MA 2: Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)

Time: Monday 9:30–12:15 Location: H16

MA 2.1 Mon 9:30 H16

Trilinear coupling and toroidicity in multiferroics — Andrea Urru[1] and •Vincenzo Fiorentini[2,3] — [1]Dept. of Physics, Rutgers University, USA — [2]Chair of Materials Science and Nanotech, TU Dresden — [3]Dept. Physics, University of Cagliary, Italy

We discuss the properties of the triple-order-parameter (ferromagnet, ferroelectric, ferrotoroid) layered-perovskite metal Bi5Mn5O17, as predicted from first-principles calculations, in the light of a Landau expansion with trilinear coupling, with particular reference to its multiple degenerate ground states with mutually orthogonal vector order parameters, giant cross-coupling magnetoelectricity, and magnetotoroidic effects.

MA 2.2 Mon 9:45 H16

Engineering magnetic domain wall energies in $BiFeO_3$ via epitaxial strain: A route to assess skyrmionic stabilities in multiferroics from first principles — •Sebastian Meyer[1,2], Bin Xu[3,4], Laurent Bellaiche[4], and Bertrand Dupé[1,2] — [1]Université de Liège, Belgium — [2]Fonds de la Recherche Scientifique, Belgium — [3]Soochow University, China — [4]University of Arkansas, USA

Epitaxial strain has emerged as a powerful tool to tune magnetic and ferroelectric properties in functional materials such as in multiferroic perovskite oxides. Here, we use first-principles calculations to explore the evolution of magnetic interactions in the antiferromagnetic multiferroic $BiFeO_3$ (BFO), one of the most promising multiferroics for future technology [1]. The epitaxial strain in BFO is varied between $\varepsilon \in [-2\%, +2\%]$. We find that both strengths of the exchange interaction and Dzyaloshinskii-Moriya interaction decrease linearly from compressive to tensile strain whereas the uniaxial magnetocrystalline anisotropy lifts the energy degeneracy of the (111) easy plane of bulk BFO. From the trends of magnetic interactions we can explain the destruction of cycloidal order in compressive strain as observed in experiments due to the increasing anisotropy energy. For tensile strain, we predict that the ground state remains unchanged as a function of strain. By using the domain wall energy, we envision a region where isolated chiral magnetic textures might occur as a function of strain [2].

[1] R. Ramesh, N. Spaldin, *Nature Mater* **6**, 21-29 (2007)
[2] S. Meyer *et al.*, *Phys. Rev. B* **109**, 184431 (2024)

MA 2.3 Mon 10:00 H16

Hidden order in Cr_2O_3 and α-Fe_2O_3 as a predictor for (anti-)magnetoelectricity — •Xanthe Verbeek[1,2], Andrea Urru[2,3], and Nicola Spaldin[2] — [1]Insitut für Physik, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany — [2]Materials Department, ETH Zurich, 8093 Zürich, Switzerland — [3]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

With first-principles calculations of Cr_2O_3 and α-Fe_2O_3, we show that the different magnetoelectric effects in these materials result from the ordering of hidden magnetic multipoles. We reveal for the first time anti-ferroically ordered magnetic multipoles in both Cr_2O_3, and isostructural α-Fe_2O_3, in which the global inversion symmetry is preserved by the different magnetic dipolar ordering. We can relate each of these multipoles and their ordering to linear, quadratic, and cubic (anti-) magnetoelectric effects, where in an anti-magnetoelectric effect the induced moments are ordered antiferromagnetically in the unit cell. We confirm the predicted induced moments using first-principles calculations, showing the lowest response in α-Fe_2O_3 a centrosymmetric magnetic material, to be a linear anti-magnetoelectric effect, revealing the presence of the magnetoelectric coupling despite the preserved global inversion symmetry. Our results demonstrate the existence of hidden magnetic multipoles leading to local linear magnetoelectric responses, even in centrosymmetric magnetic materials, and broaden the definition of magnetoelectric materials by including those showing such local magnetoelectric responses.

MA 2.4 Mon 10:15 H16

Non-trivial Spin Structures and Multiferroic Properties of the DMI-Compound $Ba_2CuGe_2O_7$ — •Peter Wild[1], Korbinian Fellner[1], Michał Dembski-Villalta[1], Markus Garst[2], Eric Ressouche[5], Tommy Kotte[3], Bertrand Roessli[4], Alexandra Turrini[4], and Sebastian Mühlbauer[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Karlsruhe Institute of Technology, (KIT), Karlsruhe, Deutschland — [3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [4]Paul Scherrer Institut (PSI), Villigen, Switzerland — [5]Institut Laue-Langevin (ILL), Grenoble, France

Antiferromagnetic $Ba_2CuGe_2O_7$, characterized by a quasi-2D structure with Dzyaloshinskii-Moriya interactions (DMI), is a non-centrosymmetric insulator that exhibits spiral spin structures with potential non-trivial topology and a variety of unconventional magnetic phase transitions. Below the Néel temperature $T_N = 3.05$K, the DMI term leads to a long-range incommensurate, almost AF cycloidal spin spiral in the ground state. Recently, a new phase with a vortex-antivortex magnetic structure has been theoretically described and experimentally confirmed in a pocket in the phase diagram at around 2.4K and an external field along the crystalline c-axis of around 2.2T. A lack of evidence for a thermodynamic phase transition towards the paramagnet in specific heat measurements and a finite linewidth in E and Q of the incommensurate peaks in neutron scattering, as opposed to the cycloidal ground state, seem to mark the vortex phase as a slowly fluctuating structure at the verge of ordering.

MA 2.5 Mon 10:30 H16

A comparison of Γ-point symmetries and phonon selection rules of spin-space and magnetic point group in $Co_2Mo_3O_8$ — •Onur Ercem[1], Felix Schilberth[1,2], Lilian Prodan[1], Vladimir Tsurkan[1], Alexander Tsirlin[3], István Kézsmárki[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary — [3]Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany

$Co_2Mo_3O_8$, which has recently come into the focus of research, as different magnetically ordered ground states can be formed and tuned by external magnetic fields or doping. $Co_2Mo_3O_8$ has a hexagonal structure, the polarization along the c-axis, and a collinear antiferromagnetic order below $T_N = 40$ K. Reflectivity measurements were performed using the FTIR spectrometer, in the frequency range from 100 to 8000 cm^{-1}, and the temperature range from 10 to 300 K could be covered. A preliminary analysis of the infrared-active modes for $E \parallel c$ reveals that 8 out of the 9 predicted A_1 modes are observed at the expected eigenfrequencies and the emergence of the mode at around 300 cm^{-1} below T_N. In $E \perp c$ at room temperature 10 modes were observed. Below T_N two new modes at 301 cm^{-1} and at 362 cm^{-1} observed. Comparison was made with lattice dynamical calculations.

MA 2.6 Mon 10:45 H16

Ferroelectric hafnium oxide-based multiferroic bilayers for magnetoelectric spin-orbit devices — •Maximilian Lederer, Johannes Hertel, Christoph Durner, Tatiana Gurieva, and Benjamin Lilienthal-Uhlig — Fraunhofer IPMS, Center Nanoelectronic Technologies, Dresden, Germany

This study investigates multiferroic heterostructures comprising $Hf_{0.5}Zr_{0.5}O_2$ (HZO) with Co/Pt top and TiN bottom electrodes on Si substrates. Using advanced deposition techniques, sub-nanometric thin films were fabricated. The research highlights achieving both ferroelectricity and perpendicular magnetic anisotropy simultaneously through a two-step annealing process. These properties are crucial for magnetoelectric spin-orbit (MESO) devices, which offer significant advantages such as lower power consumption and enhanced data storage capabilities. Insights into crystallization and diffusion processes were gained through various structural investigation methods. Additionally, the study demonstrates the manipulation of magnetic and ferroelectric domains using different microscopy techniques, underscoring the potential of MESO devices in next-generation electronic applications.

15 min. break

MA 2.7 Mon 11:15 H16

Internal fields at the V-sites and magnetic structure of

the lacunar spinel GeV_4S_8 — •Thomas Gimpel[1], Norbert Büttgen[1], Hiroyuki Nakamura[2], Vladimir Tsurkan[1], and István Kézsmárki[1] — [1]University of Augsburg — [2]Graduate School of Engineering, Kyoto

GeV_4S_8 is a multiferroic lacunar spinel that undergoes both structural (T_{JT}=30 K) and magnetic (T_N=13 K) transitions upon which the four V-sites of the V_4 tetrahedra that are equivalent in the cubic phase transform into three distinct sets of V-sites with zero-field ^{51}V NMR frequencies of 21.7, 53.6 and 65.6 MHz. This indicates that only two V-sites have the same internal magnetic field, while the other two have different ones. Based on the angular dependence of the resonance field upon the rotation of the field, we conclude that the direction of the internal field is common for the four V-sites and is parallel to one of the cubic [110]-type axes, which indicates that the magnetic space group is $Pmn2_1$.

MA 2.8 Mon 11:30 H16

Fast control of antiferromagnetic domains via pulsed electric fields in Co_3O_4 — •Isabel Täuber, Maximilian Winkler, Somnath Ghara, Lilian Prodan, and Istvan Kezsmarki — Universität Augsburg, Deutschland

Co_3O_4 shows the linear magnetoelectric effect below the Neel-temperature of 30K, with a large magnetoelectric coefficient of 14 ps/m. Besides the typical control of the AFM state by colling with electric and magnetic fields across TN, the domains can be switched by voltage pulses as short as a few ns far below the transition temperature. To improve the application ability, we focus on switching of thin films of Co_3O_4 single crystals, paving the way for the next generation of spintronics.

MA 2.9 Mon 11:45 H16

Anomalously strong magnetoelectric coupling in hexaferrite films — •Jakub Vít[1], Kwang-Tak Kim[2], Hyunju Hwang[2], Radomír Kužel[3], Milan Dopita[3], Darina Smržová[4], Kee Hoon Kim[2], and Josef Buršík[4] — [1]Institute of Physics, Czech Academy of Sciences, Czechia — [2]Center for Novel States of Complex Materials Research, Seoul National University, Korea — [3]Faculty of Mathematics and Physics, Charles University, Czechia — [4]Institute of Inorganic Chemistry, Czech Academy of Sciences, Czechia

Bulk hexaferrites are well known to exhibit strong magnetoelectric (ME) effects, often extending up to room temperature. In contrast, ME properties of hexaferrite films have been investigated only in a single recent study: In Z-hexaferrite films, the ME effect was found significantly stronger than in a crystal. [1] We continued this research by studying Y-hexaferrite films $Ba_{2-x}Sr_xCo_2Fe_{11.1}Al_{0.9}O_{22}$ on $SrTiO_3$ (111), grown by chemical solution deposition. For x=1, the magnetic-field-induced polarization reached 6.5 mC/m^2 at 10 K , i.e. 10x more than in the Z-hexaferrite films [1] and 50x more than in Y-hexaferrite crystals. [2] To elucidate these intriguing observations, microstructure of the films was studied in detail by real (SEM, TEM) and reciprocal (XRD) space techniques. Possible influence of the substrate on ME measurements was also taken into account.

[1] K. Shin et al., *Adv. Electron. Mater.* 2101294, (2022) [2] C. B. Park, et al., *Phys. Rev. Mater.* **5**, 034412 (2021)

MA 2.10 Mon 12:00 H16

Higher-order Magnetizations of Non-centrosymmetric Antiferromagnets — •Michael Paulsen[1], Silvia Knappe-Grüneberg[1], Jens Voigt[1], Allard Schnabel[1], Rainer Körber[1], Michael Fechner[2], Ivan Ushakov[3], and Dennis Meier[3] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg, Germany — [3]NTNU Norwegian University of Science and Technology, Trondheim, Norway

Antiferromagnetic materials lack macroscopic magnetic dipole fields, due to their compensated magnetic spin texture. In his seminal work, Dzyaloshinskii predicted that higher-order magnetization contributions arise in non-centrosymmetric antiferromagnets, in particular quadrupolar magnetic field contributions, and first experimental data suggested the presence of such fields in the antiferromagnetic model system Cr_2O_3. Here, we present calculations and measurements gained at cryogenic and room temperature using Superconducting Quantum Interference Devices (SQUIDs) and Optically Pumped Magnetometers (OPMs) setups, respectively, in ultra-low magnetic field environments. The results demonstrate the existence of quadrupolar far-fields and characteristic signatures in different classes of antiferromagnets. Importantly, our SQUID-based approaches are universal and can be applied to a wide range of systems, establishing new methods for characterizing materials with ultra-small magnetic remanence in general.