MLZ Heinz Maier-Leibnitz Zentrum

Conference Neutrons for Information and Quantum Technologies

June 4th - 7th, 2019
Arabella Brauneck Hotel, Lenggries, Germany

Abstract Booklet

MLZ is a cooperation between:

JÜLICH Forschungszentrum

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technical University of Munich TUM

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The Heinz Maier-Leibnitz Zentrum (MLZ): The Heinz Maier-Leibnitz Zentrum is a leading centre for cutting-edge research with neutrons and positrons. Operating as a user facility, the MLZ offers a unique suite of high-performance neutron scattering instruments. This cooperation involves the Technical University of Munich, the Forschungszentrum Jülich and the Helmholtz-Zentrum Geesthacht. The MLZ is funded by the German Federal Ministry of Education and Research, together with the Bavarian State Ministry of Education, Science and the Arts and the partners of the cooperation.

The Forschungs-Neutronenquelle Heinz-Maier-Leibnitz (FRM II): The Forschungs-Neutronenquelle Heinz-Maier-Leibnitz provides neutron beams for the scientific experiments at the MLZ. The FRM II is operated by the Technical University of Munich and is funded by the Bavarian State Ministry of Science and the Arts.

„Grüß Gott“, dear colleagues,

We like to welcome you to the MLZ conference **“Neutrons for Information and Quantum Technologies”** in Lenggries.

The conference is the fourth kind of MLZ conferences dealing with the usage and benefits of neutrons science in major areas of science and society. After the MLZ conference “Neutrons for Energy” in 2016, “Neutrons for Health” in 2017 and “Neutrons for Culture and Art” the conference is now devoted to information and quantum technology.

The conference **“Neutrons for Information and Quantum Technologies”** consists of 9 keynote talks, 12 contributed talks and a poster session, and we are proud to welcome numerous renowned speakers from Denmark, France, Korea, India, Japan, Luxembourg, Sweden and Germany joining the conference.

The conference addresses the field of neutron scattering in magnetic and quantum spin systems identifying their complex structure and dynamics. The conference will highlight diverse topics as spin calorotronics, magnon transport, magnetic 2-d van der Waals materials, new trends in spintronics, dynamics of magnetic textures, like skyrmions, domain walls and vortices, high-precision calculations of neutron scattering with the density-matrix renormalization group, and operating quantum states in single molecules. These will hopefully stimulate discussion between the participants, who up-to now have not regularly used neutron scattering as a method and long-standing neutron users. We also hope to offer a discussion platform for experiment and theoretical players in these exciting fields of magnetism. Therefore we have left ample time for discussions and an interesting short excursion in the Bavarian Alps around Lenggries.

The MLZ provides a number of instruments allowing to probe the structure and the dynamics of these systems. DNS, SANS and POLI allow for determining the structure in magnetic systems using neutron spin polarized techniques. The triple axis instruments PUMA, PANDA, MIRA and TRISP can determine the dynamics of these systems. These instruments will be presented in the poster session during the conference.

We look forward to having intense and fruitful discussions on the current status and future perspectives of neutron scattering for information and quantum technologies.

With kind regards and warm welcome

Prof. Dr. Peter Müller-Buschbaum and Prof. Dr. Stephan Förster

Scientific Director of Heinz Maier-Leibnitz Zentrum (MLZ) and Forschungs-Neutronenquelle FRM II, Technische Universität München (TUM)

Scientific Director of Heinz Maier-Leibnitz Zentrum (MLZ) and Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH

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TUESDAY, JUNE 4th

12:00	Lunch	
14:00	Welcome and Introduction	MUELLER-BUSCHBAUM, Peter
Spin caloritronics (14:15 - 16:00)		
14:15	Spin Caloritronics with Magnetic Insulators	BAUER, Gerrit
15:15	Mechanism of the Magnetocaloric Effect in the Mn5-xFexSi3 Series	BRÜCKEL, Thomas
16:00	Coffee	
Spin wave and magnonics (16:30 - 18:50)		
16:30	Magnon Transport in Spin Textures	HELMUT, Schultheiss
17:30	Temporal evolution of magnon-magnon interaction in a magnetic vortex	HULA, Tobias
17:50	Magnetic fluctuations in the iron-based superconductors	PARK, Jitae
18:10	Stripe discommensuration and spin dynamics in Pr3/2Sr1/2NiO4	DUTTA, Rajesh
18:30	Precise magnetic structure of CeRhIn5 from neutron diffraction on absorption optimized samples	HUTANU, Vladimir
19:00	Dinner	

WEDNESDAY, JUNE 5th

2D magnetic van der waals materials		
09:00	Magnetic Van der Waals materials: Discovery & Perspective	PARK, Je-Geun
10:00	Coffee	
New trends in spintronics (flexible, antiferromagnetic) (10:30 - 13:00)		
10:30	New Trends in Spintronics : Flexible and Antiferromagnetic Spintronics	BEDANTA, Subhankar
11:30	Electric field control of magnetism in heterostructures of oxide perovskites	KENTZINGER, Emmanuel
12:00	Polarized Neutron Reflectometry on superconducting/ferromagnetic superlattices	KHAYDUKOV, Yury
12:30	Semiconductor / Ferromagnetic Insulator InAs/EuS Epitaxy	LIU, Yu
13:00	Lunch	
Novel rare-earth free permanent magnets (15:00 -16:00)		
15:00	Magnetic Neutron Scattering Studies on Permanent Magnets	MICHELS, Andreas
16:00	Coffee	
Dynamics of magnetic textures: domain walls, vortices and Skyrmions: Dynamics of quantum materials (16:30 - 18:30)		
16:30	Thermal Aspects in Quantum Materials – Phonon Lifetimes Investigated by Neutron Scattering	HABICHT, Klaus
17:00	Vortex Matter Beyond SANS: From Superconductivity to Skyrmions	MUEHLBAUER, Sebastian
19:00	Dinner	

THURSDAY, JUNE 6th

Dynamics of magnetic textures: domain walls, vortices and Skyrmions: Dynamics of magnetic textures (08:30 - 11:00)		
08:30	Energetics of skyrmions in chiral magnets	PFLEIDERER, Christian
09:30	Magnetic Skyrmions – Novel spin textures for spintronics functionalities	BLUEGEL, Stefan
10:30	Polarization Analysis of the Non-Reciprocal Skyrmion Dynamics in MnSi	WEBER, Tobias
11:00	Excursion to the Stie Alm	
Poster Session (17:30-19:00)		
Revealing exotic spin states on PANDA cold TAS at MLZ		SCHNEIDEWIND, Astrid
Magnetic spin structures in amorphous DyCo thin film systems		LOTT, Dieter
Neutron studies of of [Fe(x)/Nb(1.5)]10/Nb(40nm) systems		GUASCO, Laura
TISANE: AC Coil Setup for Kinetic Neutron Scattering		BREMS, Xaver Simon
Neutron scattering on a new Nd-pychlore single crystal		SONG, Junda
Fabrication and characterization of $SrCoO_{3-\delta}$ thin films		PÜTTER, Sabine
Magnetic Guinier Law		MALYEYEV, Artem
MIEZETOP for the cold triple axis spectrometer (TAS) MIRA		GABOLD, Henrik
DNS: a versatile polarized neutron instrument at the forefront of quantum materials research		SU, Yixi
Incommensurate magnetic systems studied with the three-axis spectrometer (TAS) MIRA		GEORGII, Robert
Studies of Magnetic Symmetry and Topology Using Single and Double Polarized Options on POLI		HUTANU, Vladimir
19:00	Dinner	

FRIDAY, JUNE 7th

Molecular magnetism (09:00 - 10:00)		
09:00	Operating quantum states in single magnetic molecules	WERNSDORFER, Wolfgang
10:00	Coffee	
Numerical simulations of quantum spin systems (10:30 - 12:00)		
10:30	High-precision calculation of (neutron) scattering with the density-matrix renormalization group	SCHOLLWÖCK, Uli
11:30	Spin wave excitations of magnetic metalorganic materials	HELLSVIK, Johan
Concluding remarks & Farewell (12:00 - 12:30)		
12:30	Lunch	

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Spin Caloritronics with Magnetic Insulators

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Spin Caloritronics is the science and technology devoted to the control of the electron spin with heat in nanoscale structures and devices [1]. It is a subdiscipline of the fields of spintronics, magnetism, and thermoelectrics. A specialized conference series celebrates its 10th edition [2].

Magnetic insulators, especially yttrium iron garnet (YIG), have been crucial material for spin caloritronics since the discovery of the spin Seebeck effect in the YIG|Pt system [3]. YIG is a ferrimagnet with record-high magnetic quality, but a complex crystal structure with a large unit cell. Inelastic neutron scattering experiments [4] interpreted by atomistic simulations [5] are essential for an understanding of spin caloritronic effects.

I this talk I will review the field with emphasis on new developments.

1. G.E.W. Bauer, E. Saitoh, and B. van Wees, Nature Mater. 11, 391-399 (2012).
2. Spin Caloritronics X,Groningen (The Netherlands), May 20-24, 2019, spincal2019.webhosting.rug.nl
3. K. Uchida et al., Nature Mat. 9, 894–897 (2010).
4. A. J. Princep et al., npj Quantum Mater. 2, 63 (2017) and references therein.
5. J. Barker and G.E.W. Bauer, Phys. Rev. Lett. 117, 217201 (2016) and in preparation.

Mechanism of the Magnetocaloric Effect in the $Mn_{5-x}FexSi_3$ Series

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Due to potential energy savings for room temperature applications, the magnetocaloric effect (MCE) has attracted increasing interest in the past years. We have performed extensive studies of structure, magnetism, magnetocaloric effect and spin dynamics in the $Mn_{5-x}FexSi_3$ series of compounds [1-5]. While the magnetocaloric effect is moderate for these compounds, they are composed of abundant and non-toxic elements and can be grown as large single crystals. This allows us to perform inelastic neutron scattering studies of the spin and lattice dynamics thus giving insight into the microscopic mechanism of the MCE. For the compound $MnFe_4Si_3$ a strong response of the critical fluctuations has been detected and identified as an important feature connected to the MCE effect [4]. The compound Mn_5Si_3 exhibits an inverse magnetocaloric effect. Inelastic neutron scattering reveals that contrary to the intuitively expected behavior, the application of a magnetic field can induce additional spin fluctuations giving rise to an increase of the magnetic entropy. This mechanism provides a microscopic explanation of the inverse magnetocaloric effect [5].

[1] M. Gottschlich et al; Journal of Materials Chemistry 22 (2012), 15275
[2] O. Gourdon et al; Journal of Solid State Chemistry 216 (2014), 56
[3] P. Hering et al; Chemistry of Materials 27 (2015), 7128
[4] N. Biniskos et al; Physical Review B 96 (2017), 104407
[5] N. Biniskos et al; Physical Review Letters 120 (2018), 257205

Magnon Transport in Spin Textures

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Magnonics is a concept using magnons - the collective excitation quanta of the spin system in magnetically ordered materials - as carriers for information. Magnons are waves of the electrons' spin precessional motion. They propagate without charge transport and its associated Ohmic losses, paving the way for a substantial reduction of energy consumption in computers.

The full potential of magnonics lies in the combination of magnons with nano-sized spin textures. Both magnons and spin textures share a common ground set by the interplay of dipolar, spin-orbit and exchange energies rendering them perfect interaction partners. Magnons are fast, sensitive to the spins' directions and easily driven far from equilibrium. Spin textures are robust, non-volatile and still reprogrammable on ultrashort timescales.

I will give an introduction about magnon propagation and manipulation in microstructures with non-collinear spin textures, in particular magnons propagating in nano channels formed by magnetic domain walls. Furthermore, I will address how magnons can be excited in domain wall channels by pure spin currents originating from the spin Hall effect and nonlinear effect in magnetic vortices.

[1] K. Schultheiss, R. Verba, F. Wehrman et al. Phys. Rev. Lett. 122, 097202 (2019)
[2] K. Wagner, A. Kákay, K. Schultheiss et al. Nature Nanotech 11, 432 (2016).
[3] K. Vogt, F. Y. Fradin, J. E. Pearson, et al. Nat Comms 5, 3727 (2014).

Temporal evolution of magnon-magnon interaction in a magnetic vortex

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Brillouin light scattering microscopy (TR-µBLS) measurements on a Permalloy disk magnetized in the vortex state are presented. By applying a homogenous out-of-plane AC field with sufficiently large amplitudes it is possible to drive the spin waves in the nonlinear regime and initiate three- and four-magnon scattering processes.

Time resolved µBLS is used to show that these pumping conditions cause cascades of different types of magnon-magnon interactions. It is shown, that the temporal transition of different scattering mechanisms can be tuned by the excitation frequency and amplitude.

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Magnetic fluctuations in the iron-based superconductors

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One of the most plausible scenario for the mechanism of the unconventional superconductivity is the magnetically-mediate Cooper pair. The iron-based superconductors are much known as an unconventional type, thus a number of inelastic neutron scattering studies were reported to evidence a strong relationship between the spin excitations and superconductivity. Here we present recent progress on spin excitation studies of the iron-based superconductors mainly performed on the thermal neutron three axes spectrometer PUMA at MLZ.

Stripe discommensuration and spin dynamics in $Pr_{3/2}Sr_{1/2}NiO_4$

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Inelastic neutron scattering studies on the magnetic excitation in a stripe-ordered $Pr_{3/2}Sr_{1/5}NiO_4$ at 5K reveal that the magnetic incommensurability (ε = 0.4) as result of admixing stripe dicommensuration in the checkerboard matrix in NiO_2 plane. A suggested linear spin-wave model accounting 3D-stripe discommensuration with two-fold exchange interactions between Ni^{2+} spins, provides a good agreement with the measured spin wave dispersion up to 64 meV, notably, to describe a slight symmetric shift of the broadened peak in the energy range from 35 to 45 meV. Our results indicate that discommensuration model is essential to consolidate in the LSWT calculation to understand the microscopic effect of doped holes to the spin microstructure.

Precise magnetic structure of $CeRhIn_5$ from neutron diffraction on absorption optimized samples.

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$CeRhIn_5$ is a prototypical strongly correlated metal attracting much attention because of it peculiar magnetic and electronic properties. However, despite the intense studies two aspects of the ambient pressure magnetic structure of this heavy fermion material have remained under some debate since its discovery: whether the structure is indeed an incommensurate helix or a spin density wave, and what is the precise magnitude of the ordered magnetic moment. Contradictory results on this regard were reported in the literature. On the other side, the precise knowledge of the magnetic structure is an important prerequisite for the detailed theoretical modelling on the microscopic level. We suppose, that certain discrepancies in the previous results may be caused by the parasitic effects like strong absorption for the thermal neutrons by the elements like In or Rh and large sample sizes used in the precedent studies. By using a single crystal sample optimized for hot neutrons to minimize neutron absorption we performed a series of polarised and non-polarised neutron diffraction experiments clearly revealing both the helical type of the magnetic structure, and magnitude of the ordered moment of m = 0.54(2) μB. Moreover, studied macroscopic sample surprisingly presents a single chiral domain.

SPIN WAVE AND MAGNONICS - 17:50

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Magnetic Van der Waals materials: Discovery & Perspective

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There has been a huge increase of interests in two-dimensional van der Waals materials over the past ten years or so. Despite the impressive list of new materials and the novel physics it has come to offer, there is the conspicuous absence of one particular class of materials: magnetic van der Waals systems. It is certainly a sorry status of materials science given the huge impact the magnetic materials have had on both the fundamental understanding and the diverse applications. In this talk, I will identify and illustrate how we might be able to benefit from exploring these so-far neglected materials.

[1] Je-Geun Park, J. Phys. Condens. Matter 28, 301001 (2016)
[2] Jae-Ung Lee, et al., Nano Lett. 16, 7433 (2016)
[3] Cheng-Tai Kuo, et al., Scientific Reports 6, 20904 (2016)
[4] So Yeun Kim, et al., Phys. Rev. Lett. 120, 136402 (2018)
[5] Kenneth S. Burch, David Mandrus, and Je-Geun Park, Nature 563, 47 (2018)
[6] Kangwon Kim, et al., Nature Communications 10, 345 (2019)

New Trends in Spintronics: Flexible and Antiferromagnetic Spintronics

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Shapeable magneto-electronics is the new trends in spintronics due to the growing market of flexible electronic devices. In this context we have deposited perpendicularly magnetized Co(0.7nm)/Pt thin film on flexible substrates like Polyimide film (25 μm thick) and Kapton tapes. We observed that magnetic anisotropy is tunable via variable strain. However the domain shape may or may not change depending on the different strain mechanism.

Next I will discuss on another field of antiferromagnetic (AFM) spintronics. Pure spin current can be generated by the precession of magnetization in a ferromagnet (FM) to the neighboring heavy metal (HM) via spin pumping process. This pure spin current gets converted to a charge current due to high spin orbit coupling (SOC) of the HM which is known as inverse spin Hall effect (ISHE) process. Recently AFM materials having high SOC are found to be good replacement of HM in spin current based study. We have performed the ISHE study of CoFeB (10 nm)/ AFM (d nm) where we considered various AFM such as Mn2Au, IrMn etc. Angle dependent ISHE was performed to disentangle various spin rectification effects.

Further I will show the study on topological insulator (TI)/ferromagnetic Bi_2Se_3/YIG garnet films. Polarized neutron reflectometry experiments indicate induced magnetic moment in the TI. ISHE experiments are also performed to demonstrate that TIs are potential candidates to replace HM as they also possess high spin-orbit coupling.

Electric field control of magnetism in heterostructures of oxide perovskites

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Magnetoelectric multiferroics are promising candidates for fast, dense and cooler electronics. Numerous oxide perovskites are either magnets or traditional ferroelectrics but only a few of them display both types of order and magneto-electric coupling in a single phase. Ferromagnetic-ferroelectric or ferromagnetic-piezoelectric thin film heterostructures of oxide perovskites provide an alternative approach to achieve and study electric field control of magnetism. In such systems, the matching of lattice constants between different perovskite oxides can promote the coherent growth of heterostructures with sharp interfaces.

Here, we address the possibility of electric field control of magnetism in two systems: (a) two layers of ferroelectric $BaTiO_3$ and ferromagnetic $La_{0.67}Sr_{0.33}MnO_3$ on a Nb-doped $SrTiO_3$ substrate, and (b) a single layer of $La_{0.67}Sr_{0.33}MnO_3$ on piezoelectric $0.7(Pb(Mg_{1/3}Nb_{2/3})O_3)$-$0.3(PbTiO_3)$ substrate.

The samples are grown by oxide molecular beam epitaxy and high oxygen pressure sputtering, followed by a systematic characterization of their structural and magnetic properties in the laboratory. Atomically resolved magnetism is investigated as a function of applied electric field using a combination of polarized neutron reflectivity and advanced electron microscopy.

Polarized Neutron Reflectometry on superconducting/ferromagnetic superlattices

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Artificial heterostructures with alternating superconducting (S) and ferromagnetic (F) layers are currently attracting great attention due to a diverse set of proximity effects, including -phase superconductivity and triplet pairing [1]. The ability to control magnetic state by superconductivity is attracting attention in applied research on superconducting spintronics [2] including such new approaches as neuromorphic computing [3]. At the moment most research efforts are focused on simple S/F structures such as bi- and trilayers. However, both superconducting and magnetic properties of more complex S/F systems, such as [S/F]n superlattices, may qualitatively differ from the properties of their S/F unit cells thus opening up perspectives for novel functionalities. Tuning of parameters of such S/F “metamaterials” is a complicated task which requires involving many methods.

PNR is an effective method allowing for depth-resolved study of vector magnetic state of S/F heterostructures and its change due to proximity effects. In this talk we will discuss our recent results on magnetic proximity effect in Gd/Nb [4] and design of spin-valve based on Co/Nb [5] superlattices.

[1] M. Eschrig, Phys. Today 64, 43 (2011).
[2] A. Golubov and M. Kupriyanov, Nat. Mater. 16, 156 (2017).
[3] M. L. Schneider et. al, J. Appl. Phys. 124, 161102 (2018).
[4] Y. Khaydukov et. al, Phys. Rev. B 99, 140503(R) (2019)
[5] N.Klenov, Y.Khaydukov et.al, Beilstein J. Nanotechnol. 10, 833 (2019).

Semiconductor / Ferromagnetic Insulator InAs/EuS Epitaxy

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Material development holds promise as the basis of topological quantum computing with Majorana fermions. These quasiparticles have been predicted at ends of semiconductor nanowires (NWs) coupled to conventional superconductors. This prediction was followed by a series of experiments providing strong evidence. However, in the current system, an external magnetic field along the NW axis is always needed to realize Majorana states. Therefore, in order to integrate and scale up qubit devices, it is aimed to induce a self-sustaining parallel magnetic field on semiconductor-superconductor (SE-SU) hybrid NWs. Composite tri-crystals using ferromagnetic insulators (FMIs) in close proximity to the SE-SU structure have been proposed as a solution to lift the spin degeneracy, where the Zeeman splitting could be induced by the exchange field from the FMI.

In this work, we study hybrid InAs/EuS epitaxy as the initial basis of tri-crystal SE-SU-FMI NW systems. The EuS thin film grown on (100) Zinc Blende InAs surface is fully coherent. The interfacial band alignment preserves semiconducting nature. The exchange field exists at InAs//EuS interface. The magnetic moments are located around In atoms. The results do not only show the InAs//EuS//Al hybrid crystals as promising candidates for topological quantum computing, but also confirm EuS as a promising FMI for various spin applications.

Magnetic Neutron Scattering Studies on Permanent Magnets

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Nd-Fe-B-based permanent magnets have been continuously investigated for the last three decades due to their technological relevance as materials used in energy-related applications (e.g., motors and wind turbines). A crucial issue is the understanding of the magnetization-reversal process, which eventually may result in the preparation of dysprosium and terbium-free Nd-Fe-B alloys with characteristic magnetic parameters (coercivity, remanence, maximum energy product) that guarantee their performance also at the high operating temperatures of motors (up to 200 ◦C). In order to achieve this goal, the combination of advanced characterization techniques such as aberration-corrected high-resolution transmission electron microscopy and three-dimensional atom-probe tomography with ab-initio calculations and numerical micromagnetic modeling is required. Indeed, recent studies along these lines have provided important information regarding the nature (chemical composition, crystalline structure, ferro- or paramagnetic) of the intergranular Nd-rich phases in Nd-Fe-B magnets (including nanocomposites), which decisively determine the coercivity mechanism of these materials. In this talk we will discuss how magnetic neutron scattering, specifically small-angle neutron scattering, can contribute to the understanding of the microstructure-property relationship of Nd-Fe-B magnets and we will give an outlook on rare-earth-free Mn-Bi magnets.

Thermal Aspects in Quantum Materials – Phonon Lifetimes Investigated by Neutron Scattering

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Thermal management is a key aspect for future information technologies since non-volatile data storage and information processing in quantum circuits strongly rely on minimizing thermal decoherence effects. Among the successful strategies to control the coherence are rapid cooling and thermal isolation of quantum states, emphasizing the importance to engineer materials with very high or very low thermal conductivity. Computational materials design based on first-principle calculations holds a huge potential for identifying novel compounds with superior heat transport properties, and state-of-the-art ab initio methods, albeit based on approximations, allow to calculate wavevectordependent

relaxation rates for every phonon mode in the Brillouin zone. Exploiting the high energy resolution of inelastic neutron scattering, we have measured phonon lifetimes in the quantum paraelectric $SrTiO_3$ which allows to benchmark the predictive power of quantum theoretical calculations.
We discuss recent results obtained by neutron triple-axis spectroscopy and neutron resonance spinecho spectroscopy pin-pointing phonon lifetimes on an absolute energy scale. We further discuss Larmor diffraction measurements which deliver important information about phonon scattering at the domain walls. These experiments provide a thorough basis to resolve discrepancies between the calculated and measured lifetimes and to further develop theoretical models for lattice-mediated heat propagation.

Vortex Matter Beyond SANS: From Superconductivity to Skyrmions

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Both superconducting vortex and skyrmion lattices in chiral magnets can be regarded as macroscopic lattices, formed by topological entities. Analogous to condensed matter, a large variety of phases is also observed for vortex and skyrmion matter, resembling their particle like character and reflecting the underlying physical properties. Moreover, both vortex and skyrmion matter represent ideal model systems for questions of general importance as topological stability and decay and also domain nucleation and growth. As for superconducting vortex matter, skyrmion melting transitions, skyrmion liquids and skyrmion glass phases are expected to exist in various materials.

Neutron scattering provides an ideal tool for the investigation of both vortex and skyrmion matter. Going beyond the standard SANS approach, we present an overview how to address the static and dynamic properties of superconducting vortex and skyrmion matter by means of neutron grating interferometry (nGI), neutron diffractive imaging (nGI), time-resolved small angle neutron scattering (TISANE), ultra small angle neutron scattering (USANS) and the neutron resonance spin echo spectroscopy technique (MIEZE).

Work in collaboration with: C. Franz, T. Reimann, A. Backs,V. Pipich, M. Schulz, J. Kindervater, T. Adams, F. Haslbeck, A. Chacon, F. Jonietz, P. Böni, C. Pfleiderer, M. Garst, A. Rosch, P. Milde, L. Eng, J. Seidel.

NOTES

Energetics of skyrmions in chiral magnets

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Topological spin textures in chiral magnets such as skyrmions attract great interest as a possible route towards spintronics devices. Central to the suitability for applications are the mechanisms controlling the long-term stability and decay processes. Starting from the mechanisms of stabilization the role of kinetic arrest and supercooling will be addressed. These identify topological magnetic order far from equilibrium as an exciting approach for the exploration of the fundamentals of topological protection and in the search for novel electronic phases.

Magnetic Skyrmions – Novel spin textures for spintronics functionalities

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In this talk I give an overview primarily on chiral magnetic skyrmions – two-dimensionally localized topological magnetization solitons – in B20 magnets, films of B20 magnets, transition-metal films and heterostructures. Taking a multiscale approach from quantum mechanics of electrons, over atomistic spinmodels to micromagnetism, I draw a line of thought from the electronic structure, to the spin-orbit interaction, the magnetic spin-texture, the stability of skyrmions, and to their coexistence with antiskyrmions and bobbers. I discuss the potential and the role of Heisenberg-type exchange frustration for the properties of skyrmions followed by the recent progress made in the field of skyrmionics, i.e. skyrmions as entity of information, which have to fit to the field of spintronics, in size, ambient temperature, injection, transport, detection and manipulation at reasonable fields and currents. I look into the materials dimensions for skyrmions, the choice of heterostructures of synthetic antiferromagnets, the role of interfaces and the role of impurities. I look into the topological orbital moment of skyrmions, the Hall effects and the tunneling spin-mixing magneto-resistance as means of single skyrmion detection. Skyrmions might be only the beginning of localized magnetization textures. I may give a perspective of three-dimensional magnetic textures localized on the nanometer scale.

Polarization Analysis of the Non-Reciprocal Skyrmion Dynamics in MnSi

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The chiral magnet MnSi possesses a non-centrosymmetric chemical unit cell. The non-centrosymmetry has profound consequences for spin-wave dynamics in all ordered magnetic phases of MnSi. Namely, it introduces a Dzyaloshinskii-Moriya term, which causes magnons to be created at different absolute energies than they are annihilated. This asymmetry (”non-reciprocity”) in the dispersion is limited to reduced momentum transfer components parallel to the applied magnetic field direction, i.e. the skyrmion axis.

Using the new triple-axis spectrometer ThALES at the ILL, we performed a longitudinal polarization analysis of the skyrmion dynamics in MnSi for direction in reciprocal space both along and perpendicular to the skyrmion axis. Individual polarization-dependent dispersion branches could be clearly resolved in the first direction, while for the second direction we found a broad quasi-continuum of dispersion branches. Utilizing the Monte-Carlo convolution of a linear spin-wave model [1] and the instrumental resolution function, we achieved an excellent quantitative agreement between experiment and theory.

[1] M. Garst, et al., Journal of Physics D 50(29), 293002 (2017).
This work will be part of a comprehensive paper on skyrmion dynamics:
T. Weber, D. Fobes, J. Waizner, L. Beddrich, P. Steffens, G. Tucker, R. Bewley, M. Skoulatos, R. Georgii, P. Link, G. Ehlers, A. Bauer, C. Pfleiderer, P. Böni, M. Janoschek, and M. Garst, in preparation.

Revealing exotic spin states on PANDA cold TAS at MLZ

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Investigations of magnetic excitations focus on new magnetic materials, quantum magnetism, superconductivity, heavy-fermion or low-dimensional systems, frustrated and multiferroic materials.

The challenges of high-resolution studies can be answered only by cold neutron (TAS) spectroscopy experiments. In our days, there is a trend for extreme conditions, searching for exotic spin states. The discovery of these systems is often limited by small sample sizes or weak scattering cross sections, as well as asking for special sample environment such as high magnetic fields with low temperatures. PANDA, being a high-resolution, high-flux cold TAS spectrometer with a remarkably low background, successfully contributes with high-level experiments to a broad variety of scientific topics.

We here present a selection of recently published results where PANDA experiments significantly contributed.

Magnetic spin structures in amorphous DyCo thin film systems

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Alloys of rare-earth elements and 3d transition metals became recently again in the focus of attention due there rich variety of magnetic effects owed to the different anisotropies of both material classes.

In this work, various thin film systems containing the amorphous DyCo alloy will be discussed. Despite of their amorphous nature, the film system show non trivial magnetic ordering leading to extraordinary phenomena. Neutron scattering techniques, in particular polarized neutron reflectometry are essential to investigate such thin film systems providing the sensitivity to study the magnetic structures on a microscopic level that is essential to understand the underlying principles.
In $DyCo_4$ a large Atomic Exchange Bias effect was observed in a single film owned to the competition between the atomic exchange and the Zeemann interaction. In contact with a soft magnetic thin film of permalloy a chirality based exchange bias effect could be created. Here, the direction of the exchange bias effect can be isothermal switched by a moderate perpendicular magnetic field. The presence of an interfacial Dyzaloshinskii-Moriya is one of the keys to explain the observation.
In a very recent study, we could demonstrated how skyrmionic objects could be created in $DyCo_3$ single films. The utilization of ferrimagnetic skyrmions as well as the of novel concepts of exchange bias may be of crucial importance for the development of future applications in the field of magnetic sensors.

POSTER SESSION -17:30

Neutron studies of of [Fe(x)/Nb(1.5)]10/Nb(40nm) systems

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Thin film heterostructures are one of the most prominent and studied systems for the realization of spintronics devices, due to the different magnetic couplings and proximity phenomena that are possible to obtain. One of the most well-known examples is the RKKY exchange coupling, that leads to Giant Magnetoresistance in ferromagnet/metal/ferromagnet layers, which is nowadays at the basis of modern spintronics. An interesting question to explore is what would happen to the coupling between ferromagnetic in the presence of superconducting correlations in the normal metal spacer.

In this work we report on preliminary results on the preparation and characterization of samples of composition Al_2O_3(1 -1 0 2)//Nb(40 nm)/[Fe(x)/Nb(1.5 nm)]10/Pt(3 nm), with x = 2-4 nm, grown in DCA M600 MBE setup of JCNS. A Fe/Nb superlattice is deposited on top of a thick superconducting Nb(40 nm) buffer layer, that acts as a reservoir of superconducting pairs which will be transferred to the superlattice using proximity effect [1]. The samples were studied with SQUID magnetometry, X-ray diffraction and depth sensitive polarized neutron reflectometry (PNR), which is proved to be a powerful method for the study of magnetic state of Fe/Nb superlattices [2].

[1] S.V. Bakurskiy et al, JETP Letters 102 (9), 586-593 (2015)
[2] Ch. Rehm, D, Nagengast, F. Klose, H. Maletta, A. Weidinger EPL 38 (1997)

TISANE: AC Coil Setup for Kinetic Neutron Scattering

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We present the design and characterization of a newly built AC coil setup for TISANE measurements at the small angle scattering instrument SANS-1 at MLZ in Garching. The setup is based on an existing 2.2 T HTS magnet and a modified CC type cryostat. The new setup can generate a static magnetic field Bstat of 2.2 T superpositioned by an AC magnetic field BAC in orthogonal and parallel orientation with respect to Bstat at base temperatures of Tbase= 3 - 5 K. The magnitude of BAC ranges from 25 mT for static fields to 1.2 mT at a frequency of 10 kHz. The whole setup can be positioned such that Bstat is either parallel or orthogonal to the neutron beam. Special attention is given to the design process of the AC coil and the choice of material for the cryostat modification. The design process was supported and optimized by FEM-simulations. Measurements of the static magnetic field at different coil separations and currents and the frequency dependence of the magnetic field for different radiation shields and configurations are presented and agree well with FEM-simulations.

POSTER SESSION -17:30

Neutron scattering on a new Nd-pychlore single crystal

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Pyrochlore $Nd_2Zr_2O_7$ was found to have very special magnetic ground state in which there is a coexistence of dynamical spin-ice correlations and quantum moment fragmentation due to the dipolaroctupolar doublet ground state of Kramers Nd^{3+} ion. Through 1:1 mixing of Sc^{3+} and Ta^{5+} in B sites, the crystal field ground state of Nd^{3+} can be strongly affected, and the magnetic ground state of pyrochlore $Nd_2Zr_2O_7$ is suggested to have rather different ground state with the case of pure $Nd_2Zr_2O_7$. Polarized neutron diffuse scattering at 100 mK confrimed the long-range order together with strong diffuse scattering in the ground state. The strong diffuse scattering in the ordered state indicates a robust moment fragmentation even in the Sc-Ta mixing sample. More specially, clear mangetic peak at (0 0 2) below 500 mK suggested a different magnetic structure of $Nd_2Zr_2O_7$ in comparision with the case of pure $Nd_2Zr_2O_7$. It is concluded that doping in B sites is an effective method to modulate the magnetic ground state of Nd-pyrochlore, which can help to realize more novel quantum magnetism and collective excitations in this magnetically frustrated system.

Fabrication and characterization of $SrCoO_{3-\delta}$ thin films

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Because of its multivalent Co states and high oxygen mobility $SrCoO_{3-\delta}$ (SCO) is a promising material for energy and spintronic applications [1]. Upon changing its oxygen content it exhibits a topotactic phase transition. While $SrCoO_3$ is a ferromagnetic metal (T_C=305 K) with perovskite structure, $SrCoO_{2.5}$ is an antiferromagnetic insulator(T_N =570 K) with brownmillerite structure.
In this contribution, we focus on the fabrication of $SrCoO_{2.5}$ thin films by molecular beam epitaxy on various substrates like $SrTiO_3$ and $LaAlO_3$. As Sr and Co are coevaporated from distinct effusion cells, the first task is to obtain stoichiometric thin films. We present results of RHEED assisted stoichiometric thin film growth and of driving the topotactic transition by annealing in low oxygen gas flow. For bulk SCO it has been shown that the perovskite structure can be stabilized by adding of about 5% rare earth ions [2]. For this reason we study the effect of Sm doping on the crystal structure of SCO thin films. The magnetic properties were studied with SQUID and the crystalline properties by surface characterization methods like LEED, RHEED and XRR.

[1] H. Jeen et al., Nature Materials 12, (2013) 1057
[2] M. James et al., Solid State Sciences 6 (2004) 655

POSTER SESSION -17:30

Magnetic Guinier Law

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The so-called Guinier law represents the low-q approximation for the small-angle scattering curve from a dilute assembly of identical and randomly oriented particles. This relation has been derived for nonmagnetic particle-matrix-type systems; an important prerequisite for it to apply is the presence of a sharp interface separating particles and matrix. On the other hand, it is well known that the magnetic microstructure of nanocrystalline magnets is highly nonuniform on the nanometer length scale and characterized by a spectrum of continuously varying long-wavelength magnetization fluctuations. This results in a large and strongly field-dependent magnetic small angle neutron scattering (SANS) cross section. In this work we introduce the Guinier law for the case of magnetic SANS and provide an analysis of experimental data on a hard magnetic Nd-Fe-B-based and a soft magnetic Fe-based nanocomposite.

MIEZETOP for the cold triple axis spectrometer (TAS) MIRA

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Neutron Spin Echo is a techniques to obtain high resolution which uses the spin to record information.
It is used to observe slow phenomena, which are correlated to relaxation processes, e.g. correlations between atomic positions or spin orientations. Here these phenomena manifest itself in an inelastic broadening of the structure factor S(Q) revealing time domains of inelastic processes that are magnitudes higher than classical neutron spectrometers. One way of realization is MIEZE (Modulation of IntEnsity with Zero Effort) where the energy transfer displays in a contrast change of the oscillating signal. We implement this technique into our triple axis instrument to obtain high resolution in a broad Q-range.

POSTER SESSION -17:30

DNS: a versatile polarized neutron instrument at the forefront of quantum materials research

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With its compact design, large double-focus monochromator and wide-angle polarization analysis, DNS is optimized as a high intensity cold-neutron polarized instrument. Major instrument upgrades, including a new-generation Fe/Si supermirror based focusing polarizing bender [1], and a 300 Hz disc chopper system, have been accomplished recently. This has opened up possibilities to combine polarized neutrons with time-of-flight spectroscopy for the studies of exotic magnetic order and excitations in quantum materials, such as magnetic Dirac and Weyl semimetals, quantum spin liquid, quantum spin ice and Kitaev quantum magnets. In this poster, an overview about the recent instrument upgrades and some selected examples on our recent studies of quantum materials [2-5] will be given.

[1] K. Nemkovski, et al., J. Phys. Conf. 862, 012018 (2017).
[2] S. Gao, et al., Nat. Phys. 13, 157 (2017).
[3] V. Pecanha-Antonio, et al., Phys. Rev. B 96, 214415 (2017).
[4] V. Pecanha-Antonio, et al., Phys. Rev. B 99, 134415 (2019).
[5] Fengfeng Zhu, Xiao Wang, et al., (unpublished).

Incommensurate magnetic systems studied with the three-axis spectrometer (TAS) MIRA

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The cold-neutron three-axis spectrometer MIRA is an instrument optimized for low-energy excitations. Its excellent intrinsic -resolution makes it ideal for studying incommensurate magnetic systems. MIRA is uses advanced neutron focusing optics such as elliptic guides, which enable the investigation of small samples under extreme conditions. Scientific topics include the investigation of complex inter-metallic alloys and spectroscopy on incommensurate magnetic structures.

POSTER SESSION -17:30

Studies of Magnetic Symmetry and Topology Using Single and Double Polarized Options on POLI

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Single crystal diffractometer with polarised neutrons POLI recently implemented at Maier-Leibnitz Zentrum (MLZ) was specially designed to perform studies of complex magnetic structures and magnetic domain populations in bulk by different polarised neutron techniques. Flipping Ratio measurements using high magnetic field, uniaxial polarisation analysis in the moderate magnetic field, and Spherical Neutron Polarimetry in Zero-field are successfully implemented. The study of magnetoelectric and antiferromagnetic domains under applied electric/magnetic field as well of ferromagnetic domains by depolarisation analysis are also possible. Here we present different experimental setups available on POLI and show the examples of their applications.

Operating quantum states in single magnetic molecules

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The endeavour of quantum electronics is driven by one of the most ambitious technological goals of today's scientists: the realization of an operational quantum computer. We start to address this goal by the new research field of molecular quantum spintronics, which combines the concepts of spintronics, molecular electronics and quantum computing. The building blocks are magnetic molecules, i.e. well-defined spin qubits. Various research groups are currently developing low-temperature scanning tunnelling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors) to read and manipulate the spin state and perform basic quantum operations. We will present our recent measurements of geometric phases, the iSWAP quantum gate, the coherence time of a multi-state superposition, and the application to Grover's algorithm [1-5].

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[3] M. N. Leuenberger, D. Loss, Quantum computing in molecular magnets. Nature 410, 789-793(2001).
[4] C. Godfrin, A. Ferhat, R. Ballou, S. Klyatskaya, M. Ruben, W. Wernsdorfer, F. Balestro, Phys. Rev. Lett. 119, 187702 (2017).
[5] C. Godfrin, et al.,. npj Quant. inf. 4, 53 (2018).

High-precision calculation of (neutron) scattering with the density-matrix renormalization group

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In recent years, the density-matrix renormalization group (DMRG) method, by now the leading method for one-dimensional strongly correlated quantum systems, has been extended to the simulation of time-dependent phenomena at finite-temperature and is therefore now ideally placed to calculate momentum- and frequency-dependent scattering off magnets. In this talk, I will introduce to the method, its relation to the theory of entanglement, the important post-processing of data, and show how if produces results in excellent agreement with various experimental results (for instance, $RbCoCl_3$) and allows the detailed study of magnetic properties of materials.

Spin wave excitations of magnetic metalorganic materials

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The Organic Materials Database (OMDB) [1,2] is an open database at Nordita that is hosting about 22,000 electronic band structures, density of states and other properties for synthesized 3-dimensional organic crystals. The web interface of the OMDB offers various search tools for the identification of novel functional materials such as band structure pattern matching and density of states similarity search. In this work we extend the OMDB to include magnetic excitation properties. For inelastic neutron scattering we focus on the dynamical structure factor S(Q,ω) which contains information on the excitation modes of the material. We introduce a new dataset containing atomic magnetic moments and Heisenberg exchange parameters for which we calculate the spin wave spectra and dynamic structure factor with linear spin wave theory and atomistic spin dynamics [3]. We thus develop the materials informatics tools to identify topological magnon spectra such as Dirac crossings within the class of organic molecular crystals, and reveal mechanisms for the topological protection of the crossings.

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[1] S. S. Borysov, R. M. Geilhufe, and A. V. Balatsky, PloS one 12.2 (2017): e0171501.
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[3] J. Hellsvik, R. Díaz Pérez, R. M. Geilhufe, M. Månsson, A. V. Balatsky, in preparation.

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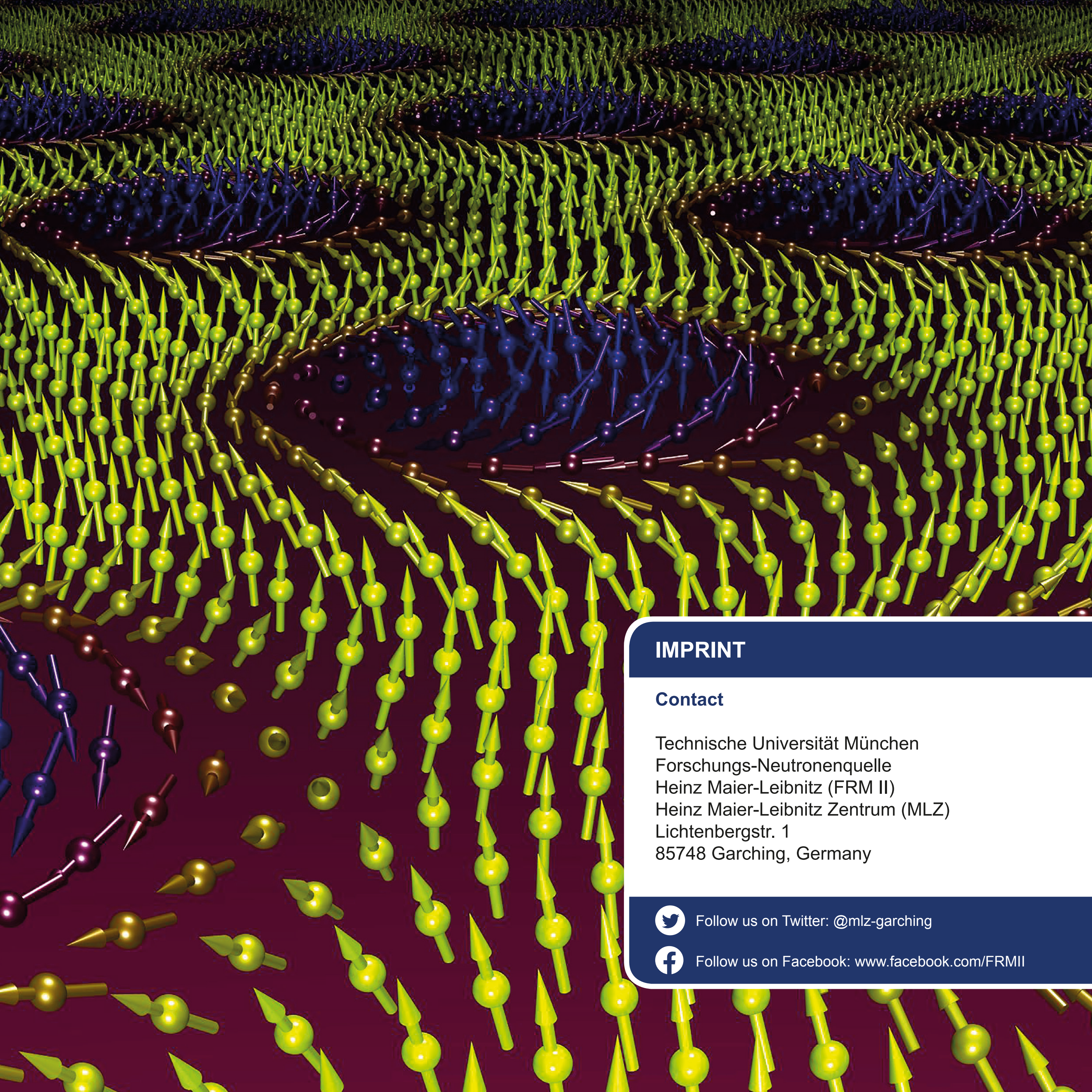

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