DS 7: Thermoelectric and Phase Change Materials

Time: Tuesday 10:00–11:30 Location: REC/B214

DS 7.1 Tue 10:00 REC/B214

Voltage-Controlled Magnetism via Electrically Triggered Metal-Insulator Transitions — •Lorenzo Fratino — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université

Phase separation is key to understanding magnetism in correlated systems like manganites. This talk will show how the resistive switching in metal-insulator transition (MIT) materials can be used to create and control artificial phase separation with voltage. In (La,Sr)MnO*, a threshold voltage triggers an electrothermal MIT, creating a paramagnetic insulating barrier inside a ferromagnetic metallic matrix [1]. We can use this to directly tune magnetic properties, achieving effects like voltage-triggered magnetic anisotropy switching [2]. We also developed a CdS/LSMO heterostructure where light injection modulates resistance drop*comparable to a 9 T magnetic field, while surprisingly decoupling the optical and magnetic responses [3]. This work establishes a versatile pathway for voltage-controlled magnetism using MIT materials [4].

References: [1] Nat. Commun. 12, 5499 (2021) [2] Phys. Rev. B 108, 174434 (2023) [3] Phys. Rev. Appl. 19, 044077 (2023) [4] Adv. Funct. Mater. 2419840 (2025)

DS 7.2 Tue 10:15 REC/B214

Thermoelectric power factors of defective scandium nitride nanostructures from first principles — •Luigi Cigarini[1], Urszula D. Wdowik[1], and Dominik Legut[1,2] — [1]IT4Innovations, VŠB Technical University of Ostrava, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

In scandium nitride (ScN), structural defects and chemical impurities strongly affect thermoelectricity (TE), although transport mechanisms remain unclear [1-3]. Reported electronic transport in ScN thin films shows large variability, and strategies to enhance TE efficiency often yield conflicting results [4,5]. Here, using the Landauer approach, we analyze how different types of imperfections affect electronic transport in ScN lattice. Defects are classified according to their symmetry (isolated, multiple contiguous, involving stacking mismatches) and chemical nature (oxygen impurities, nitrogen-site vacancies). Our theoretical results identify two dominant defect classes with opposing effects on TE performance: (i) contiguous nitrogen vacancies, which enhance el. conductivity but reduce the magnitude of the Seebeck coeff. (S), and (ii) oxygen substitutions coupled with nearby stacking mismatches, which increase the magnitude of S while hindering el. conductivity. In this way, we propose a rationale that relates part of the experimental variability to its microscopic origin [6]. [1] Phys. Rev. Mater. 3, 020301 (2019), [2] J. Mater. Chem. C 4, 3905 (2016), [3] Phys. Rev. B 86, 195140 (2012), [4] J. Appl. Phys. 113, 153704 (2013), [5] Appl. Surf. Sci. Adv. 25, 100674 (2025), [6] Preprint: arXiv:2509.14762.

DS 7.3 Tue 10:30 REC/B214

Understanding Charge Transport in ZnO Quantum Dots Through Combined Thermoelectric and High-Field Measurements — •Henrik Holzhauser, Morteza Shokrani, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

ZnO Quantum Dot (QD) solids are an attractive material for a wide range of applications. ZnO QDs also make an excellent model system for QD solid in general owing to the ability to tune the effective diameter of ZnO QD via UV illumination, and the effective electronic localization length via ligands. The charge transport in QD solids is typically explained as thermally activated tunnelling or hopping between the localized states of individual QDs. As such, the electric conductivity is both electric field and temperature dependent. In comparison, the Seebeck effect in QD solids, especially in connection with the electrical conductivity, is not as precisely understood. Here, we combine measurements of the Seebeck coefficient for various ZnO QDs with electric field- and temperature-dependent conductivity measurements, all performed at lattice temperatures ranging from 100 to 300K. We used bare ZnO QDs and ZnO QDs with ligands of various lengths and measured all QD solids at multiple UV-induced effective diameters. The wide range of experiments allows us to obtain a comprehensive understanding of the dominant mechanisms and the characteristic energy and length scales in the system. We find that transport is dominated by energetic disorder resulting from a diameter-dependent charging energy, in combination with an effective localization energy that reflects both wavefunction decay and morphology.

15 min. break

DS 7.4 Tue 11:00 REC/B214

Classification of Metal - Insulator Transitions: Insights from characteristic Property Changes and related Quantum Mechanical Bonding Descriptors — •Tim Bartsch[1], Raagya Arora[4], Carl-Friedrich Schön[1], Umesh Waghmare[3], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [3]Theoretical Sciences Unit, School of Advanced Materials JNCASR Jakkur, Bangalore 560064, India — [4]John A. Paulson School of Engineering and appled science, Havard University, Cambridge Massachusetts

The nature of the transition between metals and insulators is one of the most fascinating topics in condensed matter physics. The end points of this transition are well-defined, i.e. a solid which has a non-vanishing electrical conductivity σ in the limit T * 0 K is a metal, while an insulator is characterized by σ = 0 S/m (T * 0 K). In 1980, Rosenbaum and co-workers investigated the metal-insulator transition in phosphorus-doped silicon, by measuring the low-temperature resistivity of samples with different doping concentrations. Here, we are pursuing a rather different goal. We are looking at a range of different crystalline insulators and check whether they can be classified as pressure-controlled MITs based on characteristic changes in their properties. Such pressure-driven MITs occur in all insulating solids at sufficiently high pressures when the orbital overlap of neighboring atoms increases sufficiently to favor a metallic state.

DS 7.5 Tue 11:15 REC/B214

Effect of Ge doping and thickness on anomalous Nernst effect in Fe4N thin films — •Robin K. Paul[1], Jakub Vít[2], Karel Knížek[2], Petr Levinský[2], Ondřej Kaman[2], Mariia Pashchenko[2], Lenka Kubíčková[2], Kyo-Hoon Ahn[2], Markéta Jarošová[2], Joris More-Chevalier[2], Stanislav Cichoň[2], Tomáš Kmječ[3], Jaroslav Kohout[3], Marcus Hans[4], Stanislav Mráz[4], Jochen M. Schneider[4], Giovanni d'Andrea[1], Lambert Alff[1], Esmaeil Adabifiroozjaei[1], Leopoldo Molina-Luna[1], Oliver Gutfleisch[1], and Imants Dirba[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Institute of Physics of the CAS, Praha, Czech Republic — [3]Charles University, Praha , Czech Republic — [4]RWTH, Aachen, Germany

Anomalous Nernst Effect(ANE)-based devices have recently emerged as a promising alternative to Seebeck based ones, offering simpler geometries. However, their adoption is constrained by lower efficiencies compared to Seebeck-based counterparts. This study focuses on exploring materials with high ANE coefficients. Among the candidates, Fe_4N has attracted attention due to its cost-effectiveness, and tunability through elemental doping. DFT calculations indicate that doping Fe_4N with Ge can enhance its ANE coefficient. In this work, thin films of doped $Fe_{4-x}Ge_xN$ were fabricated onto MgO substrates. The evolution of crystal structure and microstructure are systematically characterized correlating with Nernst effect. ANE is also reported to increase with decrease in film thickness which was investigated by preparing Fe_4N films of thickness from 5nm to 50nm.