TT 21: Electron Theory of Magnetism and Correlations (joint session MA/TT)

Time: Monday 15:00–18:00 Location: POT/0151

TT 21.1 Mon 15:00 POT/0151

Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$ — Varun Venkatasubramanian[1], Makoto Shimizu[2], •Daniel Guterding[3], and Harald O. Jeschke[1] — [1]Research Institute for Interdisciplinary Science, Okayama University, Okayama, Japan — [2]Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan — [3]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany

The nodal-line ferrimagnet $Mn_3Si_2Te_6$ exhibits a pressure-induced insulator-to-metal transition (IMT), which coincides with pronounced anomalies in its magnetic ordering temperature and anomalous Hall conductivity. We employ density functional theory (DFT) in combination with classical Monte Carlo simulations to elucidate the origin of these effects. Pressure-dependent Heisenberg Hamiltonians extracted from DFT reveal a strong evolution of exchange couplings across the structural transition from the trigonal to the monoclinic phase, producing a dome-shaped variation of the ferrimagnetic ordering temperature in quantitative agreement with experiment. While our simulations capture the pressure-driven IMT and magnetic evolution, the anomalous Hall response cannot be fully explained by intrinsic Berry curvature effects, indicating additional extrinsic contributions.

[1] V. Venkatasubramanian, M. Shimizu, D. Guterding, and H. O. Jeschke, *Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$*, arXiv:2509.18238

TT 21.2 Mon 15:15 POT/0151

Near Room-Temperature Ferromagnetism and Insulator-Metal Transition in van der Waals Material $CrGeTe_3$ — Daniel Guterding[1], Jihaan Ebad-Allah[2], Gili Scharf[3], Han-Xiang Xu[4], Makoto Shimizu[5], Junya Otsuki[6], Alon Ron[3], Christine Kuntscher[2], and •Harald O. Jeschke[6] — [1]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany — [2]Augsburg University, Augsburg, Germany — [3]Tel Aviv University, Tel Aviv, Israel — [4]Chinese Academy of Sciences, Beijing, China — [5]Kyoto University, Kyoto, Japan — [6]Research Institute for Interdisciplinary Science, Okayama University, Okayama, Japan

We investigate how pressure tunes the electronic and magnetic properties of the van der Waals ferromagnet $CrGeTe_3$, a promising material for near room-temperature applications. Using DFT+DMFT, we trace the transition from semiconducting to metallic ferromagnet [1]. Optical conductivity reveals a mid-infrared feature, signalling orbital-selective correlations, while a double-exchange mechanism stabilizes high-temperature ferromagnetism [2]. The anomalous Hall effect shows extrinsic behaviour beyond pure Berry curvature effects [3]. These results highlight the interplay of magnetism and electronic correlations in achieving tunable ferromagnetism in $CrGeTe_3$, suggesting that pressure and charge carrier doping offer promising routes to control magnetism and transport in layered materials.

[1] H.-X. Xu *et al.*, Phys. Rev. B **108**, 125142 (2023)
[2] J. Ebad-Allah *et al.*, Phys. Rev. B **111**, L140402 (2025)
[3] G. Scharf *et al.*, Phys. Rev. Res. **7**, 013127 (2025)

TT 21.3 Mon 15:30 POT/0151

Ground State of the Topological Insulator Candidate Eu_2AuGe_3 — •Vinicius Estevo Silva Frehse[1], Aleksandr Sukhanov[1], Artem Korshunov[2], Eugen Weschke[3], Aly Abdeldaim[4], Priscila Rosa[5], and Marein Rahn[1] — [1]Universität Augsburg, Augsburg, Germany — [2]Donostia International Physics Center, San Sebastián, Spain — [3]Helmholz Zentrum Berlin, Berlin, Germany — [4]Diamond Light Source, Didcot, UK — [5]Los Alamos National Laboratory, Los Alamos, USA

Eu_2AuGe_3 is an unusual rare earth germanide in which quasi-trigonal europium sheets are interleaved with Au-Ge honeycomb layers, where high-throughput calculations indicate potential for topological band inversions. Bulk and transport data have revealed a series of (re-)ordering transitions upon cooling, as well as metamagnetic transitions at low temperature. Recently, we identified a broad transition around $T_{CDW} = 130$ K as the continuous freezing-out of a buckling mode of the honeycomb layers.

Here, we present preliminary evidence from neutron and resonant elastic X-ray scattering, which hints at helical magnetic order below $T_N = 11$ K. Unexpectedly for the nominally spin-only divalent europium, the magnetic order also appears to be accompanied by a modulated orbital order parameter. This phase is preceded by a transition at 23 K, where we observe a subtle doubling of the *ab*-plane, possibly related to the charge density wave formed during T_{CDW}.

TT 21.4 Mon 15:45 POT/0151

Electronic structure, magnetic and optical properties of antiferromagnetic 3*d*-oxides from a Wannier-localized optimally-tuned screened range-separated hybrid functional — •Alexander Shick[1,2], Guy Ohad[2], Jeffrey Neaton[3,4], and Leeor Kronik[2] — [1]FZU-Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Weizmann Institute of Science, Rehovoth, Israel — [3]University of California, Berkeley, USA — [4]Lawrence Berkeley National Laboratory, Berkeley, USA

We apply the recently developed Wannier-localized, optimally tuned, screened range-separated hybrid (WOT-SRSH) functional to prototypical bulk antiferromagnetic insulators — MnO, NiO, and hematite (Fe_2O_3). Comparison to calculations based on well-established functionals, namely PBE0, and HSE06, as well as to self-consistent quasiparticle GW and dynamic mean field theory calculations, and to experiment, shows that the WOT-SRSH functional provides a good quantitative description of band gaps, spin magnetic moments, photoemission, and optical absorption spectra. This establishes WOT-SRSH as a uniform, non-empirical framework for band theory of electronic, magnetic, and optical properties of magnetic insulators.

TT 21.5 Mon 16:00 POT/0151

Spectroscopic evidence of Kondo resonance in 3*d* van der Waals ferromagnets — •Deepali Sharma[1,2], Neeraj Bhatt[1], Asif Ali[1], Rajeswari Roy Chowdhury[1], Chandan Patra[1], Ravi Prakash Singh[1], and Ravi Shankar Singh[1] — [1]IISER Bhopal, Bhopal, India — [2]TU Dortmund, Dortmund, Germany

Two-dimensional van der Waals (vdW) ferromagnets drive the advancement in spintronic applications and enable the exploration of exotic magnetism in low-dimensional systems. The entanglement of the dual−localized and itinerant−nature of electrons lies at the heart of the correlated electron systems giving rise to exotic ground state properties such as complex magnetism, heavy fermionic behavior, Kondo lattice formation, etc. Through temperature-dependent electronic structure of vdW ferromagnets, Co substituted Fe_3GeTe_2, probed using high-resolution photoemission spectroscopy and density functional theory combined with dynamical mean field theory (DFT + DMFT), we provide direct evidence of the emergence of Kondo resonance peak driven by complex interplay between localized and itinerant electrons. Further, in overall agreement with the experimental electronic structure and magnetic properties, DFT + DMFT also reveals non-Stoner magnetism. The findings provide a way forward to the understanding of complex interplay between electronic structure, exotic magnetism, and heavy fermionic behavior leading to the Kondo scenario in 3*d* vdW ferromagnets.

TT 21.6 Mon 16:15 POT/0151

T-linear and quadratic transport across the Cuprate and Nickelate phase diagram : pseudogap, strange-metal and Fermi-liquid — •Dongwook Kim[1], Motoharu Kitatani[2], Juraj Krsnik[3], and Karsten Held[4] — [1]Wiedner Hauptstraße 8-10, 1040 Wien — [2]3-2-1 Koto, Kamigori-cho, Ako-gun, Hyogo 678-1297, Japan — [3]Trg Republike Hrvatske 14. HR-10000 Zagreb Croatia — [4]Wiedner Hauptstraße 8-10, 1040 Wien

We investigate DC resistivity and nodal quasiparticle (QP) scattering in hole-doped cuprates-nickelate type superconductors by ladder dynamical vertex approximation (LDΓA). In the pseudogap regime of doping $\delta = 0.1$-0.175, we observe a crossover from T-linear to T^2 resistivity at low T. For dopings $\delta = 0.2$-0.25, the resistivity remains fully T-linear down to the lowest temperatures, indicating strange-metal behavior associated with a nearby quantum critical point (QCP). At higher doping of $\delta = 0.3$ the T^2 recovery reappears, signaling exit from the quantum-critical regime. The nodal QP scattering rate and the first-Matsubara-frequency rule analysis independently confirm the same FL*NFL crossover, providing consistent support for the T-dependent transport obtained within LDΓA

15 min break

TT 21.7 Mon 16:45 POT/0151

Toward ab-initio simulation for resonant inelastic X-ray scattering in strongly correlated materials — •Yun Yen[1,2], Matthias Krack[2], and Michael Schüler[2,3] — [1]Institute for Theoretical Physics, Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]PSI Center for Scientific Computing, Theory and Data, Villigen PSI, Switzerland — [3]Department of Physics, University of Fribourg, Fribourg, Switzerland

X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) can be used to study low-energy excitations in complex materials, which are challenging to interpret due to strong correlations during the photoexcitation processes. We aim to develop ab-initio methods for XAS and RIXS, by constructing Anderson impurity models using Wannier-based tight-binding parameters and constrained random phase approximation. The spectrums are then computed via exact diagonalization and Krylov subspace methods. We will show a benchmark on spin spiral materials, where the d-d excitation intensity dependence can be related to the onset of magnetic order with the support of our methods.

TT 21.8 Mon 17:00 POT/0151

Magnetic Persistence in PrAlGe via RIXS and XAS modeling — •Juan Felipe Pulgarin Mosquera[1,2], Yun Yen[3], Tianlun Yu[4], Yeong-Ah Soh[4], Thorsten Schmitt[4], and Michael Schueler[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, Villigen PSI, Switzerland — [2]University of Fribourg, Department of Physics, University of Fribourg, Fribourg , Switzerland — [3]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [4]PSI Center for Photon Sciences, Villigen-PSI, Switzerland

The interplay between topological electronic states and magnetism is in the spotlight of condensed matter for potential applications. PrAlGe is a prime candidate in this context, with several works reporting it as a magnetic Weyl semimetal. However, the microscopic relationship between the magnetic ordering, anomalous Hall effect and local spectroscopic signatures remains an open question. We study this phenomenon based on a combination of X-ray spectroscopy and first-principle calculations. We present our ab-initio approach to computing X-ray absorption spectroscopy and resonant inelastic X-ray scattering based on accurate Anderson Impurity model derived from density-functional theory with Hubbard corrections. This comparison is crucial for understanding the experimental finding that the ferromagnetic transition occurs at $T_c \sim 16$ K, significantly lower than the temperature scale at which the AHE and circular dichroism vanish $T_{AHE} \sim 35$ K). The survival of circular dichroism above T_c serves as a local probe for the persistence of local magnetic moments.

TT 21.9 Mon 17:15 POT/0151

Ab initio spin Hamiltonians and magnetism of Ce and Yb triangular-lattice compounds — Leonid V. Pourovskii[1,2], •Rafael D. Soares[3], and Alexander Wietek[3] — [1]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [2]Collège de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

We calculate the crystal-field splitting, ground-state Kramers doublet and intersite exchange interactions within the ground-state doublet manifold for a representative set of Ce and Yb triangular-lattice compounds. These include the putative quantum spin liquids (QSL) $RbCeO_2$ and $YbZn_2GaO_5$ and the antiferromagnets $KCeO_2$ and $KCeS_2$. The calculated nearest-neighbor (NN) couplings are antiferromagnetic and exhibit noticeable anisotropy. The next-nearest-neighbor (NNN) couplings are ferromagnetic in the Ce systems and dominated by classical dipole–dipole interactions in the Yb case. Solving the resulting effective spin-1/2 models by exact diagonalization up to $N = 36$ sites, we predict ordered magnetic ground states for all systems, including the two QSL candidates. We explore the phase space of an anisotropic NN + isotropic NNN triangular-lattice model finding that a significant antiferromagnetic NNN coupling is required to stabilize QSL phases, while the NN exchange anisotropy is detrimental to them. Our findings highlight a possibly important role of deviations from the perfect triangular model in real materials.

TT 21.10 Mon 17:30 POT/0151

Transition metal dihalides: from band structure to magnetic properties — •Alexander Yaresko[1], Sebastien Hadjadj[2], and Maxim Ilyn[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Centro de Física de Materiales, Donostia-San Sebastián, Spain

Transition metal dihalides TX_2 (T=Fe, Ni, X=Cl, Br) have recently attracted attention because of successful growth of monolayer-thick TX_2 films on various substrates, such as Au or $NbSe_2$, allowing to study 2D magnetism. We compare results of band structure calculations for bulk and monolayer FeX_2 and NiX_2. By mapping the total energies calculated for helical spin structures with various q to the Heisenberg model we show that the change of magnetic order within a layer from ferro- in $NiCl_2$ to helimagnetic in $NiBr_2$ can be explained by the increased strength of antiferromagnetic (AF) 3-rd neighbor exchange interaction J_3 which competes with FM nearest neighbor J_1. We found that inter-layer coupling J_{2c} stabilizes FM order within a layer. Thus, one can expect stronger tendency to a helimagnetic state in a NiX_2 monolayer.

In contrast to NiX_2, J_1 estimated from LDA+U spin-spiral calculations for FeX_2 is weak but shows substantial dependence on the strength of the Coulomb repulsion U. In agreement with experimental findings, calculations including spin-orbit coupling result in appreciable easy axis anisotropy with Fe magnetic moments normal to layers.

We also discuss various microscopic contributions to intra- and inter-layer exchange interactions.

TT 21.11 Mon 17:45 POT/0151

Coexistence of charge order and antiferromagnetism in three-dimensional Hubbard-Holstein model: A study (exploring phases) at and away from half-filling — •Sandip Halder and Moshe Schechter — Ben-Gurion University of the Negev, Beer-Sheva, Israel

The physics of correlated electron systems has long been explored through the Hubbard model and its extensions, including models with long-range hopping. Likewise, phenomena arising from electron-phonon coupling- such as charge order and superconductivity- have been extensively studied within the Holstein model, though largely in lower dimensions. In transition-metal oxides, however, both electron correlations (U) and electron-phonon coupling (V) coexist intrinsically, motivating a comprehensive study of the Hubbard-Holstein model in three dimensions.

Using an exact diagonalization-based semi-classical Monte Carlo (s-MC) method, we investigate the intriguing properties of this model. At half-filling, the system undergoes a first-order transition between a charge-ordered (CO) phase and an antiferromagnetic (AF) phase as U and V are varied. In the AF regime, near the phase boundary, hole doping drives the system from the AF state (n=1) to a CO state (n=0.5), and eventually to a disordered phase at low densities. Notably, a robust coexistence of AF and CO emerges around x=0.35 (n=0.65), with T_{CO} exceeding T_N, consistent with experiments on $La_{2-x}Sr_xNiO_4$. The study provides new insight into correlated materials and guiding future experimental explorations.