MA 4: Electron Theory of Magnetism and Correlations

Time: Monday 9:30–11:45 Location: H19

MA 4.1 Mon 9:30 H19

Tunable Half-Metallicity and Ferromagnetism in Gated single layer g-C3N4 via Nitrogen Lone Pair Depletion. — •Pietro Nicolò Brangi, Francesca Martini, Pier Luigi Cudazzo, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Graphitic carbon nitride (g-C3N4) is a promising catalyst for water splitting and hydrogen production, with nitrogen lone pairs arising from broken carbon-nitrogen bonds in its heptazine structure. These strongly localized and weakly hybridized lone pairs form ultraflat bands potentially leading to correlated states when doped.

Using first-principles calculations, we show that field-effect hole-doping in single-layer g-C3N4 depletes these lone pairs, generating ultraflat bands at the Fermi level and unveiling a rich phase diagram. At low hole concentrations, a half-metallic state emerges with tunable magnetization, increasing linearly with carrier density and reaching up to 1 Bohr magneton /3 f.u.. At an integer filling of one hole per cell, a band-insulating ferromagnetic state is stabilized, followed by an interplay of metallic and half-magnetic phases with further doping, ultimately leading to a second ferromagnetic insulating state.

Our work highlights nitrogen-based lone-pair systems as a novel platform for strongly correlated states, with implications for magnetism even at small electric fields, hinting at unexplored potential in photocatalysis.

MA 4.2 Mon 9:45 H19

Investigation of crystalline environment for Fe oxides using XAS and XPS:A DFT+MLFT approach — •Hamza Zerdoumi, Ruiwen Xie, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt,Germany

Fe oxides are versatile materials with applications spanning catalysis, memory storage, and photoelectrochemical decomposition of seawater for clean hydrogen production. Taking Fe_2O_3 as an example, there exist five distinct phases, i.e., α-Fe_2O_3, β-Fe_2O_3, γ-Fe_2O_3, ϵ-Fe_2O_3, and ζ-Fe_2O_3, each exhibiting unique properties. Therefore, it is intriguing to clarify how the local crystalline environment can shape the electronic structure and hence tailor the corresponding functionalities. In this study, we simulate X-ray photoelectron spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) spectra using a combination of density functional theory (DFT) and multiplet ligand field theory (MLFT). By analyzing individual spectral bands corresponding to iron sites in various crystal structures, we examine the correlation between local symmetry and the simulated spectra. Our work highlights how variations in local environments influence the spectroscopic features of iron oxide polymorphs, offering valuable insights into their diverse properties.

MA 4.3 Mon 10:00 H19

Domain wall engineering in distorted Kagome magnet — •Avdhesh Kumar Sharma[1], Premakumar Yanda[1], Samuel Harrison Moody[2], Chandra Shekhar[1], and Claudia Felser[1] — [1]Max Planck Institute for chemical physics of solids, 01187 Dresden, Germany — [2]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

In condensed matter, Kagome material can host interplay of nontrivial topology, correlations, and magnetism due to their unique lattice and band structure. Recently, RTX series with ZrNiAl structure have gained attention due to possessing kagome lattice continuously breaking translation symmetry i.e., distorted kagome lattice. Intriguingly, HoAgGe has been predicted to have a kagome spin ice state and break the the reversal like symmetry and show two degenerate states in anomalous Hall effect. Along this line, we have synthesized single crystals of TbAgGe to investigate the magnetic and electrical transport properties in detail. It crystallizes in a hexagonal crystal structure with space group P-62m. It exhibits long-range AFM ordering of Tb3+ ions at Néel temperatures 29K, 25K and 20K. Further, it shows metamagnetic transitions when H || c, which might result in a non-coplanar spin structure in the system and goes to ferromagnetic (FM) state at high fields. Moreover, it shows significant anomalous Hall effect near the metamagnetic transitions, which is attributed to originating from the magnetic domain walls. Our findings suggest that RTX family with distorted kagome lattice can be an excellent platform to study the interplay of domain wall magnetism and topology.

MA 4.4 Mon 10:15 H19

Magnetic-circular dichroism on low-lying excitations in antiferromagnetic Fe2Mo3O8 — •Kirill Vasin[1], Istvan Kézsmárki[1], Sándor Bordács[2], and Joachim Deisenhofer[1] — [1]University of Augsburg, Augsburg, Germany — [2]Budapest University of Technology and Economics, Budapest, Hungary

We report the observation of a strong magnetic circular dichroism (MCD) and Faraday effect in the polar honeycomb antiferromagnet $Fe_2Mo_3O_8$ in the terahertz (THz) range. Using a common linear detection scheme with polarizers on both the emitter and detector set to the same angle, we observe seemingly thickness-dependent features and broadening in the transmission spectrum near narrow resonances in the Faraday configuration. These features are absent in the Voigt geometry with the same static magnetic field configuration, confirming that they arise from Faraday rotation (or MCD). By analyzing the zero-field spectrum and fitting Lorentz oscillators in the time-domain, we resolved oscillators parameters of the observed strong and narrow THz excitations with high accuracy. Using these parameters, we successfully reconstructed our field- and thickness-dependent transmission spectra, highlighting the role of Faraday rotation in the observed phenomena.

Our findings demonstrate the importance of considering detection schemes in Time-Domain THz spectroscopy and provide insights into methods of measuring MCD and Faraday rotation without ellipsometry techniques in «single-shot» transmission measurements for aniferromagnets.

MA 4.5 Mon 10:30 H19

Pressure-induced effects on the electronic band topology, magnetic order, and transport properties in FeSn — •Artem Chmeruk[1], Lilian Prodan[2], and Liviu Chioncel[3] — [1]University of Augbusrg — [2]University of Augbusrg — [3]University of Augbusrg

The family of kagome metals offers a fruitful platform for investigating the interplay between electronic band structure topology and various properties such as magnetism, electrical and optical response, etc. A rather promising topic of research is to control the positions of various topological features such as band (anti-) crossings of different dimensions (nodal points, lines, etc.) by some external parameters. For example, applying an external magnetic field could lead to band reconsctruction and therefore move the band crossings to different locations in the BZ. In a similar fashion, external pressure provides an opportunity to control these topological features both in terms of their location in the momentum space and on the energy scale. The possibility of moving such crossings closer to the Fermi level would immediately have an effect on the various observable quantities such as anomalous Hall conductivity. In this work, we study the effect of pressure on the magnetic order and the electronic band structure in FeSn up to 10 GPa. Furthermore, we investigate changes in the Berry curvature and its influence on the transport properties.

MA 4.6 Mon 10:45 H19

Emergent Majorana Metal from a Chiral Spin Liquid — •Shi Feng[1,2], Penghao Zhu[2], Kang Wang[3], Tao Xiang[3], and Nandini Trivedi[2] — [1]Technical University of Munich, Garching, Germany — [2]The Ohio State University, Columbus, USA — [3]Institute of Physics, Chinese Academy of Sciences, China

We propose a novel mechanism to explain the emergence of an intermediate gapless spin liquid phase (IGP) in the antiferromagnetic Kitaev model in an externally applied magnetic field, sandwiched between the well-known gapped chiral spin liquid (CSL) and the gapped partially polarized (PP) phase. We propose in moderate fields π-fluxes nucleate in the ground state and trap Majorana zero modes. As these fluxes proliferate with increasing field, the Majorana zero modes overlap creating an emergent Z_2 Majorana metallic state with a 'Fermi surface' at zero energy. We further show that the Majorana spectral function captures the dynamical spin and dimer correlations obtained by the infinite Projected Entangled Pair States (iPEPS) method thereby validating our variational approach. The emergence of the IGP as a Majorana metal at zero temperature indicates a new class of gapless QSLs alongside the commonly recognized Dirac spin liquids and $U(1)$

spinon Fermi surfaces in prevailing theories, bringing new insights into the nature of various candidate QSL phases of matter stabilized by moderate magnetic fields.

MA 4.7 Mon 11:00 H19

Tuning the order of a deconfined quantum critical point
— Anika Goetz[2], •Natanael C. Costa[1], and Fakher Assaad[2] — [1]Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil — [2]Institut für Theoretische Physik und Astrophysik, Universitat Würzburg, Würzburg, Germany

We consider a Su-Schrieffer-Heeger model in the assisted hopping limit where direct electron hopping is subdominant. At fixed electron-phonon coupling and in the absence of Coulomb interactions the model shows a deconfined quantum critical point between a $(0, \pi)$ valence bond solid in the adiabatic limit and a quantum antiferromagnetic (AFM) at high phonon frequencies. Here we show that by adding terms to the model that reinforce the AFM phase, thereby lowering the critical phonon frequency, the quantum phase transition becomes strongly first order. Our results does not depend on the symmetry of the model. In fact by adding a Hubbard-U term to the model lowers the $O(4)$ symmetry to SU(2), such that the DQCP we observe has the same UV symmetries as other models that account for the same quantum phase transitions.

MA 4.8 Mon 11:15 H19

The Laughlin vortex crystal in ideal Chern bands — •Saranyo Moitra and Inti Sodemann — Leipzig University, Leipzig, Germany

We have uncovered a novel phase transition of the celebrated Laughlin Fractional quantum Hall wave-function from its topologically ordered fluid phase onto a power-law-correlated vortex crystal in flat Chern bands with ideal quantum geometry. We will present a theory of ground state correlations and collective modes of these states across this transition and discuss their potential relevance to anomalous fractional quantum Hall phenomena in platforms such as moiré MoTe2, twisted bilayer graphene and pentalayer graphene.

MA 4.9 Mon 11:30 H19

Forestalled Phase Separation as the Precursor to Stripe Order — •Aritra Sinha and Alexander Wietek — Max Planck Institute for the Physics of Complex Systems, Nothnitzer Strasse 38, Dresden 01187, Germany

Stripe order is a prominent feature in the phase diagram of the high-temperature cuprate superconductors and has been confirmed as the ground state of the two-dimensional Fermi Hubbard model in certain parameter regimes. Upon increasing the temperature, stripes and the superconducting state give way to the enigmatic strange metal and pseudogap regime, whose precise nature poses long-standing, unresolved puzzles. Using modern tensor network techniques, we discover a crucial aspect of these regimes. Infinite projected entangled pair state (iPEPS) simulations in the fully two-dimensional limit reveal a maximum in the charge susceptibility at temperatures above the stripe phase. This maximum is located around hole-doping p=1/8 and intensifies upon cooling. Using minimally entangled typical thermal states (METTS) simulations on finite cylinders, we attribute the enhanced charge susceptibility to the formation of charge clusters, reminiscent of phase separation where the system is partitioned into hole-rich and hole-depleted regions. In contrast to genuine phase separation, the charge cluster sizes fluctuate statistically without a divergent charge susceptibility. Hence, while this precursor state features clustering of charge carriers, true phase separation is ultimately forestalled at lower temperatures by the onset of stripe order.