MA 58: Computational Magnetism II

Time: Friday 9:30–12:45 Location: POT/0151

MA 58.1 Fri 9:30 POT/0151

Prototype for Magnetic Multiscale Modelling Suite (MaMMoS) — •Hans Fangohr[1], Samuel RJ Holt[1], Martin Lang[1], Swapneel Pathak[1], Andrea Petrocchi[1], Wilfried Hortschitz[2], Santa Pile[2], Alena Vishina[3], M Nur Hasan[3], Georgia A Marchant[3], Timoteo Colnaghi[4], Christina Winkler[4], Jonas Winkler[5], Nora Dempsey[6], Thomas G Woodcock[5], Andreas Marek[4], Heike C Herper[3], and Thomas Schrefl[2] — [1]MPSD, Hamburg, Germany — [2]UWK, Krems, Austria — [3]Uppsala University, Sweden — [4]MPCDF, Garching, Germany — [5]IFW, Dresden, Germany — [6]Institute Neel, Grenoble, France

Magnetic materials require multiscale modelling across electronic, atomistic, micromagnetic and device levels. MaMMoS provides a unified Python framework that links these steps and avoids manual data translation. Based on ground-state magnetic parameters from DFT databases, it computes their temperature dependence using atomistic spin-dynamics, and passes them directly to micromagnetic solvers for modelling hysteresis and switching. Common analysis tools (e.g., coercivity, remanence) are included, and benchmarking and optimisation are possible. Planned extensions include machine-learning based modules to replace simulations with faster, approximate estimates. We present the current prototype to attract early adopters and invite community feedback.

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MA 58.2 Fri 9:45 POT/0151

A Fourier-Space Approach to Physics-Informed Magnetization Reconstruction from Nitrogen-Vacancy Measurements — •Alexander Setescak[1], Florian Bruckner[1], Dieter Suess[1], Young-Gwan Choi[2,3], Hayden Binger[2], Lotte Boer[2], Claire Donnelly[2], Uri Vool[2], and Claas Abert[1] — [1]University of Vienna, Vienna, Austria — [2]Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany — [3]University of Ulsan, Ulsan, Republic of Korea

Reconstructing complex magnetization textures from nitrogen-vacancy (NV) magnetometry stray-field measurements presents a challenging inverse problem. In this work, we introduce a physics-informed method that addresses this by incorporating the full micromagnetic energy directly into the variational formulation.

Built on a PyTorch backend, our forward model integrates an auto-differentiable micromagnetic framework with FFT-based stray-field calculations and Fourier-space upward continuation. This enables efficient gradient-based optimization via the adjoint method and allows the sensor-sample distance to be treated as an optimization parameter. By doing so, we eliminate the experimental uncertainty arising from unknown NV implantation depths and surface oxidation layers.

Validation on synthetic data demonstrates high-fidelity reconstruction of spin textures and precise sensor height estimation. Furthermore, when applied to experimental NV measurements of the van der Waals magnet $Fe_{3-x}GaTe_2$, the framework reconstructs skyrmion bubbles that are consistent with theoretical micromagnetic behavior.

MA 58.3 Fri 10:00 POT/0151

First principals calculation of current-induced spin-transfer and spin-orbit torques — •Tamás Véber[1], László Oroszlány[1,2], Zoltán Tajkov[1,3], Marcell Sipos[1], and Branislav K. Nikolic[4] — [1]Eötvös Loránd University, Budapest, Hungary — [2]Wigner Research Centre for Physics, Budapest, Hungary — [3]HUN-REN Centre for Energy Research, Budapest, Hungary — [4]University of Delaware, USA

The study of two dimensional magnetic materials - especially those possessing strong spin-orbit coupling - has great promise both in terms of providing new theoretical discoveries, as well as practical applications like smaller and more energy efficient magnetoresistive RAM (MRAM) technologies. The theoretical study of such systems has been well-established in recent decades. However, no single ecosystem exists in which all the simulation and post-processing steps can be performed in a cohesive way. We aim to fill this gap by providing a chain of cross-compatible software for this purpose - and where it is possible, do this in the form of open-source libraries. In this work we lay out such an implementation for obtaining current-induced spin torques - like spin-transfer torque (STT) and spin-orbit torque (SOT) - in the linear response regime from ab initio results. We demonstrate this method on a set of magnetic two dimensional few-layer materials, comparing our results with the literature.

MA 58.4 Fri 10:15 POT/0151

Multi-spin Hamiltonians from symmetry considerations — •Levente Rózsa — HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — Budapest University of Technology and Economics, Budapest, Hungary

Spin Hamiltonians are central to modeling magnetic materials. These Hamiltonians must reflect the symmetry of the underlying crystal [1]. Going beyond the most extensively studied two-spin interaction terms, for example the introduction of the isotropic biquadratic exchange interaction, has proven successful in describing special types of magnetic ordering in classical and quantum magnets. Four-spin generalizations of the anisotropic Dzyaloshinsky-Moriya interaction have also been proposed [2,3].

Here, we present a general formalism for deriving symmetry-adapted multi-spin interactions up to arbitrary order in the spin Hamiltonian. This method provides an alternative to perturbative expansions [2] which become difficult to tract as the number of spins and the complexity of the interactions increases. We identify all possible interaction terms containing four spins, and describe their transformation properties under rotations. We propose procedures for deriving these interactions from first-principles calculations, and for calculating the magnetic ground states stabilized by them.

[1] J. Bouaziz et al., Phys. Rev. B 112, 014406 (2025). [2] S. Brinker et al., New J. Phys. 21, 083015 (2019). [3] A. Lászlóffy, L. Rózsa et al., Phys. Rev. B 99, 184430 (2019).

MA 58.5 Fri 10:30 POT/0151

Above-Room-Temperature Magnetism in the Fe3GeTe2 and Fe3GaTe2 monolayer — •Anjali Jyothi Bhasu[1], Bendegúz Nyári[1], László Oroszlány[2], László Udvardi[1], and László Szunyogh[1] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki ut 8., HU-1111 Budapest, Hungary — [2]Department of Physics of Complex Systems, Eötvös Loránd University, 1117 Budapest, Hungary

Room-temperature ferromagnetism that remains robust at the nanoscale is a key requirement for next-generation spintronic and information storage technologies. Using density-functional methods, we investigate monolayers of the van der Waals magnets Fe3GeTe2 and Fe3GaTe2, both of which exhibit magnetic ordering under ambient conditions. We compute the magnetic interaction parameters using the LKAG torque formalism as well as the spin-cluster expansion combined with the relativistic disordered local moment formalism. Special emphasis is placed on how these interactions vary with the Hubbard parameter U, which controls electron-electron correlations within the DFT+U framework. We then estimate the energetically favored magnetic structure by evaluating the Fourier transform of the tensorial coupling matrices. The order-disorder transition temperatures are obtained from large-scale Monte Carlo simulations, and we find that the simulated transition temperatures depend sensitively on the value of U.

MA 58.6 Fri 10:45 POT/0151

Micro and macroscopic quantum details of complex spin-textures — •Wenhan Chen[1,2], Sangeeta Sharma[1,3], and John Kay Dewhurst[2] — [1]Max-Born-Institut (MBI) im Forschungsverbund Berlin e.V,Max-Born-Str 2A, Berlin — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle (saale) — [3]Freie Universität Berlin, Berlin

Studying large-scale systems from first principles remains challenging because conventional DFT becomes prohibitively expensive. The recently proposed ultra-long-range DFT (ULR-DFT) aims to address this systematically while retaining full quantum-mechanical detail.

In our preliminary work, ULR-DFT successfully reproduces micrometre-scale ferromagnetic domains and domain walls, while also providing quantum-level information such as band structures and response functions. Applied to B20 chiral magnets, it captures helical states and skyrmion textures in agreement with experiments. Over-

all, ULR-DFT is promising for both fundamental research and device modelling, including band-structure engineering for spintronic applications.

15 min break

MA 58.7 Fri 11:15 POT/0151

Automated Defect Detection in Magnetic Imaging Data Using Latent Measures and U-Net Segmentation — •Ross Knapman[1,2], Nasim Bazazzadeh[1,3], Kübra Kalkan[1], Atreya Majumdar[1], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Institute of Mechanics, Faculty of Engineering, University of Duisburg-Essen, 45141 Essen, Germany — [3]Radiology Department, Massachusetts General Hospital, 175 Cambridge St., Boston, MA 02114, USA

Detecting and characterising local inhomogeneities is essential for understanding and optimising magnetic materials. We present an automated framework that combines physics-based latent measures with deep convolutional segmentation for robust defect identification in magnetic imaging data. Time-resolved micromagnetic simulations with randomly distributed defects are used to compute three per-pixel descriptors: temporal mean, temporal standard deviation, and a latent-entropy measure that quantifies local dynamical complexity [1,2]. Each measure serves as input to a U-Net architecture trained for pixel-level segmentation of defect regions. Performance is evaluated under additive and multiplicative noise to test robustness. This approach demonstrates how integrating physics-motivated feature construction with deep learning enables reliable automated analysis of magnetic textures and defect landscapes in simulation and experiment.

[1] Horenko, I. et al., Comm. App. Math. and Comp. Sci 16, 267 (2021). [2] Rodrigues, D. R. et al., iScience 24, 102171 (2021).

MA 58.8 Fri 11:30 POT/0151

Dynamical mean-field theory for spin systems at finite temperature: cluster extension — •Przemyslaw Bieniek[1], Timo Gräßer[2], and Götz Uhrig[1] — [1]Condensed Matter Theory, TU Dortmund University, Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]Institute of Molecular Physical Science, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Dynamical mean-field theory (DMFT) is an established numerical technique for approximately solving fermionic many-body problems. It maps the full quantum system to an impurity problem and uses a self-consistency condition to connect back to expectation values of the original model. In recent years, a method inspired by DMFT applicable to spin systems (spinDMFT) was developed. It is in agreement with numerical techniques and has already proven successful in explaining nuclear magnetic resonance experiments. However, it was derived only in the case of infinite temperature.

Based on spinDMFT, we develop a dynamical mean-field theory for spin systems at finite temperatures. The algorithm computes spin correlations in imaginary time. It maps the spin system to a single-site problem with a time-dependent mean field and uses a self-consistency condition to connect the values of the mean-field to quantum expectation values. The single-site approach is extended to a cluster algorithm, allowing for the computation of nonlocal expectation values. We benchmark the algorithm by comparing the resulting correlations with numerical approaches. We discuss the potential applications of the method and possible extensions.

MA 58.9 Fri 11:45 POT/0151

A Computational Framework for Bare and Interacting Longitudinal Susceptibility in Magnetic Materials — •Rohit Pathak[1], Vladislav Borisov[1,2], Mikhail I. Katsnelson[2,3], Anna Delin[4,5], and Olle Eriksson[1,2] — [1]Uppsala University, Sweden — [2]Wallenberg Initiative Materials Science for Sustainability, Uppsala, Sweden — [3]Radboud University, Netherlands — [4]KTH Royal Institute of Technology, Sweden — [5]Wallenberg Initiative Materials Science for Sustainability, Stockholm, Sweden

We present a computational framework for calculating the non-interacting and interacting spin susceptibilities in magnetic materials using the Relativistic Spin-Polarized Toolkit (RSPt) [1]. The ground-state electronic structure is obtained from self-consistent DFT calculations, followed by the computation of site-resolved Matsubara Green's functions, whose convolution yields the bare susceptibility. The interacting χ^{zz} is evaluated by solving the ADA–TDDFT Dyson equation $K = (1 - XU)^{-1}X$, based on previously developed theory [2]. Applications to bcc Cr, $BaFe_2As_2$, and FeSe show that the calculated $\chi(\mathbf{q})$ peaks reproduce the known magnetic ordering vectors. This framework enables systematic exploration of spin-density-wave phenomena in correlated electron systems.

[1] J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, and O. Grechnyev, Full-Potential Electronic Structure Method (Springer, 2010).

[2] M. I. Katsnelson and A. I. Lichtenstein, J. Phys.: Condens. Matter 16, 7439 (2004).

MA 58.10 Fri 12:00 POT/0151

Proximity-Induced Magnetic Phases in CrI3 Monolayers Coupled to Transition-Metal Dichalcogenide Monolayer — •Zoltan Tajkov[1], Laszlo Oroszlany[1], Amador Garcia Fuente[2], Jaime Ferrer[2], Jaroslav Fabian[3], and Daniel Pozsar[1] — [1]Eotvos Lorand University, Budapest, Hungary — [2]University of Oviedo, Oviedo, Spain — [3]University of Regensburg, Regensburg, Germany

We investigate the emergence of altered magnetic phases in a CrI3 monolayer induced by proximity effects with WTe2. Using density functional theory (DFT) calculations within the SIESTA framework, we analyze the magnetic properties via a novel approach for extracting the magnetic exchange interaction and onsite anisotropy tensors in extended Heisenberg spin models, explicitly incorporating relativistic effects. This method, based on the Liechtenstein-Katsnelson-AntropovGubanov torque formalism, evaluates energy variations upon infinitesimal spin rotations. Our results provide insight into how a 2D magnet is influenced when coupled to a material with strong spin-orbit coupling. Additionally, we explore the impact of varying twist angles, considering the incommensurability of the CrI3 and WTe2 unit cells.

MA 58.11 Fri 12:15 POT/0151

Acoustic Wave Group Velocity under Magnetic Field — •Dominik Legut[1,2], Ievgeniia Korniienko[1], and Pablo Nieves[3] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czechia — [2]Charles University, Prague, Czechia — [3]University of Oviedo, Oviedo, Spain

Recently, we derived a spin-lattice model for ferromagnetic cubic crystals[1]. Then we analyzed the effect of the magneto-elasticity on the group velocities for high symmetry directions[2]. Here we present a different approach to determine the group velocity of the acoustic waves in any crystals and under the effects an external magnetic field for cubic and hexagonal symmetry. The group velocity is obtained by calculating Christoffel matrix elements and their partial derivative with respect to the phase velocity direction, and inserting them in an analytical expression for the group velocity. The effect of that external magnetic field is computed through the induced effective corrections to the elastic tensor which depend on the magnetic susceptibility tensor and the magnetoelastic constants. We present examples of dry sandstone, cubic CoPt and hcp Co to show complex landscapes of fractional change in group velocity as a function of ray direction, as well as a field dependence consistent with the Simon effect[3]. We have developed web-based applications where these effects can be analyzed and visualized in 3D[4].

[1] P. Nieves et al.: Phys. Rev. B **103**, 094437 (2021)
[2] P. Nieves et al.: Phys. Rev. B **105**, 134430 (2022)
[3] I. Korniienko, et al.: Results in Physics, **73**, 108264 (2025)
[4] P. Nieves et al.:, SoftwareX **33**, 102472 (2026)

MA 58.12 Fri 12:30 POT/0151

machine learning prediction of magnetic ordering in chiral induced multiferroic hybrid MOFs — •Gayathri Palanichamy, Biplab Sanyal, and Jonas Fransson — Materials Theory Division, Angstrom Laborartory, Uppsala Univesity, Sweden

Chiral hybrid metal organic frameworks with Ruddlesden Popper type halide layers provide a versatile platform for engineering multiferroicity by combining molecular chirality with transition metal magnetism. In this work, we develop a machine learning framework to identify multiferroic candidates in systems where chiral A-site organic molecules break inversion symmetry to induce ferroelectricity, while B-site transition metal centers govern magnetic ordering. First principles calculations confirm that the chiral distortion stabilizes a spontaneous polarization, and selected compositions exhibit coexisting ferroelectricity and ferromagnetism. To efficiently explore this large chemical and structural space, we construct feature descriptors capturing molecular chirality, distortion modes, metal ligand coordination metrics, and octahedral connectivity. Random Forest and Deep Neural

Network models are trained to classify magnetic ground states (FM, AFM A, AFM C, AFM G) and achieve an R* score of 0.94, enabling reliable prediction of magnetic ordering across diverse chiral MOFs. Our approach also identifies previously unexplored chiral Ruddlesden Popper candidates with potential multiferroic behavior. This work establishes a data driven strategy toward building a chiral magnetic MOF repository, providing design principles for future spintronic and multifunctional materials.