resonant spin echo spectrometer RESEDA — ●JONATHAN LEINER^{1,2}, CHRISTIAN FRANZ^{1,2,3}, JOHANNA JOCHUM^{1,2}, and CHRISTIAN PFLEIDERER^{1,2} — ¹Technical University of Munich, Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — ³JCNS at MLZ, FZ Jülich GmbH, Garching, Germany

The RESEDA (Resonant Spin-Echo for Diverse Applications) instrument has been optimized for neutron scattering measurements of quasi-elastic and inelastic processes over a wide parameter range. One spectrometer arm of RESEDA is configured for the MIEZE (Modulation of Intensity with Zero Effort) technique where the measured signal is an oscillation in neutron intensity over time, which is prepared by two precisely tuned radio-frequency (RF) flippers. With MIEZE, all of the spin-manipulations are performed before the beam reaches the sample, and thus the signal from sample scattering is not disrupted by any depolarizing conditions there (i.e. magnetic materials). The MIEZE spectrometer is being further optimized for the requirements of small-angle neutron scattering (MIASANS), a versatile combination of the spatial and dynamical resolving power of both techniques. We present the progress on (i) installing new superconducting solenoids as part of the RF flippers to significantly extend the dynamic range (ii) design and installation of modular options for both reflecting guides

and evacuated flight paths with absorbing walls for background reduction (iii) installation of a new detector on a translation stage within a vacuum vessel for flexibility with angular coverage and resolution.

MA 18.19 Fri 10:00 P

Microfocused optical spin-wave spectroscopy with vector magnetic fields — ●YANNIK KUNZ, MICHAEL SCHNEIDER, BJÖRN HEINZ, LARS NIKLAS HESS, PHILIPP PIRRO, VITALIY VASYUCHKA, and MATHIAS WEILER — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

The field of magnonics aims to exploit spin waves for information processing purposes. Experimental techniques that allow accurate spin-wave spectroscopy in magnonic microstructures are needed to tailor magnonic devices. The micro-focused frequency-resolved magneto-optic Kerr effect (FR-MOKE) can be used for spatially resolved spin-wave measurements in the frequency-domain with phase resolution, empowered by vector network analysis [1]. Here we present a FR-MOKE setup that provides 3D vector magnetic fields to study linear and non-linear spin-wave dynamics in micropatterned magnonic conduits in all field geometries. The setup allows simultaneous integration of micro-focused Brillouin Light Scattering and time-resolved MOKE to access both coherent and incoherent spin-wave dynamics as a function of frequency and/or time. We characterize the setup performance through optical spin-wave spectroscopy measurements of metallic and insulating magnonic devices. [1] L. Liamsberger et al. *IEEE Magn. Lett.* 10, 5503905 (2019)

MA 18.20 Fri 10:00 P

Time-Resolved Imaging of Ferromagnetic Resonances in the Oldenburg Ultrafast Transmission Electron Microscope (UTEM) — ●JONATHAN WEBER, NIKITA PORWAL, MICHAEL WINKELHOFER, and SASCHA SCHÄFER — Carl-von-Ossietzky Universität Oldenburg, Deutschland

Recent progress in the development of laser driven, high-brightness photocathodes offers a path to investigate magnetization dynamics with unparalleled resolution by employing a Lorentz imaging scheme in an ultrafast transmission electron microscope [1,2].

Aiming to extend the accessible frequency range, we develop a setup for Lorentz-imaging detected ferromagnetic resonances. Beyond the nanometer spatial resolution, inherent to transmission electron microscopy, a setup for fs-temporal resolution is presented, employing nano-localized photoemission from a Schottky-field emitter in the Oldenburg UTEM. The laser system which is used for the generation of ultrashort electron pulses is also utilized as a master clock for the synchrotronization of phase-locked microwave signals [3]. Making use of a custom-made sample holder we pass these signals to a microresonator which excites precessions of the magnetic moments in nanostructured Py films at GHz frequencies. With this advanced excitation scheme we aim to further establish ultrafast Lorentz microscopy as a powerful tool to characterize magnetic dynamics on the nanoscale.

- [1] T. Eggebrecht et al. *Phys. Rev. Lett.* 118, 097203 (2017)
- [2] N. R. da Silva et al. *Phys. Rev. X* 8, 031052 (2018)
- [3] M.R. Otto et al. *Struct. Dyn.* 4, 051101 (2017)

MA 18.21 Fri 10:00 P

Force-detected magnetic resonance of nanometer thin films: measuring copper nuclear spins with a nanoladder sensor — ●GESA WELKER¹, MARTIN HÉRITIER², MARTIN DE WIT¹, TIM FUCHS¹, JAIMY PLUGGE¹, FREEK HOEKSTRA¹, ALEXANDER EICHLER², CHRISTIAN DEGEN², and TJERK OOSTERKAMP¹ — ¹Leiden Institute of Physics, Leiden University, The Netherlands — ²ETH Zurich, Switzerland

Magnetic Resonance Force Microscopy (MRFM) is a non-invasive 3D imaging technique that can be used to characterize biological and solid-state samples on the nanoscale. Small ensembles of spins are detected by measuring the attonewton forces they exert on an ultrasoft cantilever. State of the art for biological samples is the imaging of a single tobacco mosaic virus with nanometer resolution (Degen, 2009), based on the detection of nuclear ¹H (proton) spins. An important goal in the field is improving measurement sensitivity in order to achieve higher image resolution, the ultimate goal being single-nuclear-spin resolution. In this poster we present a new type of force sensor for MRFM, designed for increased sensitivity and operation at millikelvin temperatures to reduce thermal noise. The sensor combines a nanoladder cantilever (spring constant 16 $\mu\text{N/m}$) with a micromagnet of 1.1 μm radius. Using the new sensor, we unambiguously identified a copper

nuclear resonance signal.

MA 18.22 Fri 10:00 P

Finite-element dynamic-matrix approach to calculate spin-wave dispersions in waveguides with arbitrary cross section — ●LUKAS KÖRBER^{1,2}, GWEN QUASEBARTH^{1,2}, ANDREAS OTTO², and ATTILA KÁKAY¹ — ¹Helmholtz-Zentrum Dresden - Rossendorf, Dresden Germany — ²Technische Universität Dresden

One of the key objectives in curvilinear magnetism is the determination of the spin-wave dispersion and mode profiles in magnetic waveguides with surface curvature. Due to the geometrical complexity, dynamic micromagnetic simulations are often used to obtain quantitative predictions where only approximate analytical approaches are available. However, especially in geometries which require an accurate modeling of the sample surface, these dynamic micromagnetic simulations become computationally exhausting. To address this challenge, we present a finite-element dynamic-matrix approach to efficiently calculate the dispersion and spatial mode profiles of spin waves propagating in waveguides with arbitrary cross section where the equilibrium magnetization is invariant along the propagation direction. This is achieved by solving a linearized version of the equation of motion of the magnetization numerically only in a single cross section of the waveguide at hand. To take account of the dipolar interaction we present an extension of the well-known Fredkin-Koehler method to plane waves. As an application of our method, we present the first results on the spin-wave dispersion in nanotubes with thick shell which exhibits higher-order standing modes along the radial direction as well as an extremely strong dispersion asymmetry compared to thin-shell nanotubes.

MA 18.23 Fri 10:00 P

Automated spin-dynamics simulations with AiiDA-Spirit — ●PHILIPP RÜSSMANN¹, JORDI RIBAS SOBREVIELA^{1,2}, MORITZ SALLERMANN¹, and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — ²RWTH Aachen University, Aachen, Germany

The Spirit framework (spirit-code.github.io) allows to perform spin-dynamics simulations of magnetic materials based on the solution of the Landau-Lifshitz-Gilbert equation. These calculations can be used, for example, to find the magnetic ground state based on exchange coupling parameters, to calculate the Curie Temperature with a Monte Carlo method or perform geodesic nudged elastic band calculations for the minimal energy transition path between two magnetic states. We present the AiiDA-Spirit plugin (aiida-spirit.readthedocs.io) that connects the Spirit code to the AiiDA framework. AiiDA allows to perform automated calculations while keeping track of the data provenance between calculations. The AiiDA-Spirit plugin is able to use exchange coupling parameters calculated based on first-principles calculations within the AiiDA-KKR package (aiida-krk.readthedocs.io). This facilitates multi-scale modelling, bridging the gap from the atomic scale of quantum mechanical simulations to the micrometer scale of magnetic structures and devices. — We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG) under Germany's Excellence Strategy – Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 – 390534769.

MA 18.24 Fri 10:00 P

Energy-efficient control of magnetization reversal in bistable nanowires — ●MOHAMMAD BADARNEH¹, GRZEGORZ KWIATKOWSKI¹, and PAVEL BESSARAB^{1,2} — ¹University of Iceland, Reykjavík, Iceland — ²ITMO University, St. Petersburg, Russia

We explore theoretical limits for the energy-efficient control of switching phenomena in bistable magnetic nanowires. We calculate optimal control paths (OCPs) for the magnetization switching as functions of the switching time, damping and various parameters of the nanowires. Following an OCP involves concerted rotation of the magnetic moments in such a way that the system's internal modes are effectively used to aid magnetization switching. OCP calculations demonstrate that short nanowires reverse their magnetization via coherent rotation which can be induced by applying uniform external magnetic field with frequency defined by a collective in-phase precession of the magnetization [1]. If the length of the wire exceeds a certain critical length, standing spin wave emerges during magnetization switching [2]. Such spin wave assisted magnetization switching has recently attracted much attention as a promising technique to reduce the switching field for magnetic recording. Our results demonstrate that optimal switching mechanisms and corresponding control stimuli can be predicted

from first principles, contributing to the development of low-power technologies.

[1] G.J. Kwiatkowski *et al.*, Phys. Rev. Lett. **126**, 177206 (2021)

[2] M.H.A. Badarneh *et al.*, Nanosyst. Phys. Chem. Math. **11**(3), 294 (2020)

MA 18.25 Fri 10:00 P

Exchange interactions in hematite from first principles — ●ANDRÁS DEÁK¹, TOBIAS DANNEGGER², MARTIN EVERS², LÁSZLÓ SZUNYOGH^{1,3}, and ULRICH NOWAK² — ¹Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary — ²Fachbereich Physik, Universität Konstanz, Germany — ³MTA-BME Condensed Matter Research Group, Budapest University of Technology and Economics, Hungary

Antiferromagnets have lately appeared in the forefront of spintronics research, with exciting novel magnonic spin transport applications for collinear insulating antiferromagnets. We will detail our investigations of hematite (α -Fe₂O₃), a well-known collinear insulating antiferromagnet showing weak ferromagnetism.

We assess magnetic ordering in the material using the Screened Korringa–Kohn–Rostoker (SKKR) multiple scattering theory. We use a multiscale description by deriving spin model parameters from first principles and investigating the ground state spin configuration and its stability using this model. With this approach we can tackle the nature of the weak ferromagnetic distortion in this antiferromagnet, and provide spin model parameters that can be used in large-scale simulations of magnon dynamics effects.

MA 18.26 Fri 10:00 P

Quantum effects in thermally activated domain wall switching in ferromagnets — ●GRZEGORZ J. KWIATKOWSKI¹ and PAVEL F. BESSARAB^{1,2} — ¹Science Institute of the University of Iceland, Reykjavík, Iceland — ²ITMO University, St. Petersburg, Russia

Most widely used data storage technologies are based on nanoscale magnetic structures [1]. In order to improve both memory retention and energy efficient writability one needs to increase stability of magnetic samples without a change in energy barrier which directly affects the costs or rewriting the memory. Due to this fact it is vital to optimise the preexponential factor in Arrhenius law, which requires one to properly study the effect of internal degrees of freedom on thermal switching processes [2,3]. We present analytic estimation of rate of escape for domain wall switching in 3D samples with focus on how results scale with internal parameters and sample size. Since for spin waves minimum excitation energy is larger than average thermal fluctuation for high frequency modes we employ Bose-Einstein statistics, which leads to nontrivial temperature dependencies of the preexponential factor opening up new possibilities for enhancing stability of magnetic structures. This work was funded by the Russian Science Foundation (Grant No. 19-72-10138) and the Icelandic Research Fund (Grant No. 184949-052).

[1] W. A. Challener *et al.* Nature Photonics volume 3, pages 220-224 (2009) [2] P. F. Bessarab, V. M. Uzdin and H. Jónsson Physical Review Letters **110**:2, 020604 (2013) [3] G. Fiedler *et al.* Journal of Applied Physics **111**, 093917 (2012)

MA 18.27 Fri 10:00 P

Energy-efficient control of magnetic states — MOHAMMAD BADARNEH¹, GRZEGORZ KWIATKOWSKI¹, SERGEI VLASOV², IGOR LOBANOV², VALERY UZDIN², and ●PAVEL BESSARAB^{1,2} — ¹University of Iceland, Reykjavík — ²ITMO University, St. Petersburg, Russia

Control of magnetization switching is critical for the development of novel technologies based on magnetic materials. Transitions between magnetic states can follow various pathways which are not equivalent in terms of energy consumption and duration. In this study, we propose a general theoretical approach based on the optimal control theory to design external stimuli for efficient switching between target magnetic states. The approach involves calculation of optimal control paths (OCPs) for the desired magnetic transition. Following an OCP involves rotation of magnetic moments in such a way that the strength of the external stimulus is minimized, but the system's internal dynamics is effectively used to aid the switching. All properties of the switching pulses including temporal and spatial shape can be derived from OCPs in a systematic way. Various applications of OCP calculations are presented, including energy-efficient switching of a nanomagnet by means of external magnetic field [1] or electric current, and spin-wave assisted magnetization reversal in nanowires [2].

This work was funded by the Russian Science Foundation (Grant No.

19-72-10138), the Icelandic Research Fund (Grant No. 184949-052).

[1] G.J. Kwiatkowski *et al.*, Phys. Rev. Lett. **126**, 177206 (2021).

[2] M.H.A. Badarneh *et al.*, Nanosyst. Phys. Chem. Math. **11**, 294 (2020).

MA 18.28 Fri 10:00 P

Magnon topology in chiral crystals: Multifold crossings and nodal planes — ●NICLAS HEINSDORF, XIANXIN WU, and ANDREAS SCHNYDER — Max Planck institute for condensed matter physics

We investigate the topology of magnon excitations in magnets with chiral space groups. The presence of (magnetic) screw rotations lead to symmetry enforced Weyl points and nodal planes in the magnon band structure. In addition, there are multifold crossings pinned at high-symmetry points. We systematically analyze the band topology of these crossings and calculate their topological charges. In particular, we find that the magnon nodal planes carry a quantized topological charge similar to magnon Weyl points. Analogous to the protected spin currents on the surface of topological insulators, the topologically nontrivial magnon crossings result in protected surface modes of heat quanta. We propose several candidate materials and calculate their magnon band structures, topological invariants, and topologically protected surface modes.

MA 18.29 Fri 10:00 P

Magnetic interactions in correlated systems from first principles — ●VLADISLAV BORISOV¹, YAROSLAV O. KVASHNIN¹, NIKOLAOS NTALLIS¹, QICHEN XU², REBECCA CLULOW¹, PETER SVELDINDH¹, DANNY THONIG³, PATRIK THUNSTRÖM¹, MANUEL PEREIRO¹, ANDERS BERGMAN¹, ERIK SJÖQVIST¹, ANNA DELIN², LARS NORDSTRÖM¹, and OLLE ERIKSSON^{1,3} — ¹Uppsala University, SE-75120 Uppsala, Sweden — ²KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden — ³Örebro University, SE-70182, Örebro, Sweden

The formation of non-trivial magnetic textures, such as skyrmions, depends on the interplay between the Heisenberg and Dzyaloshinskii-Moriya (DM) interactions. In this work, we discuss a general theoretical framework based on density functional (DFT) and dynamical mean-field theories which allows to calculate these interactions accurately from first principles including electronic correlations.

First, we demonstrate that dynamical correlations can lead to non-monotonic variations of magnetic exchange, for example, in skyrmionic B20 compounds MnSi and FeGe and low-dimensional system of Co/Pt(111) bilayer [1].

Secondly, we use the proposed theoretical approach to study the doped B20 compounds Fe_{0.75}TM_{0.25}Si (TM = Co, Rh, Ir) and Co_{0.75}TM_{0.25}Si (TM = Fe, Ru, Os) and predict that skyrmions can be stabilized in all these compounds and the DM interaction is enhanced in the *4d*- and *5d*-doped systems. We also report successful synthesis for (Fe,Ir)Si and (Co,Ru)Si and measurements for the later.

1. PRB 103, 174422 (2021).

MA 18.30 Fri 10:00 P

Local spin Hamiltonians from model electronic structure theory — SIMON STREIB¹, VLADISLAV BORISOV¹, MANUEL PEREIRO¹, ANDERS BERGMAN¹, ERIK SJÖQVIST¹, ANNA DELIN^{2,3}, MIKHAIL KATSNELSON⁴, OLLE ERIKSSON^{1,5}, and ●DANNY THONIG⁵ — ¹Department of Physics and Astronomy, Uppsala University, Sweden — ²Department of Applied Physics, KTH Royal Institute of Technology, Sweden — ³Swedish e-Science Research Center (SeRC), KTH Royal Institute of Technology, Sweden — ⁴Institute for Molecules and Materials, Radboud University, The Netherlands — ⁵School of Science and Technology, Örebro University, Sweden

The derivation of spin Hamiltonians from ab initio calculations is an important tool for modeling effective precession fields in the dynamics of magnetic materials since a full electronic description of the dynamics is computationally very demanding. In this work, we contrast two different – "local" and "global" – approaches. The global approach aims at describing arbitrary spin configurations, whereas the local approach is only valid for small magnetic fluctuations locally around a given spin configuration. We argue that global symmetry requirements, such as time-reversal symmetry, do not necessarily restrict local spin Hamiltonians if the dependence of the effective exchange parameters on the magnetic state is taken into account. We present a general formalism to map model electronic structure theory to a local spin Hamiltonian and we check our formalism by means of numerical calculations for low-dimensional structures, like dimers and chains [1].

[1] S. Streib *et al.*, Phys. Rev. B **103**, 224413 (2021)

MA 18.31 Fri 10:00 P

An automated tool for generation of optimal Voronoi tessellation of crystal structures by the inclusion of void sites — ●ROMAN KOVÁČIK and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The performance of the electronic structure calculation within the Korringa-Kohn-Rostoker Green function method strongly relies on a good convergence with respect to the angular momentum expansion. This in turn depends on an as close-packed as possible definition of the atomic structure, due to the Voronoi tessellation used to partition the space. Hence, for the crystal structures with low packing density, an appropriate set of void sites has to be defined, which we address in our newly developed python tool.

The lower and upper bound of the number of void sites is estimated from the packing density, using simple geometrical arguments or assuming atomic radii of the present species. Within these bounds, a number of all distinct sets of Wyckoff positions is generated, corresponding to the space group of the input structure and yet unoccupied by present atoms. In case of a free coordinate in a particular Wyckoff position, a user defined number of random initial positions are tried. The fitness of the resulting Voronoi tessellation is examined as a function of the radius of void sites from the minimum ratio of inscribed and circumscribed sphere and the maximum ratio of circumscribed sphere and nearest neighbor distance over the Voronoi cells. Solutions are presented for several trivial and non-trivial crystal structures.

MA 18.32 Fri 10:00 P

Light-, temperature-, and x-ray-induced spin-crossover transition of molecules adsorbed on a graphite surface — ●JORGE TORRES¹, LALMINTHANG KIPGEN¹, SASCHA OSSINGER², SANGEETA THAKUR¹, CLARA W.A. TROMMER², IVAR KUMBERG¹, RAHIL HOSSEINFAR¹, EVANGELOS GOLIAS¹, SEBASTIEN HADJADJ¹, JENDRIK GÖRDES¹, CHEN LUO³, KAI CHEN³, FLORIN RADU³, FELIX TUCZEK², and WOLFGANG KUCH¹ — ¹Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany — ²Christian-Albrechts-Universität zu Kiel, Institut für Anorganische Chemie, Kiel, Germany — ³Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

When iron spin-crossover molecules (SCM) are irradiated by light, their spin configuration can be excited from the ground state S_0 to an excited state S_1 and from there even to a metastable state of different multiplicity. For Fe(II) complexes this corresponds to a transition from low-spin (LS) to high-spin (HS) states. When the temperature is changed, this transition takes place in terms of thermodynamic effects. In this work we deposited different sub-, mono- and multilayer coverages of $[\text{Fe}\{\text{pzpy}\}\text{pz}]_2$ on highly oriented pyrolytic graphite and measured them by X-ray absorption spectroscopy. Analysis of the HS and LS fraction showed that for almost all samples the light-induced excited spin-state trapping (LIESST) effect resulted in twice the HS fraction than the thermally induced spin-state transition. The transition temperature $T_{1/2}$ (50% HS and 50% LS) is located at 300 K, opening a window for potential applications at room temperature.

MA 18.33 Fri 10:00 P

Hyperthermia setup for efficient nanoparticle heating — ●DANIEL KUCKLA, AMIRARSALAN ASHARION, JULIA-SARITA BRAND, VINZENZ JÜTTNER, and CORNELIA MONZEL — Heinrich-Heine-Universität Düsseldorf

All biological systems are temperature dependent. Of special interest is the influence of elevated temperatures on malignant tissue and how this can be exploited for medical treatments. One approach called "magnetic hyperthermia" uses bio-functionalized magnetic nanoparticles (MNPs) which heat in an alternating magnetic field. By targeting MNPs to the malignant cells, a spatially selective heating of tissue is realized. Here, we present a hyperthermia setup, which allows to image the behaviour of cells marked with MNPs on a microscope while being subjected to an alternating magnetic field. We provide a comprehensive characterization of the setup components and magnetic fields generated, as well as strategies to limit off-target power dissipation. We further quantify the heat generated by MNPs in well-defined in vitro and biomimetic environments. The efficient generation of high-frequency magnetic fields and direct observation of MNP responses will provide valuable information on the heat generation mechanism in different environments.

MA 18.34 Fri 10:00 P

Spectroscopic studies of a Fe(II) spin-crossover complex in the room temperature regime — ●LEA SPIEKER¹, STEPHAN SLEZIONA¹, GÉRALD KÄMMERER¹, CAROLIN SCHMITZ-ANTONIAK², TORSTEN KACHEL³, SOMA SALAMON¹, DAMIAN GÜNZING¹, TOBIAS LOJEWSKI¹, NICO ROTHENBACH¹, ANDREA ESCHENLOHR¹, KATHARINA OLLEFS¹, SENTHIL KUMAR KUPPUSAMY⁴, MARIO RUBEN^{4,5}, UWE BOVENSIEPEN¹, PETER KRATZER¹, MARIKA SCHLEBERGER¹, and HEIKO WENDE¹ — ¹Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — ²Jülich Research Center — ³Helmholtz Center Berlin — ⁴Karlsruhe Institute of Technology — ⁵CNRS-University of Strasbourg

Spin-crossover complexes with a bi-stable spin-state switching in the room temperature regime, influenced by external stimuli such as light, pressure, temperature, or X-rays, are desirable for applications. With different spectroscopic methods, like Raman- and X-ray absorption spectroscopy, we investigated a Fe(II) complex showing a phase transition from a diamagnetic low-spin ($S=0$) to a paramagnetic high-spin ($S=2$) state in the room temperature regime ($T_{1/2\uparrow} = 330$ K) with a broad thermal hysteresis of $\Delta T = 50$ K. Unique changes of the molecular bondings during a temperature-induced phase transition are confirmed by Raman spectroscopy measurements combined with density functional theory calculations. In addition, X-ray absorption spectroscopy measurements reveal a thermally reversible soft X-ray induced excited spin-state trapping effect in the room temperature regime. Financially supported by CRC 1242 Project A05 (Project-ID 278162697).

MA 18.35 Fri 10:00 P

High-frequency Electron Paramagnetic Resonance studies on a pentagonal-bipyramidal V(III) complex — ●LENA SPILLECKE, CHANGHYN KOO, and RÜDIGER KLINGELER — Kirchhoff-Institute for Physics, Heidelberg University, Germany

We present detailed high-frequency/high-field electron paramagnetic resonance (HF-EPR) studies as well as magnetic susceptibility measurements down to 400 mK on the first pentagonal-bipyramidal Vanadium(III) complex with a Schiff-base N_3O_2 pentadentate ligand. [1] By detailed measurements on loose and fixed powder samples we rationalized precisely the crystal field parameters and g -value information of this complex and also quantified small but finite intermolecular dimer-like antiferromagnetic magnetic coupling of $J = -1.1$ cm⁻¹. Especially the observation of intermolecular coupling is somehow surprising considering the isolated character and large distance between the V(III) centers. However, theoretical analysis reveals that the interaction between distant V(III) centers is mediated via π -stacking contacts between the ligands of neighboring complexes. In conclusion this work gives a deep insight into the magnetic properties of a V(III) complex and demonstrates how HF-EPR spectroscopy can act as powerful tool for the investigation of magnetic properties.

[1] *Bazhenova et al., Dalton Trans.* 49, 15287-15298 (2020)

MA 18.36 Fri 10:00 P

High-frequency EPR study on the exchange couplings in 3d-4f heterometallic complexes with diverse structures — ●CHANGHYUN KOO¹, LENA SPILLECKE¹, SILVIA MENGHI¹, SEBASTIAN SCHMIDT², YAN PENG², NAUSHAD AHMED³, MAHESWARAN SHANMUGAM³, ANNIE K. POWELL², and RÜDIGER KLINGELER¹ — ¹Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — ²Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany. — ³Department of Chemistry, Indian Institute of Technology, Mumbai, India.

3d-4f heterometallic complexes are suggested to enhance the magnetic anisotropy barrier in single molecular magnets (SMM) candidate metal organic complexes as combining benefits of 3d and 4f magnetic ions. Though the exchange coupling between 3d and 4f ions, J_{3d-4f} , is essential, its quantitative determination is still challenging. In this presentation, the precise J_{3d-4f} values in several 3d-4f heterometallic complexes with various molecular structures, i.e. Cu_2Ln with linear bonding, Fe_4Ln_2 with ring-like structure, and Fe_2Ln_2 butterfly-like structure ($\text{Ln} = \text{Tb}, \text{Dy}, \text{Ho}, \text{Yb}, \text{and Gd}$) are determined by means of the high-frequency electron paramagnetic resonance (HF-EPR) technique. Based on the current studies, the effect of the exchange interaction on the magnetic properties of the complexes is discussed.

MA 18.37 Fri 10:00 P

Thermal- and Light-Induced Spin-Crossover Characteristics of a Functional Iron(II) Complex at Submonolayer Coverage on HOPG — ●SANGEETA THAKUR¹, EVANGELOS GOLIAS¹, IVAR KUMBERG¹, KUPPUSAMY S. KUMAR², RAHIL HOSSEINFAR¹, JORGE

TORRES¹, LALMINTHANG KIPGEN¹, CHRISTIAN LOTZE¹, LUCAS M. ARRUDA¹, FLORIN RADU³, MARIO RUBEN², and WOLFGANG KUCH¹ — ¹Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany — ²Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — ³Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

The role of molecule-substrate interactions on the thermal- and light-induced spin-state switching characteristics of 0.4 monolayer of a functional spin-crossover(SCO)-complex $[\text{Fe}(\text{H}_2\text{B}(\text{pz})_2)_2\text{COOC}_{12}\text{H}_{25}\text{-bipy}]$ on a highly oriented pyrolytic graphite (HOPG) substrate was studied using x-ray absorption spectroscopy [1]. A spin-state coexistence of 42% low-spin (LS) and 58% high-spin (HS) is observed for the complex at 40 K, in contrast to the complete spin-state switching observed in the bulk and in SiO_x-bound 10 nm thick films [2], highlighting the role of molecule-substrate interactions. The 100% HS state obtained after light irradiation at 10 K indicates the occurrence of efficient on-surface light-induced spin switching, encouraging the development of light-addressable molecular devices based on SCO complexes.

[1] S. Thakur et al. J. Phys. Chem. C 125, 25, (2021).

[2] K. S. Kumar et al., Adv. Mater. 30, 1705416, (2018).

MA 18.38 Fri 10:00 P

Modeling spin-phonon relaxation in organic semi-conductors from first-principles — ●UDAY CHOPRA, ERIK R. MCNELLIS, and JAIRO SINOVA — Johannes Gutenberg University, Staudingerweg 7, Mainz 55128

Spin-orbit coupling (SOC) is one of the major causes of spin-relaxation in organic semiconductors. It generally works in conjunction with other factors, for example a hopping driven spin-flip mechanism [1,2]. In this work, we explore spin-relaxation caused due to molecular vibrations. We present a model to estimate the spin-phonon couplings using finite-differences within harmonic approximation from a first-principles approach. Using these couplings we are able to derive the spin-relaxation times (T1) between the Zeeman energy levels for Raman-like processes using the Fermi's Golden rule. Our model assumes a relaxation mediated via two phonons via an intermediate state. This enables us to evaluate and predict the temperature dependence of T1 and analyse the contribution of relevant phonon-modes that dominate the relaxation. We present our findings using organic-semiconductors and single-molecule magnets to demonstrate transferability across different systems. [1] Chopra et al. Phys. Rev. B 100, 134410 (2019) [2] Chopra et al. J. Phys. Chem. C 123, 19112, (2019)

MA 18.39 Fri 10:00 P

Optical control of 4f orbital state in rare-earth metals — N. THIELEMANN-KÜHN¹, ●T. AMRHEIN¹, W. BRONSH¹, S. JANA², N. PONTIUS², R. ENGEL³, P. MIEDEMA³, D. LEGUT⁴, K. CARVA⁵, U. ATXITIA¹, B. VAN KUIKEN⁶, M. TEICHMANN⁶, R. CARLEY⁶, L. MERCADIER⁶, A. YAROSLAVTSEV^{6,7}, G. MERCURIO⁶, L. LE GUYADER⁶, N. AGARWAL⁶, R. GORT⁶, A. SCHERZ⁶, M. BEYE³, P. OPPENEER⁷, M. WEINELT¹, and C. SCHÜSSLER-LANGEHEINE² — ¹Freie Universität Berlin — ²HZB — ³DESY — ⁴IT4Innovations — ⁵Charles University — ⁶European XFEL — ⁷Uppsala University

High density magnetic storage devices base on materials with large magneto crystalline anisotropy (MCA) that needs to be overcome by laser heating above the Curie temperature to enable bit writing [1]. In a time-resolved X-ray absorption experiment at the European XFEL we found that the MCA itself can be manipulated on fs time scales by an optical stimulus [2]. In 4f rare-earth metals the magnetic moment and high MCA stems from the 4f system that is not directly accessible with optical wavelengths. We show, however, that the direct excitation of 5d electrons drives 4f-5d inelastic electron scattering and 4f-5d electron transfer, initiating orbital excitations in the 4f shell that change the MCA tremendously. Besides the technological relevance of such handle on MCA, 4f electronic excitations directly alter exchange and electron-phonon coupling and thus contribute to a more fundamental understanding of non-equilibrium dynamics.

[1] W. Challener et al. Nature Photon 3, 220-224 (2009).

[2] arXiv:2106.09999

MA 18.40 Fri 10:00 P

Characterization of superconducting niobium lumped-element-resonators for strong magnon-photon coupling to yttrium-iron-garnet (YIG) structures — ●PHILIPP GEYER¹,

KARL HEIMRICH¹, PHILIP TREMPER¹, FRANK HEYROTH², SANDRA GOTTSWALS¹, and GEORG SCHMIDT^{1,2} — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany — ²Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Nanotechnikum Weinberg, 06120 Halle (Saale), Germany

In the past years the field of hybrid quantum magnonics appears a promising candidate for quantum information processing. Here, magnons can be an important mediator for coupling between different quantum states [1]. We investigate superconducting Nb lumped-element-resonators grown on annealed sapphire (0001) substrates. The resonators are fabricated by optical lithography, Nb sputtering and lift-off. The deposition of niobium was done by argon ion sputtering at room-temperature and the niobium was not covered by a protecting layer. Nevertheless, we observe for 50 nm thin films superconducting transition temperatures above 7 K and sufficiently high critical B-fields. Our work is focused on resonators which excite preferably high localized magnetic fields. YIG particles will be transferred from high quality free standing YIG microstructures to achieve strong coupling between microwave photons and magnons [3]. [1] D. Lachange-Quirion et al. Science, Vol. 367, Issue 6476, pp. 425-428 (2020) [2] P. Trempler et al. Appl. Phys. Lett. 117, 232401 (2020)

MA 18.41 Fri 10:00 P

Mapping the Stray Fields of a Micromagnet Using Spin Centers in SiC — ●MAURICIO BEJARANO^{1,2}, FRANCISCO JOSE TRINDADE GONCALVES¹, MICHAEL HOLLENBACH^{1,2}, TONI HACHE^{1,3}, TOBIAS HULA^{1,3}, YONDER BERENCÉN¹, JÜRGEN FASSBENDER¹, MANFRED HELM¹, GEORGY V. ASTAKHOV¹, and HELMUT SCHULTHEISS¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — ²Technische Universität Dresden, 01062 Dresden, Germany — ³Technische Universität Chemnitz, 09107 Chemnitz, Germany

We report on utilizing an ensemble of V_{Si} centers as a room-temperature sensor of static stray fields generated by magnetic microstructures patterned on top of a SiC substrate. We use optically-detected magnetic resonance (ODMR) to measure the impact of the stray fields on the intrinsic V_{Si} resonance frequencies. The spin resonance at the spin centers is driven by a micrometer-sized microwave antenna patterned next to the magnetic element. The antenna pattern is made to ensure that the driving microwave fields are delivered locally and more efficiently compared to conventional millimeter-sized circuits. We observe a spatially dependent frequency shift of the V_{Si} resonances which enables us to determine the field contribution from the magnetic element in its close vicinity. Our results are a first step toward developing magnon-quantum applications by deploying local microwave fields and stray fields at the micrometer length scale. This work was supported in part by the German Research Foundation under Grants SCHU 2922/4-1 and AS 310/5-1.

MA 18.42 Fri 10:00 P

Optical read-out of the Néel vector in metallic antiferromagnet Mn₂Au — ●V. GRIGOREV¹, M. FILIANINA¹, S. YU. BODNAR¹, S. SOBOLEV¹, N. BHATTACHARJEE¹, S. BOMMANABOYENA¹, Y. LYTUVNENKO¹, Y. SKOURSKI², D. FUCHS³, M. KLAUE¹, M. JOURDAN¹, and J. DEMSAR¹ — ¹Institute of Physics, Uni Mainz, 55128 Mainz, Germany — ²HLD-EMFL, HZDR, 01328 Dresden, Germany — ³IQMT, KIT, 76344 Eggenstein-Leopoldshafen, Germany

Metallic antiferromagnets with broken inversion symmetry on the two sublattices, strong spin-orbit coupling and high Néel temperatures offer new opportunities for applications in spintronics. Especially Mn₂Au, with high Néel temperature and conductivity, is particularly interesting for real-world applications. The read-out of the staggered magnetization, *i.e.* the Néel vector is limited to studies of anisotropic magnetoresistance or X-ray magnetic linear dichroism. Here, we report on the in-plane reflectivity anisotropy of Mn₂Au (001) films, which were Néel vector aligned in pulsed magnetic field. In the near-infrared, the anisotropy is $\approx 0.6\%$, with higher reflectivity for the light polarized along the Néel vector. The observed magnetic linear dichroism is about four times larger than the anisotropic magnetoresistance, suggesting the dichroism in Mn₂Au is a result of the strong spin-orbit interactions giving rise to anisotropy of interband optical transitions, in-line with recent studies of electronic band-structure. The considerable magnetic linear dichroism in the near-infrared could be used for ultrafast optical read-out of the Néel vector in Mn₂Au.