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ABSTRACT BOOKLET

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INVITED & FLASH TALKS

Talk 1

Theory of infinite-layer nickelate superconductors

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The discovery of superconductivity in infinite-layer nickelates [1] marked a new age of superconductivity: the nickel age. Using density functional theory, dynamical mean-field theory and dynamical vertex approximation (DΓA [2]), we successfully predicted the phase diagram T_c vs. Sr-doping of $Nd_{1-x}Sr_xNiO_2$ with - for an unconventional superconductor-unprecedented accuracy with defect-free films synthesized only 3 years later [4]. Also the normal state spin spectrum well agrees with resonant inelastic x-ray spectroscopy (RIXS) [5] and the one-particle spectrum with angular-resolved photoemission spectroscopy (ARPES) [6], including waterfalls [7].

With this excellent agreement to later experiments, we can now with some confidence predict the phase diagram of finite-layer nickelates [8] and that infinite-layer nickelates have a much higher T_c under 100GPa of pressure even without any chemical doping [9].

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Talk 2

Modelling quantum behaviour using many-body methods in (apparently) non-quantum materials

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The word "Quantum materials" brings automatically to mind exotic materials and phases like unconventional superconductors, Majorana Fermions, skyrmions, topological materials, entanglement etc, and a whole host of open questions come forward. However, the so-called "non-quantum" materials can also give rise to very interesting "quantum" behaviour due to electron correlation in the open *d* shell. In this talk, we examine "quantum" behaviour in (apparently) non-quantum materials in terms of the interplay of strong correlations with magnetism, doping, and strain in transition metal oxides using quantum many body methods.

Transition metal oxides come in many forms and structures but mostly have open *d* shells. We consider the perovskite geometry and compare their properties with layered geometry. First, we consider a typical perovskite oxide material with Jahn-Teller (JT) distortions. $LaMnO_3$ is one such perovskite oxide with strong JT distortions giving rise to an antiferromagnetic insulating ground state. Inspired by the puzzling experimental findings of an exotic ferromagnetic insulating state when $LaMnO_3$ forms heterostructures with $SrTiO_3$, which is generally believed to give rise to a conducting 2D electron gas, we explore the electronic and magnetic state of $LaMnO_3/SrTiO_3$ superlattices. Using *ab initio* DMFT calculations, we find that a ferromagnetic insulating state emerges due to intrinsic effects of strong correlations in the system, in agreement with experimental studies. We also predict that, due to electronic correlations, the emerging 2D electron gas is located at the $LaMnO_3$ side of the interface. This is in sharp contrast to DFT results that locate the electron gas on the $SrTiO_3$ side [1]. Importantly, we also clarify that the epitaxial strain is a key ingredient for the emergence of the exotic ferromagnetic insulating state. This becomes clear from calculations on both biaxial and uniaxially strained $LaMnO_3$ systems, also showing ferromagnetism which is not seen in the unstrained bulk material [2].

Next, we consider a similar isoelectronic JT distorted but layered material $LiMnO_2$ and explore the impact of Li doping (or lithiation/delithiation). We observe that an antiferromagnetic insulating state stabilising a high Néel temperature is the ground state in $LiMnO_2$ similar to bulk $LaMnO_3$ as expected. We developed a fast sign-problem free method to carry out multiple-impurity DMFT calculations to study the effect of delithiation. However, on delithiation we find various exotic quantum states emerge such as ferrimagnetic correlated metals, charge-disproportionated ferromagnetic correlated metals with large

quasiparticle weights, ferromagnetic metals with small quasiparticle weight, as function of x, all in high spin states. For x=0.67-0.33, a mix of +3/+4 oxidation states of Mn is observed. We explore the temperature vs. de-lithiation phase diagram and conclude that delithiation or doping is a key ingredient for emergence of exotic correlated phase transitions [3].

In the layered material changing the transition metal Mn to Ni and considering $LiNiO_2$ which although in its formal oxidation state of +3 should be JT distorted shows suppression of JT distortion as well as a very low Néel temperature, raising questions regarding the origin of its insulating behaviour. *Ab initio* DMFT calculations on rhombohedral non-JT distorted $LiNiO_2$ show a gap of combined Mott and charge-transfer character as well as show the presence of a ligand hole $3d^8L^1$ state, due to negative charge transfer, with excellent match of Ni K edge, O K edge XAS as well as O ResPES experiments. This also explains the suppression of the JT distortion due to the ligand hole on the O and the $3d^8L^1$. The paramagnetic insulating state has a band gap of ~0.6 eV, in excellent agreement with experiments and is in sharp contrast to DFT calculations at various levels which show a metallic ground state. We further show that whereas DFT shows the presence of an unphysical metallic Drude peak in optical absorption spectra, DMFT calculations capture the correct form of the optical absorption spectra and have an excellent match with the calculated band gap as well [4,5,6]. Increasing the amount of Li now in $LiNiO_2$ with an extra Li in the Ni layer resulting in the composition of Li_2NiO_3 which also has no JT distortion lead to the increase in the amount of Ni-O covalency and the ligand holes on the Ni 3d state to rise to $3d^8L^2$ [6,7]. Hence, we demonstrate a range of quantum effects as the impact of doping, and strain on magnetism and the electronic structure of these “non-quantum” materials and their interplay with strong electronic correlations which are captured by quantum many body theory.

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Talk 3

Giant Negative Thermal Expansions Induced by Electronic Phase Transitions

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Negative thermal expansion (NTE) materials which shrink on heating attract the keen attention because these can compensate for the thermal expansion of structural materials by making composites and solve the critical problems caused by the thermal expansion. We utilize $6s^2$ lone pair activity of Pb^{2+} and Bi^{3+} and valence skipping nature of these ions for exploration of NTE materials [1]. $PbVO_3$ is a $PbTiO_3$-type compound with an enhanced polar tetragonal structure (c/a = 1.23) owing to d_{xy} orbital ordering of V^{4+} (d^1). Hole doping by Bi^{3+} substitution for Pb^{2+} decreases the polar distortion and enables temperature induced polar-nonpolar transition accompanied by ~ 9 % volume shrinkage [2,3]. Similarly, ferroelectric transition temperature of $BiFeO_3$ can be reduced by A- and B-site substitutions and NTE has been achieved [4]. $BiNiO_3$ is a perovskite compound stabilized by high-pressure (HP) synthesis at 6 GPa. It has a characteristic valence distribution of $Bi^{3+}_{0.5}Bi^{5+}_{0.5}Ni^{2+}O_3$ and undergoes a pressure induced intermetallic charge transfer transition resulting in $Bi^{3+}Ni^{3+}O_3$ HP phase above 4 GPa. This transfer causes Ni's valence to change from Ni^{2+} to Ni^{3+}, leading to the Ni–O bond contracting and unit cell volume decreasing by 2.5% [5]. In the case of d $BiNi_{1-x}Fe_xO_3$, the charge transfer transition between Bi^{5+} and Ni^{2+} can be induced by heating at ambient pressure (AP), leading to an NTE [6,7]. Similarly, $PbCrO_3$ exists in a $Pb^{2+}_{0.5}Pb^{4+}_{0.5}Cr^{3+}O_3$ valence distribution at AP and exhibits a 9.8% pressure-induced volume collapse [8]. We investigated the phase relation of $PbCrO_3$ in the pressure-temperature space and found that, contrary to $BiNiO_3$, $PbCrO_3$ returns to the ambient pressure phase when the temperature is increased under pressure. The slope of the phase boundary in the P-T phase diagram of $BiNiO_3$ is negative because the metallic $Bi^{3+}Ni^{3+}O_3$ HP-LT phase has higher entropy than $Bi^{3+}_{0.5}Bi^{5+}_{0.5}Ni^{2+}O_3$. On the other hand, the glassy distribution of Pb^{2+} and Pb^{4+} enhances the entropy of the $Pb^{2+}_{0.5}Pb^{4+}_{0.5}Cr^{3+}O_3$ phase and the phase boundary has a positive slope [9]. Large thermal expansion rather than NTE is expected in $PbCrO_3$ if the high-pressure phase is stabilized by chemical substitutions and indeed, $Pb_{0.7}Ca_{0.3}CrO_3$ exhibits approximately 12% unit cell volume expansion on heating between 300 – 400 K [9].

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Talk 4

Thermal expansion in Cross-Coupled order parameter oxides

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The enigmatic phenomenon of colossal volumetric and uniaxial negative thermal expansion (NTE) in Ca_2RuO_4 has long challenged understanding due to its intertwined electronic, structural, and magnetic degrees of freedom. Through ab initio molecular dynamics (AIMD), normal-mode decomposition techniques, and anharmonic Grüneisen analysis, we reveal the microscopic origin of its anisotropic expansion. The uniaxial NTE near the metal-to-insulator transition (MIT) arises from phonons with negative Grüneisen parameters coupled to pronounced elastic anisotropy. Octahedral tilts are central yet non-rigid, involving intrinsic shape changes rather than rigid unit modes [npj Comput. Mater. **11**, 356 (2025), Chem. Mater. **33**, 7665-7674 (2021)]. AIMD captures the thermal evolution of RuO6 rotations, tilts, and antipolar Ca displacements, which modify local tetragonal distortions of the RuO6 octahedra and drive the MIT. Our findings provide microscopic insight into negative thermal expansion (NTE) in Ca_2RuO_4 and highlight strategies to engineer phase transitions and thermal responses in A_2BO_4 oxides through tailored cross-coupling between order parameters.

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Talk 5

Quantum oscillations in the magnetization and density of states of non-interacting and interacting insulators

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The Fermi surface, the defining characteristic of metals, leads to oscillatory behavior of various observables as a function of the inverse magnetic field. It was thus a great surprise when such oscillations were seen in insulators without any Fermi surface, like in Kondo insulators. I will first briefly discuss a general theory [1] of quantum oscillations (QOs) in non-interacting hybridization-gap insulator and show that it exhibits distinct frequencies for Shubnikov de Hass (SdH) and deHass-van Alphen (dHvA) oscillations for low-energy density of states and magnetization oscillations, respectively, unlike in a metal. Kondo insulators are, however, strongly correlated systems where the interaction effects cannot be a priori ignored. We generalize the periodic Anderson model to a solvable Sachdev-Ye-Kitaev (SYK)-like interactions for the f-electrons and study the effects of interactions on QOs in Kondo insulators. We find that while the QO frequencies remain almost unaffected by interactions, there are striking differences between SdH and dHvA oscillations, with the SdH amplitude strongly enhanced due to the renormalization of the effective gap. We also present an asymptotic low-temperature analysis to complement and analytically understand our numerical results.

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Talk 6

Magnetic octupolar versus electric quadrupolar ground states of Osmium oxides

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Spin-orbit coupling in localized electrons can lead to the formation of electric or magnetic multipoles and associated exotic phenomena. We have studied the cubic double perovskite Ba_2CaOsO_6 with Os^{6+} ($5d^2$) ions that exhibits a phase transition to a "hidden ordered" state using various spectroscopic techniques, that is, x-ray absorption spectroscopy (XAS), resonant inelastic x-ray scattering (RIXS), Raman scattering, and x-ray magnetic circular dichroism (XMCD) [1,2]. The lowest $J_{eff} = 2$ state of the d^2 multiplet showed a residual cubic splitting into a non-Kramers E_g doublet ground state and T_{2g} triplet excited state. The absence of any structural distortion from the cubic symmetry suggests that the Eg ground state is a magnetic octupolar state. Multiplet calculation under fictitious magnetic fields has revealed that exchange interaction between nearest-neighbor octupoles is strong enough to stabilize the ferro-octapolar order. This work has been done in collaboration with J. Okamoto, G. Shibata, Yu. S. Ponosov, A. Tanaka, H. Hayashi, K. Yamaura, H. Y. Huang, A. Singh, C. T. Chen, N. Kawamura, S. V. Streltsov, and D. J. Huang.

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Talk 7

Advances in electron and optical spectroscopy from density functional theory

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Talk 8

Phonons with Angular Momentum Generated by Magnetism

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Phonons carrying angular momentum have recently attracted interest as they could enable novel ways to act on the spin magnetic moment in spintronic devices [1]. It remains however a question how chiral phonons can be generated and utilized. Here we employ theoretical methods and ab-initio-based calculations to investigate how chiral phonons can emerge in magnetic materials. Starting from a general spin-lattice Hamiltonian we derive a magnon-phonon Hamiltonian up to second order in magnon and phonon operators and use ab-initio calculations to compute the coupling terms, choosing bcc Fe as a typical example. Diagonalization of the Hamiltonian gives the hybrid magnon-phonon quasiparticles (magnon-polarons) in the Brillouin zone. Our calculations show the emergence of chiral phonons from selective magnon-phonon coupling in inversion-symmetric magnetic systems, particularly along high-symmetry directions. Our calculations reveal finite zero-point phonon angular momentum and strong anomalous thermal Hall responses linked to finite (spin) Berry curvatures. Our results suggest the existence of chiral phonons to occur in many magnetic materials [2].

A second question which we address is the possible excitation of phonons with angular momentum due to femtosecond laser-induced demagnetization, as has been suggested by recent ultrafast electron diffraction measurements [3] to be an intermediate state to the Einstein-de Haas effect [4]. To investigate this proposed mechanism, we study the coupled electron-nuclear dynamics during ultrafast demagnetization of $L1_0$ FePt, using Ehrenfest nuclear dynamics simulations combined with time-dependent density functional theory (TDDFT). Our calculations demonstrate that upon femtosecond demagnetization atomic rotations of the Fe and Pt atoms appear, i.e., the generation of phonons carrying finite angular momentum [5]. We analyze the origin of these atomic rotations and show that both ultrafast demagnetization and generation of phonons with angular momentum arise from symmetry constraints imposed by spin-orbit coupling, thus providing insight in spin-phonon interaction at ultrafast timescales.

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Talk 9

Quantifying altermagnetism and its connection with topology

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Altermagnetism has emerged as an interesting form of antiferromagnetism, where the opposite spin bands from different sublattices do not overlap. Although interesting from many aspects, a measure of an altermag net's strength is yet to be defined. Here, we mathematically construct a possible measure of altermagnetism and demonstrate its usefulness on a few model systems and real materials. Further, taking an example of altermagnetic Weyl semimetal CrSb, we demonstrate how the symmetries responsible for altermagnetism allow triple-point crossings and Dirac crossings. Based on a model Hamiltonian inspired by our DFT results, we try to understand the requirements for realizing such exotic topological phases in altermagnetic CrSb.

Talk 10

Reentrant metal -insulator and magnetic transitions in some novel oxide materials

Prabuddha Sanyal

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A formalism is proposed for obtaining an effective spin model from a spin-Fermion model for Double Perovskite and Double Double Perovskite materials. The effective spin-only model can be simulated using Monte Carlo method to obtain a magnetic phase diagram for these materials. This effective spin model was validated for Double Perovskites by comparing with an Exact Diagonalization Monte Carlo (ED-MC) study of the original spin-Fermion model, which in this case is a 2-sublattice Kondo lattice model for double exchange. A novel Antiferromagnetic Metal phase was predicted, which was later confirmed for a new real material, La-overdoped Sr2FeMoO6, using *ab initio* methods as well as experimentally. This model for double exchange was later extended to another double perovskite, Sr_2CrOsO_6, by adding a superexchange term, and its high ferromagnetic T_c of 700K, despite being an insulator, was explained. By doping Sr_2CrOsO_6 with La and Na, we obtain a novel half-metal with a high T_c, which may be important for spintronics. A Reentrant Metal-Insulator Transition was obtained as a function of doping. I also proposed a new model for La_2NiMnO_6 (LNMO), and explained the Reentrant Spin-Glass Transition in disordered LNMO using ED-MC simulations. A new model Hamiltonian (3+1 sublattice Kondo lattice model) is proposed for Double Double Perovskites $CaMnNiReO_6$ and $CaMnCoReO_6$, and an effective spin model is derived using the abovementioned formalism. Their exotic ferromagnetic and ferrimagnetic order over multiple magnetic sublattices was explained using Monte Carlo simulation of this effective spin model.

Talk 11

Ligand-Driven Emergent Magnetism in Quasi-2D Chromium Chalcogenides

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Low-dimensional magnets provide an ideal platform for tuning exchange interactions and realizing emergent magnetic phases. In this talk, I will present our results on two iso-structural chromium chalcogenides, $SbCrS_3$ and $SbCrSe_3$, based on DFT+U calculations combined with spin dynamics simulations. Both compounds crystallize in the orthorhombic Pnma structure where Cr^{3+} ions (d^3, S = 3/2) form quasi-two-dimensional layers of edge-sharing CrX_6 octahedra that create double chains along the b direction. Despite their structural similarity, the two systems exhibit distinct magnetic ground states: $SbCrS_3$ stabilizes an antiferromagnetic order with competing exchanges, while $SbCrSe_3$ is a ferromagnetic insulator with dominant ferromagnetic couplings. Orbital-resolved analysis reveals that ligand substitution from S to Se modifies the superexchange pathways and reverses the effective magnetic interactions. The weak interlayer coupling makes these materials effectively quasi-two-dimensional magnets. Furthermore, we show that uniaxial strain can tune the electronic structure and magnetic interactions, enabling strain-driven magnetic and metal-insulator transitions. These results demonstrate that ligand substitution and strain provide effective routes to engineer magnetism in quasi-two-dimensional chromium chalcogenides.

* This work is carried out in collaboration with Sk. Soyeb Ali (currently a PhD student).

Talk 12

Spin Filtering with Insulating Altermagnets

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Altermagnetic (AM) materials, characterized by nonrelativistic momentum-dependent spin splitting in their electronic band structures, present new opportunities for the next generation of ultrafast AFM spintronics. So far, however, most research studies have focused on AM metals that can be utilized in spintronic devices such as AFM tunnel junctions (AFMTJs), while the functional properties of insulating AM materials remain largely unexplored.

Here, we propose employing AM insulators (AMIs) as efficient spin-filter materials. By analyzing the complex band structure of rutile-type AMIs MF_2 (M = Fe, Co, Ni), we demonstrate that the evanescent states in these AMIs exhibit spin- and momentum-dependent decay rates, resulting in substantial momentum-dependent spin polarization of the tunneling current [1]. Using a spin-filter tunneling model [2], we estimate a sizable TMR ratio of 150 -170% in spin-filter magnetic tunnel junctions (SF-MTJs) based on AMIs CoF_2 and NiF_2, provided the Fermi energy is tuned near the valence band maximum (VBM). Our results demonstrate that AMIs provide a viable alternative to conventional ferromagnetic or ferrimagnetic spin-filter materials, potentially advancing the development of next-generation AFM spintronic devices.

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Talk 13

Downfolding from First Principles to Effective Models: A Journey with Tanusri

Roser Valenti

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In this talk, I will provide an overview of the power of downfolding methods for extracting effective low-energy models, including generalized Hubbard and spin models, and present a few examples and applications to correlated systems.

Talk 14

Creating Holographic Quantum Matter with Graphene

Arindam Ghosh

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The emerging interest in holographic quantum matter stems from its ability to provide a unifying platform to describe diverse systems, concepts and phenomena in physics, such as the high-Tc cuprates and strange metals; propagation and thermalization of quantum information, to even some foundational concepts in the theories of quantum gravity. Due to the strong interaction among the constituent particles in this class of materials the conventional quasi-particle picture breaks down, and the thermalization of nonequilibrium quantum states proceeds through emergent hydrodynamic modes. It has been challenging to realize a holographic analogue on a solid-state platform, primarily due to the presence of intrinsic disorder and paucity of adaptable experimental strategies. In this talk, I shall present some new experimental results on the electrical and thermal transport measurements in extremely high-quality graphene devices and show that the electron-hole plasma close to the charge neutrality point, or the Dirac point, of very high-quality graphene is an archetypal holographic quantum material. I shall give evidence of the universal dc transport, breakdown of the Widemann-Franz law, and approach to the holographic limit of minimally dissipative flow of charge. These results establish a robust experimental paradigm to explore the linkage between fundamental dissipative time scales and eigenstate thermalization in strongly correlated quantum condensed matter systems.

Talk 15

The Phantom of the Lattice: Unconventional Manifestations of the Jahn-Teller Physics

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Talk 16

Strong and weak coupling phases of J = 3/2 electrons on the honeycomb lattice

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Talk 17

Disorder and Correlations, can we do that?

Markus Aichhorn

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Transport properties of real materials are governed primarily by two scattering mechanisms: electron–lattice interactions and electron–electron correlations. Both of them are difficult to treat, handling both eDects simultaneously remains a major theoretical challenge. In this talk, we present recent work toward incorporating disorder effects into ab-initio descriptions of correlated materials. First, we examine the role of disorder at extremely high temperatures, such as those found in the Earth's core. By combining molecular-dynamics simulations with dynamical mean-field theory (DMFT), we analyze how these scattering processes influence the thermal conductivity of iron under Earth-core conditions. Second, we investigate the metal–insulator transition in the alloy system $SrV_xTi_{1-x}O_3$. While the material is metallic for $x > 0.5$, it becomes a Mott insulator for concentrations around $x = 0.5$ and below. We demonstrate that supercell calculations can reproduce this transition. However, this approach requires choosing representative supercell configurations for the disordered alloy. To address this ambiguity, we present initial results using an alloy-theoretical framework, the generalized quasi-chemical approach, which enables a continuous description across compositions and removes the need to select specific supercells. Although first results are promising, we also discuss the open questions and possible limitations of this approach.

Talk 18

Heusler alloys as spintronic and spin-caloritronic materials

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Ferromagnetic/antiferromagnetic/ferrimagnetic Heusler alloys have emerged as one of the most important materials in the field of applied magnetism in the recent past. These alloys are truly multifunctional and can be exploited for various applications. Apart from the ferromagnetic shape memory related effects, Heusler alloys also play a vital role in spintronics. Spintronic materials can be classified into many groups, such as half metallic ferromagnets, spin gapless semiconductors, magnetic semiconductors etc. Antiferromagnets and ferrimagnets attract a lot of interest in spintronics. All these categories have been found from the Heusler family. Several novel materials and novel phenomena have been discovered as a result of extensive experimental and theoretical investigations. Recently, the role of Heusler alloys as spin caloritronic materials is confirmed. In this talk, I will present some of the work that we have carried out in a variety of Heusler alloys in which the electronic band structure is systematically tuned to synthesize novel and better materials. The talk will also cover some of the very novel aspects that have come out of the extensive studies carried out on different classes of materials.

Talk 19

DFT combined with interpretable ML for discovery of materials

Ranjit Thapa

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Descriptors obtained through computational studies play an important role in designing a catalyst for several catalytic reactions. A good descriptor can explain the catalytic activity used to design new sustainable energy materials with high selectivity towards a particular reaction. During the last one decade we have solved two specific problems (i) general electronic descriptor for carbon-based materials and (ii) beyond d-band center as electronic descriptor for metal center-based catalysts (ongoing). This method is to understand and fast identify the catalysts used for various reactions in sustainable energy systems (Fuel Cells, Water Splitting, CO_2ER).

Specifically I will discuss how we develop the Quantum mechanics/Machine Learning based model equation to predict the catalytic activity. Then we validated the predictive model equation with experimental results (collaborative work). In short, to find the ΔG_{OH} values and theoretical overpotential on 66 sites, we need to do 198 density functional theory (DFT) based calculations (three intermediate for each site). Which needs huge resources and is also time-consuming. But by applying our SVR model we can predict the ΔG_{OH} values and overpotential for these active sites by doing three DFT calculations of the host surface only.

Second the d-band center is a well-known descriptor used for various reactions, however it fails to give correlation where the electronic environment is slightly different for the same metal. The approach of using multi-descriptor instead of single descriptors is proposed to address this problem. The d-band frontier and the d-band occupancy scaled by width corrected band center together correlates with activity for the same metal site under varying electronic environments. 432 active sites tested for catalytic activity using DFT and 105 possible descriptors are individually assessed for activity correlation and optimized using Principal Component Analysis (PCA) and eight machine learning algorithms.

Also, I will discuss the APP we are developing named as “Padarth Khoj” focused on finding catalysts materials.

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Talk 20

A Universal Framework for Controlling Non-Relativistic Spin Splitting in Antiferromagnets

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The recent discovery of non-relativistic spin splitting (NRSS) in antiferromagnets has generated considerable interest, both for its fundamental implications, challenging the long-held notion that electronic bands in antiferromagnets are necessarily spin degenerate, and for its potential applications in antiferromagnetic spintronics. In my talk, I will present our recent findings [1,2], which reveal that these unconventional antiferromagnets host hidden magnetic octupolar order, that allows control of NRSS by tuning the geometry of the surrounding nonmagnetic atoms through specific phonon modes, without changing the Néel order itself. Our results provide a universal framework for engineering spin splitting across a broad class of materials and highlight the intricate coupling between charge, spin, and lattice degrees of freedom.

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Talk 21

Hydrogen-Metal Interactions: Mechanisms, Challenges, and Pathways to Durable Materials for a Sustainable Energy Future

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As the world moves toward a sustainable and low-carbon energy future, hydrogen stands out as a clean and efficient energy carrier for applications in mobility, storage, and power systems. However, a key challenge limiting its widespread deployment is hydrogen embrittlement, which degrades the structural integrity of a material system ultimately leading to its mechanical failure. The understanding of such failure mechanisms is essential in advancing hydrogen technologies. In this talk, I will give an overview into the mechanistic underpinnings of hydrogen trapping and embrittlement in structural metals such as aluminum, zirconium, and steel. Using density functional theory I analyze how defects (stacking faults, grain boundaries, and hydrides) influence hydrogen behaviour by either trapping atoms or facilitating their diffusion. For instance, in aluminum alloys, it is found that the co-segregation of Mg and H to free surfaces provides the fundamental driving force for grain boundary embrittlement, whereas Sn strongly binds with H at the grain boundary without increasing the embrittlement tendency. In zirconium alloys, such as Zircaloy-4, Sn segregation to stacking faults and hydride phases plays a critical role in microstructural evolution under hydrogen exposure. Based on these insights, effective alloying strategies can be developed to improve the resistance to hydrogen embrittlement.

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Talk 22

Surprises from Mn^{2+} emissions in doped semiconductor nanocrystals

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The highly efficient, sub-bandgap, orange emission from Mn^{2+} dopants in semiconductor quantum dot hosts has been the subject of over two thousand publications, owing to its broad scientific interest and technological potential. This emission, universally attributed to the $^4T_1 \rightarrow {}^6A_1$ transition of Mn^{2+}, is characterized by a long lifetime of the order of milliseconds and negligible self-absorption due to the large Stokes shift, making it promising for diverse applications. Surprisingly, the fundamental mechanism by which energy is transferred from the host to the Mn $^4T_1$ state, believed to occur extremely rapidly on the sub-ns scale, has not been understood to date.

In our work,[1,2] we investigate how the first excited multiplet state of Mn^{2+} ($^4T_1$) is populated from its $^6A_1$ ground state, which evidently requires spin-nonconserving processes following photoabsorption in host semiconductor nanocrystals. This seemingly simple question leads to several fundamental issues: What are the energy-transfer pathways from the host excited states to Mn^{2+}? How is the significant excess energy of the host excited state, compared to the energy of the Mn^{2+} $^4T_1$ state, defining the large Stokes shift, dissipated?

In this talk, I shall address these issues using $Mn@CsPbCl_3$ as a generic platform and temperature-dependent steady-state and time-gated photoluminescence experiments as probes, investigating the microscopic processes involved. I shall show how the experimental results constrain the possible models, leading to rate equations that can be analytically solved and account for all observations.

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Talk 23

Altermagnetism in Phase Space

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Momentum space properties such as topology, unconventional superconductivity, and altermagnetism originate from an underlying connection between local orbitals and Bloch states. Traditional approaches typically rely on either Wannier-orbital representation or a Bloch state approach and hence often struggle to transform between real and momentum space descriptions. In this talk, I will introduce a phase-space approach where the symmetries of the Bloch states and the symmetry of the local orbitals are defined in the same symmetry class. Within this framework, the quantum states, Hamiltonian, and emergent order parameters are described using the same set of symmetry representations, which enables a systematic classification of the non-interacting parameters and interaction terms responsible for emergent phases. I will mainly apply the method to 2D RuO_2 to uncover the role of sublattice-momentum couplings in generating the characteristic spin textures of the altermagnetic phase. I will also present our machine-learning framework for predicting 2D altermagnets and identifying their order-parameter symmetries. If time permits, I will discuss how the same approach can be extended to predict unconventional pairing symmetries in monolayer $IrTe_2$.

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Talk 24

Title : To be announced

Prof. Silke Biermann

École Polytechnique, France

TBA

Talk 25

Exploring the Anomalous Hall Effect in Transition Metal Intercalated Dichalcogenide

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Quasi-two-dimensional layered magnetic materials with strong spin–orbit coupling and electron–electron correlations provide an important platform for exploring novel electronic and magnetic phenomena. Metallic transition-metal dichalcogenides with the general formula TX_2 (T = metal, X = S, Se, Te) have therefore attracted considerable attention as two-dimensional magnetic systems.

Magnetic-atom–intercalated dichalcogenides form a particularly important class of such materials. In these compounds, magnetic ions are inserted into the van der Waals gaps of layered dichalcogenides, producing compounds of the type M_xTX_2, where M is a magnetic element (e.g., Fe, Cr, Mn, Co, Ni) and TX_2 is a host material such as TaS_2, NbS_2, or $TiSe_2$. These systems provide an excellent platform for studying low-dimensional magnetism.

$Fe_{0.27}TaS_2$ is a representative van der Waals material in which Fe atoms are intercalated between two TaS_2 layers. The compound undergoes ferromagnetic ordering below the Curie temperature T_C= 90 K. When cooled in a moderate magnetic field (≥500 Oe), the sample acquires a large magnetization. Upon subsequent warming in the zero field, this magnetization persists, indicating the presence of thermo-remanent magnetization (TRM). Remarkably, the thermoremanence survives up to about 160 K, well above T_C . Magnetization analysis suggests short-range magnetic correlations in the form of a Griffiths-like singularity extending to approximately $2T_C$. The thermoremanence is also reflected in a pronounced anomalous Hall effect observed even in zero magnetic field. However, unlike the TRM, the thermoremanent Hall signal disappears immediately above T_C , indicating that the anomalous Hall effect requires long-range magnetic order.

The origin of the thermoremanence in $Fe_{0.27}TaS_2$ can be attributed to strong magneto-crystalline anisotropy arising from the Ising-like nature of the spins. The compound exhibits strong uniaxial anisotropy with the crystallographic c-axis as the easy axis. During field cooling with the field applied along the c-axis, the spins align along this easy axis. After removing the magnetic field, the system remains magnetized because a free-energy barrier separates the up- and down-spin states. As a result, magnetization persists on warming, causing the observed thermoremanence and the anomalous Hall effect in zero applied field.

Talk 26

Title: To be announced

Prof. Bernd Büchner

IFW Dresden, Germany

TBA

Talk 27

Complex Magnetic Order in Mn_3-based Antiferromagnets: Insights from neutron diffraction and EXAFS

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Antiferromagnets containing triangular magnetic sublattices, such as hexagonal DO_{19}-type Mn_3X (X = Sn, Ge, Ga), cubic Mn_3X (X = Ir, Pt, Rh), and antiperovskite compounds Mn_3AN or Mn_3AC (A = Ga, Sn, Ni), often exhibit multi-q antiferromagnetic structures**.** These modulated or non-collinear magnetic orders typically arise from competing magnetic exchange interactions and geometric frustration inherent to these high-symmetry crystal lattices. Understanding the origin and stability of such complex magnetic configurations remains an important challenge in condensed matter physics.

Over the years, we have investigated some of these systems using a combination of average and local structural probes, including neutron diffraction and extended X-ray absorption fine structure (EXAFS) spectroscopy, to elucidate the relationship between local structural distortions and the emergence of complex magnetic order. In this talk, we present our results on a few cubic and hexagonal antiferromagnets exhibiting multi-q magnetic ordering**,** highlighting the subtle influence of structural disorder on their magnetic ground states [1–6].

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Talk 28

Spin-Orbit Driven Novel Magnetism in 2d Systems

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In this talk, we shall explore the interplay between symmetry, Coulomb correlations and spin-orbit coupling in a representative two dimensional honeycomb system $OsCl_3$ with d^5 electronic configuration. Theoretically it has been predicted that the system transforms from a ferromagnetic Chern insulator to a Mott Insulator as a function of Coulomb correlations encoded in the Hubbard U parameter. We shall demonstrate that, in the Chern insulating phase, the interplay between magnetism and mirror symmetries renders the in-plane ferromagnetic state a versatile platform for realizing nontrivial topological phases, with the orientation of magnetic moments at lattice sites serving as a key tuning parameter. In the strong correlation limit, the J_{eff}=1/2 Mott insulating phase of the compound is modeled by Hubbard-Kanamori (HK) Hamiltonian incorporating spin-orbit coupling and electron correlations. Exact diagonalization (ED) calculations of the HK Hamiltonian on a two-site cluster are performed to construct the effective magnetic Hamiltonian. The ground-state magnetic properties are explored using the semiclassical Luttinger-Tisza approach as well as exact diagonalization calculations identifying the magnetic ground state to be zigzag antiferromagnetic ordering in close proximity to a spin liquid phase [1-3]. We shall also compare and contrast J_{eff}=1/2 magnetism in a d^7 triangular-lattice monolayer cobaltate, $CoBr_2$ [4] with d^5 systems.

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Talk 29

Engineering Quantum Transport in van der Waals materials

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Spin–orbitronics has gained tremendous attention in recent years, offering a promising route for efficient information transfer and storage beyond traditional electronics. Two of the important phenomena in this context are the orbital/spin Hall effect (OHE/SHE), and the Rashba–Edelstein effect. Both correspond to a response to the applied electric field. While the former accounts for a transverse orbital/spin current, the latter leads to a non-zero accumulation of the magnetic moments and thus magnetizes the material. Thanks to strong spin-orbit coupling, topological features, and easy manipulation of symmetry, the van der Waal materials have emerged as promising candidates for spin-orbitronics. In this talk, we will explore various mechanisms, such as heterostructure engineering, magnetic proximity effects, and time reversal symmetry breaking, etc. to tune the spin and orbital Hall conductivities in this class of materials. The emphasis of the talk will be on demonstrating Giant Damping-like Spin-Torque Conductivity in a GeTe/Py and $PtSe_2$/Py van der Waals Heterostructures, and Orbital and Spin Rashba Edelstein effect in Janus transition metal dichalcogenides. Finally, we will demonstrate possible ways of finding the best performing SHE materials out of a general class using AI&ML.

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Talk 30

Magnetostrictronics: Estimate exchange of magnetic anisotropy and lattice elastic energies from first-principles calculations

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The outcome of strain while magnetized was observed by Joule, 1842; and it is now-a-days digitized with computational first-principles modelling and calculations [1-2]. Harvesting and then utilizing these internal *quantum mechanical energies* of a hard magnetic solid is sustainable approach by exploring its microscopic origin of crystalline spin-anisotropy to the crystal orbital-field effects [3-4]. Novelties are thus, raised due to its phenomenological implementation and possible future applications from fundamentals to functionalities which would be guided by the bi-directional energy exchange between the *elastic* and *magnetic* anisotropic energies in hard magnetic solids [5-6]. Hence, modulating the device transport properties without *external* electric and or magnetic-field has become a pioneering domain of research, in the recent time quantum materials research of *quantum & mechanical energies* of solids [7-8]. Here, modelling and quantification of magnetocrystalline anisotropic energy (MCAE) and its correlation with associated magneto-elastic stress-strains are key to the next generation magnetostrictive applications – pioneering step to the domain *magnetostrictronics* [9-10]. An accurate first-principles calculations in the scarcity of the computational limitations of first principles calculations and numerical instabilities at the few meV of energy scale limits this exploration [9-10]. This has been now re-investigated in the available limit of the numerical stability and accuracy of the density functional theory (DFT) calculations for these two $L1_0$-*A*Pt order alloys (*A*= Fe, Mn) with some future notes about the reliability of plane-wave DFT codes [9-10]. In the presentation, I will discuss this novel route to the bi-directional energy *exchange* via *magnetostrictronics* (Figure 1).

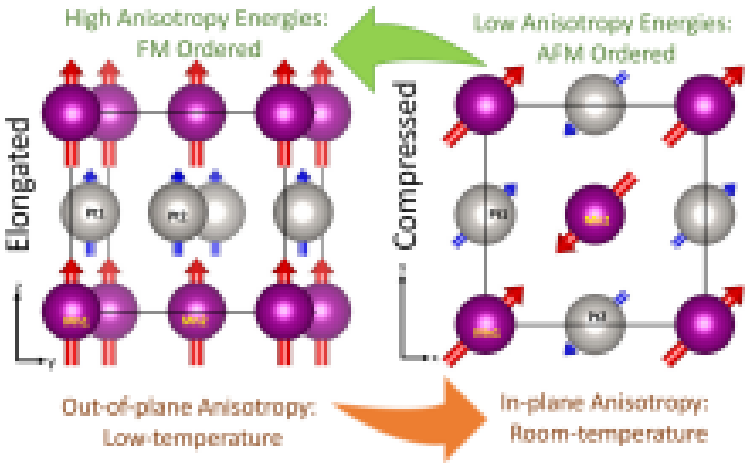

Figure 1: Spin-anisotropic energies and associated lattice distortion schematics

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Talk 31

Trend in interfacial charge transfer, emergent electronic and magnetic structure and topological properties in the 3d/5d superlattices $LaBO_3/SrIrO_3$ (B = Mn, Fe, Co, Ni)

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Using a first-principles study, we investigate the systematic behavior of n-type and p-type $LaBO_3/SrIrO_3$ superlattices with B = Mn, Fe, Co, Ni, moving from left to right across the 3d transition metal row of the periodic table. Our study unravels a clear trend in terms of interfacial charge transfer, and electronic, magnetic, and topological properties.

For p-type superlattices, the charge is transferred to the $SrIrO_3$ block for all four systems, with the charge transfer strength dictated by B-Ir covalency. However, a marked distinction occurs for n-type superlattices, where interfacial charge transfer occurs to the $LaBO_3$ block for B = Co, Ni, which have a nominal d-occupancy greater than Ir^{4+}, and to the $SrIrO_3$ block for B = Fe, Mn, which have a nominal d-occupancy smaller than or equal to that of Ir^{4+}. This makes the $SrIrO_3$ essentially nonmagnetic for n-type $LaFeO_3/SrIrO_3$ and $LaMnO_3/SrIrO_3$.

The band structure of the magnetic $SrIrO_3$ block with ferromagnetic Ir–Ir exchange and spin-orbit coupling supports $C = 2$ double Weyl points, giving rise to appreciable values of intrinsic anomalous Hall conductivity for both n-type and p-type $LaCoO_3/SrIrO_3$ and $LaNiO_3/SrIrO_3$. Our calculations further predict only p-type $LaMnO_3/SrIrO_3$ and $LaFeO_3/SrIrO_3$ to exhibit anomalous Hall conductivity, which is expected to be heavily suppressed for $LaFeO_3/SrIrO_3$ due to the weakening of Ir–Ir ferromagnetic exchange arising from the proximity to the antiferromagnetic $LaFeO_3$ block.

Our comprehensive study should provide a microscopic understanding of some of the recent experimental observations and will serve as a guide to future experiments.

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POSTERS

Poster 1

Basis Adaptive Algorithm for Quantum Many-Body Systems on Quantum Computers

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A new basis adaptive algorithm for hybrid quantum-classical platforms is introduced to efficiently find the ground-state (gs) properties of quantum many-body systems. The method addresses limitations of many algorithms, such as Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) etc by using shallow Trotterized circuits for short real time evolution on a quantum processor. The sampled basis is then symmetry-filtered by using various symmetries of the Hamiltonian which is then classically diagonalized in the reduced Hilbert space. We benchmark this approach on the spin-1/2 XXZ chain up to 24 qubits using the IBM Heron processor. The algorithm achieves sub-percent accuracy in ground-state energies across various anisotropy regimes. Crucially, it outperforms the Sampling Krylov Quantum Diagonalization (SKQD) method, demonstrating a substantially lower energy error for comparable reduced-space dimensions. This work validates symmetry-filtered, real-time sampling as a robust and efficient path for studying correlated quantum systems on current near-term hardware.

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Poster 2

Tuning magnetic ground states of RMn_6Sn_6 (R = Lu, Mg) kagome metals by dimensionality reduction: Route to ferromagnetism and large anomalous Hall effect

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The ternary intermetallic compounds, RMn_6Sn_6 (R = rare-earth or alkali or alkaline-earth metal) hosting Kagome bilayer of Mn, present a class of systems that naturally allows for the interplay of magnetism and topology. In search of ferromagnetic members in these systems, we show that dimensional reduction can be an effective means to achieve ferromagnetism and large anomalous Hall conductivity. Focusing on two specific members with R = Lu and Mg, our first-principles calculations show that dimensional confinement through the construction of experimentally relevant atomistically thin single bilayer kagome geometry of Mn atoms gives rise to a ferromagnetic metal with multiple Weyl points along with spin-orbit-coupling induced gapped bands. The calculated anomalous Hall conductivity in the thin film geometry turns out to be 287 and 178 Ω^{-1} cm^{-1}, comparable to that found for bulk RMn_6Sn_6 with alkali or alkaline-earth metal at R site. This is of interest as thin-film geometry can be efficiently integrated to devices.

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DOI: 10.1103/h9ym-4cp2

Poster 3

Spin-orbit driven $J_{eff} = 1/2$ magnetism in a d^7 triangular-lattice monolayer cobaltate

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Recent theoretical and experimental advances have identified cobaltates with a high-spin d^7 electronic configuration as promising hosts for spin-orbit entangled $J_{eff} = 1/2$ magnetism that can support bond-dependent exchange interactions [1,2]. In two-dimensional triangular lattices, the coexistence of such exchange frustration along with usual geometric frustration gives rise to a rich landscape of competing magnetic phases, establishing monolayer triangular d^7 cobaltates as a compelling platform for frustrated magnetism. Here we investigate a representative triangular lattice monolayer cobaltate $CoBr_2$, where first-principles density functional theory (DFT) calculations reveal a dominant nearest-neighbor t_{2g} - e_g hopping channel that enhances the ferromagnetic Kitaev-type exchange interactions. In contrast, the nearest-neighbor Heisenberg term is highly sensitive to a direct t_{2g} - t_{2g} hopping path and electronic correlations. The magnetic exchange parameters are evaluated using the hopping amplitudes obtained from DFT calculations within an exact diagonalization framework [3]. We construct the first (J_1) and third (J_3) nearest neighbor Heisenberg exchange dependent J_1 - J_3 magnetic phase diagram in the physically relevant regime and identify multiple competing ground states, including ferromagnetic, stripy, spiral, and 120° antiferromagnetic orders. The Luttinger-Tisza analysis further predicts a Z_2 vortex crystal phase, while exact diagonalization reveals a bond-nematic phase promoted by quantum fluctuations. Going beyond the conventional bond-independent XXZ picture typically applied to Co^{2+} systems, our results on monolayer $CoBr_2$ establish d^7 cobalt dihalides as a promising platform to explore the interplay of long-range Heisenberg and bond-dependent exchange interactions that can stabilize diverse magnetic ground states on a triangular lattice [4].

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Poster 4

$Na_2Ir^{IV}Cl_6$: An Ideal J_{eff} = ½ Vacancy-Ordered Halide Perovskite Single Crystals Exhibiting Cubic Structure and Antiferromagnetism

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Vacancy-ordered halide perovskites (VOPs) have been known for more than 100 years, but their exact crystal structures and microscopic information are to date a puzzle. VOP iridates offer a chemically well-defined platform to investigate the influence of on-site Coulomb repulsion, crystal field and spin-orbit coupling. Na-based VOP iridates are being reported for their hydration dependent structural and magnetic uncertainty. Here, we report the synthesis and comprehensive characterization of anhydrous Na_2IrCl_6 single crystals. Single crystal X-ray diffraction at 165 K reveals a cubic structure in the *Fm*-3*m* space group composed of regular isolated $\{IrCl_6\}$ octahedra, and powder X-ray diffraction confirms phase purity. Thermogravimetric analysis establishes the absence of lattice water and demonstrates thermal stability up to 453 K. X-ray photoelectron spectroscopy confirms the +4 oxidation state of iridium. Magnetic susceptibility measurement indicates antiferromagnetic ordering at $T_N \approx 2.63$ K with a large frustration parameter ($f = | \Theta_{cw}/T_N | = 29.4$) that suppressed long range magnetic ordering mediated by Ir-Cl-Cl-Ir supersuperexchange pathways. The effective magnetic moment $\mu_{eff} = 1.71\ \mu_B$ is consistent with a J_{eff} = ½ state expected for Ir^{4+} in the cubic crystal field. The cubic phase reported here contrasts with previously described monoclinic Na_2IrCl_6 and highlights the strong structural and physical property relationship in Na-based VOP iridates.

Poster 5

Magneto-Transport Anomalies Driven by the Complex Phase Diagram of Helimagnetic MnP

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The helimagnetic MnP, a member of the binary pnictide family, has been extensively studied for its rich magnetic phase diagram, which includes helical, conical, and fan-like magnetic structures [1], as well as multiple magnetic phase transitions associated with a Lifshitz critical point [2]. In contrast, its magneto-transport properties have remained relatively unexplored. In this work we have investigated the magnetoresistance (MR) and Hall resistivity properties of high-quality MnP single crystals, which undergoes a paramagnetic to ferromagnetic transition at around $T_C \sim 295$ K and a subsequent ferro to helimagnetic transition around $T_{SCR} \sim 52$ K, with particular emphasis on the low temperature (T) phase. Low-T MR measurements reveal an anomalous response in low field, followed by a large, non-saturating linear field dependence in high magnetic fields (up to ±15 T). The origin of the large linear MR may be attributed to the presence of a semi-Dirac like band dispersion protected by nonsymmorphic symmetry [3,4]. Hall measurements in the range $100K \leq T \leq 330K$ exhibit an anomalous Hall effect (AHE) predominantly governed by skew scattering, with a finite contribution from side-jump and/or intrinsic mechanisms. Below $T < 100$ K, the Hall data further reveal the presence of a topological Hall effect (THE) in both the FAN phase and the SCR phase.

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Poster 6

Neel order, spin-spiral, and spin liquid ground state in frustrated three dimensional system $CaMn_2P_2$: A DFT+U and spin dynamics study

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We investigate the magnetic ground state and phase transitions in the frustrated three-dimensional system $CaMn_2P_2$ using first-principles calculations combined with spin-dynamics simulations. Our density functional theory (DFT) calculations, incorporating Hubbard U corrections, reveal that $CaMn_2P_2$ exhibits an indirect gap semiconducting ground state with a localized Mn^{2+} ($3d^5$, $S = \frac{5}{2}$) electronic configuration and negligible spin orbit coupling effects. The computed exchange interactions show that the magnetic behavior is well described by an isotropic Heisenberg Hamiltonian. In this model, there are two major couplings: the nearest-neighbor (NN) interaction J_1 couples the two Mn layers along the c-axis and next NN J_2 is in the a-b plane where Mn ions form a hexagonal layer structure. Our results show that both J_1 and J_2 are antiferromagnetic in nature and as a consequence J_2 induces frustration owing to the in-plane triangular geometry of the Mn-ions. The J_1 is found to promote long-range antiferromagnetic order, while the J_2 is responsible for spin canting and disorder. Our spin-wave analysis confirms that the system stabilizes a spin-spiral ground state with a propagation vector $q = (\frac{1}{6}, \frac{1}{6}, 0)$ in agreement with neutron diffraction experiments. By tuning the J_2/J_1 ratio, we construct a phase diagram that reveals a transition from a collinear Neel antiferromagnetic state to spin-spiral phases with different propagation vectors, and eventually to a disordered phase at large frustration. Atomistic spin-dynamics simulations capture the temperature evolution of the magnetism and reproduce the experimentally measured magnetic specific heat as well as transition temperature with good accuracy. Furthermore, for large J_2/J_1, we identify a low-temperature phase with slow spin relaxation and persistent fluctuations, suggesting a spin-liquid-like state. Our study provides a microscopic understanding of frustration-induced magnetism in $CaMn_2P_2$ and establishes it as a realization of the J_1-J_2 model in a three-dimensional lattice for exploring emergent magnetic phases.

*The work has been carried out in collaboration with the co-authors.**[1]**

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Poster 7

Strain as a topological selector in altermagnetic CrSb

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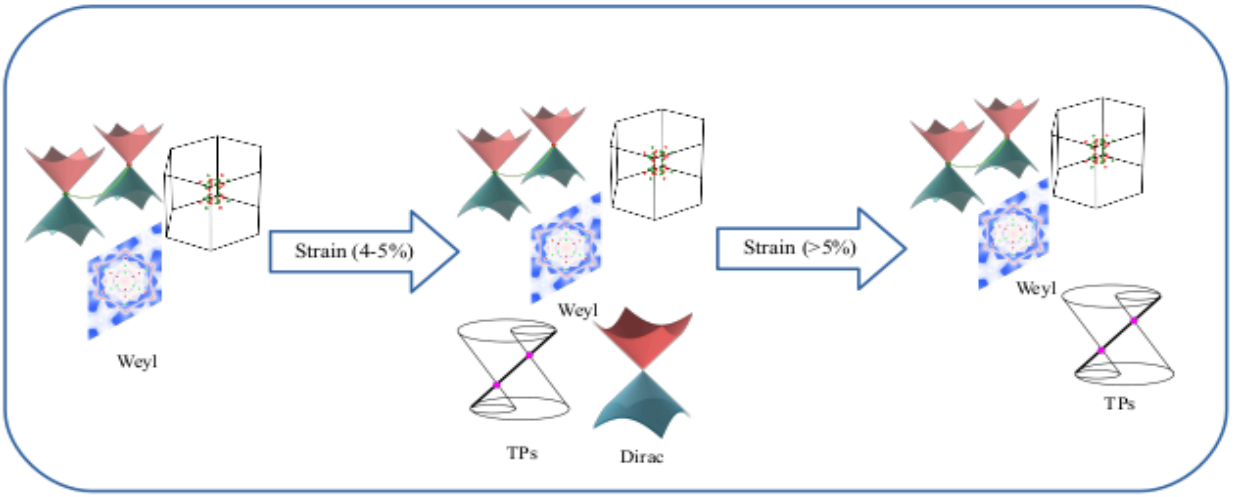

Altermagnetism combines fully compensated magnetic order with a magnetic symmetry that relates inequivalent spin sublattices, offering a promising, still underexplored platform for unconventional topological phases. In this work we show that both isotropic tensile strain and electron localization, controlled by an effective Hubbard interaction U_{eff}, can act as efficient and systematic topological control parameters in the altermagnetic Weyl semimetal CrSb. While CrSb hosts Weyl fermions at equilibrium, modest tensile strain of 4–5% stabilizes additional symmetry allowing Dirac crossings and triple-point fermions, with further strain selectively favoring the triple-point phase. We propose a 3D low energy Hamiltonian that captures the interplay between the Hubbard interaction U and the sublattice symmetry of the altermagnet, giving rise to an interaction driven Dirac crossing. Our results establish CrSb as a model altermagnet in which either strain or electron localization can selectively access and control the distinct topologies inherent to the altermagnets.

Poster 8

Application of machine learning for solving materials science problems

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The integration of machine learning (ML) into materials science has revolutionized our ability towards materials exploration, unlocking new frontiers in material optimization and innovation. In this study, we explored applications of machine learning in solving a diverse class of materials science problems. In the first example, a machine-learned force field is developed for MAX compound Ti_2AlC to explore its non-linear elastic behavior, the underlying mechanism and the effects of vacancies in the aforementioned elastic behavior [1]. The next work involves semiconductor heterostructures, particularly, its type derived from the bandstructures of the constituent semiconductors [2]. In another set of work, we have delved into the domain of nanoscale binary metal alloys to investigate the driving factors determining their core-shell preference using a ML scheme[3], and catalytic properties in Pd containing nanoalloys [4]. In the final example we have utilized ML in developing a microscopic understanding of formation of atomic wires of appreciable length by using experimentally obtained data in training [5]. Using a supervised learning scheme, we have found optimal conditions for Au chain formation. We have further applied an unsupervised learning scheme for the classification of individual breaking traces, thus identifying junction structures associated with longer chains. Our findings are corroborated by ab-initio molecular dynamics simulations.

Collaborators:

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Poster 9

Crucial role of Fe-Fe magnetic interactions in layered triangular antiferromagnet in dictating Li-ion cathode material's efficiency

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The efficiency of the Li-ion battery is mostly understood from the redox reactions capacity. Incidentally one of the most prospective Li-ion cathode materials belongs to the class of polyanionic compounds with Fe. If Fe is in +3 or +4 state, it has partially filled 3d- shell, with unpaired spin configuration, which can lead to the exotic magnetic ground state. However, very little effort has been made in the direction to understand the role of the magnetism in deriving the observed redox reaction capacity in the context of the Li-ion battery. In this work we are doing density functional theory based electronic structure investigation of the Fe based Li-ion cathode material to understand the role of the Fe magnetic moment and Fe-Fe magnetic exchange interaction in the electrochemistry of the battery with the support from experiments. We found that in the charging process when the Li-ion takes out from the cathode, the magnetic moment of the Fe decreases monotonically. The calculated magnetic exchange interactions clearly show the anti-ferromagnetic ordering of the triangular Fe sublattice. As a result strong magnetic frustration appears in the system. In the charging process (delithiation) the magnetic interactions vary non-monotonically. Initially calculated results indicated the possibilities of the mixed valent Fe state and we are trying to understand the evolution of the charge state and spin state during the charging cycle through NEB calculations.

Collaborators:

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Poster 10

Disorder mediated fully compensated ferrimagnetic spin-gapless semiconducting behaviour in Cr_3Al Heusler alloy

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Spin-gapless semiconductors (SGSs) that host fully compensated ferrimagnetism (FCF) are highly sought for energy-efficient and stray-field-free spintronics, yet their realization in chemically disordered systems has remained elusive. Here, we demonstrate that the binary Heusler alloy Cr_3Al —despite adopting a fully A2-disordered structure—exhibits a rare coexistence of SGS transport and an FCF ground state. Single-crystalline and polycrystalline Cr_3Al samples were synthesized, and structural analyses using single-crystal XRD, synchrotron powder XRD, and neutron diffraction reveal complete Cr/Al site mixing. Magnetization, X-ray magnetic circular dichroism (XMCD), and temperature-dependent neutron diffraction establish a compensated ferrimagnetic state with a vanishing ordered moment of 0.1(1) μ_B/f.u and a high Curie temperature of 773 ± 2 K. ElectricalB/f.u and a high Curie temperature of 773 ± 2 K. Electrical ~0.1(1) μB/f.u and a high Curie temperature of 773 ± 2 K. Electrical and thermal transport measurements uncover SGS characteristics, including weak temperature dependent conductivity, low Seebeck coefficients, and electron-hole compensated transport. Hall measurements show unusual temperature-dependent carrier concentrations consistent with disorder modified electronic states. First-principles calculations reproduce the experimentally observed negligibly small magnetization (0.0072 μ_B/f.u and a high Curie temperature of 773 ± 2 K. ElectricalB/f.u) and reveal a vanishing spin-up band gap— supporting SGS behavior driven by chemical disorder. Our results identify Cr_3Al as the first experimentally verified A2-disordered Heusler alloy exhibiting FCF-characteristics and SGS transport, positioning it as a disorder-tolerant platform for next-generation, high-temperature spintronic devices.

Poster 11

Symmetry-Induced Spin Textures and Orbital and Spin Hall Effects in a Non Centrosymmetric Polar Systems

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In non-centrosymmetric systems, the gradient of the electrostatic potential generates a momentum dependent effective magnetic field in the electron's rest frame. This field locks the electron spin to its momentum, lifting spin degeneracy and producing complex spin textures in reciprocal space [1,2,3]. These textures are governed by crystal symmetry and play a crucial role in generating orbital and spin Hall effects. Using first-principles density functional theory (DFT) calculations combined with low-energy k·p models, we identify diverse spin textures in the polar system Ta_2CS_2. In particular, we observe higher-order Rashba effects at Γ point and valley-dependent Zeeman splitting at the non-time-reversal-invariant K and K′ points. To quantify the Hall responses in both the orbital and spin sectors, we construct an effective tight-binding model [4]. Our analysis reveals that the valleys at the K and K′ points exhibit pronounced orbital polarization, leading to a large orbital magnetic moment through orbital–valley locking. As a consequence of the strong orbital Berry curvature associated with these valley textures, Ta_2CS_2 exhibits a remarkably large orbital Hall conductivity, significantly exceeding that reported for typical two-dimensional transition-metal dichalcogenides. When spin–orbit coupling (SOC) is included, the spin Hall conductivity remains comparatively small, highlighting the predominantly orbital nature of the transverse response. Finally, we demonstrate that stacking two layers further enhances the Hall responses. In the bilayer configuration, the orbital character at the valleys couples to the layer degree of freedom, resulting in orbital–layer locking and a substantial increase in both orbital and spin Hall conductivities. Our results establish non-centrosymmetric MXenes as a promising platform for realizing large orbital Hall effects and tunable orbital and spin transport in two dimensional materials.

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Poster 12

Two-sublattice double exchange driven magnetism in Cr-based two-dimensional magnets

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Two-dimensional (2D) magnets are of significant interest for spintronics applications. This has stimulated extensive research on van der Waals (vdW) layered compounds with ferromagnetic (FM) layers coupled through weak FM or antiferromagnetic (AFM) interlayer interactions. However, most 2D ferromagnets derived from vdW materials exhibit low Curie temperatures (Tc), with Tc strongly suppressed in the monolayer limit compared to the bulk. According to the Mermin–Wagner theorem **[1]**, long-range magnetic order is forbidden in isotropic 2D Heisenberg systems at finite temperature; thus, 2D magnetism is typically stabilized by magnetic anisotropy in addition to isotropic superexchange interactions. Because magnetic anisotropy is usually small, Tc in 2D systems is generally lower than in bulk counterparts.

An exception to this is CrSBr, which in bulk is reported to exhibit FM intralayer and AFM interlayer coupling with a high magnetic transition temperature of 132 K **[2]**. Subsequently, the CrSBr monolayer has been theoretically predicted **[3]** and experimentally synthesized **[4]**. Remarkably, the CrSBr monolayer shows an even higher FM transition temperature of 146 K. Motivated by this observation, we analyze its unusual electronic structure using a combination of numerical approaches **[5]**. We find that magnetism is driven by a two-sublattice double-exchange mechanism, which accounts for both the high transition temperature of CrSBr and the strongly reduced Tc in the related compound $CrPS_4$. The same mechanism also explains the observed negative, hysteretic magnetoresistance in bilayer CrSBr. Furthermore, we predict that the transition temperature can be further enhanced in the 2D semiconducting magnet CrSeBr and the 2D metallic magnet CrTeBr.

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Poster 13

Unveiling the physical properties of Fe-doped cosmic silicate nanostructures from a computational perspective

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One of the most intriguing challenges in astrochemistry revolves around the hunt for suitable reservoirs of the fundamental elements that are found to be depleted from gas phase observations in the interstellar and circumstellar environments [1]. Iron (Fe), the most abundant refractory transition metal is one such element whose possible existence in some form of condensed phase has been anticipated for a long time [2]. Numerous speculations and observations have identified several Fe-bearing compounds [3,4,5] in the astrochemical environment which may serve as potential candidates for sequestering the "missing iron" in the cosmos. In this regard, the structure of cosmic silicate dust grains (of olivine (Mg_2SiO_4) and pyroxene ($MgSiO_3$) stoichiometries) brings hope due to the compatibility of Fe substitution in its Mg-site. Not only that, the detection of Fe-bearing amorphous silicates [6,7] along with other astronomical findings offer strong evidence to consider the cosmic silicates as an effective confiscator of Fe. It is to be noted that these dust grains play a very crucial role in the cosmic life cycle of matter. Once released from the stellar outflows to the interstellar medium, they face a very challenging journey experiencing fragmentation and reformation by high energy particles and radiation. This results in a diversity of the sizes, shapes and chemistry. Subject to such processes, the cosmic silicates are very likely to be nanosized. Ultimately, they combine to form larger bodies in the planet forming disks. Hence, these nanosilicates can be considered important forerunners of planetary formation.

While Mg-bearing silicate dust grains dominate the cosmos, even small concentrations of Fe can significantly modulate their physical properties. In this study we have investigated the influence of Fe (concentrations ranging from 0% to 50%) on the structural, electronic, magnetic and spectroscopic properties of nano-silicates using quantum chemical density functional theory. Our simulations indicate that the formation energy (at 0K) of these

nanosilicates reduces in the presence of Fe, thereby demonstrating the potential of the nanoclusters to confiscate Fe. This study not only pinpoints the degree to which Fe amends the fundamental properties of these nanosilicates, but also provides insights into the spectroscopic properties which can aid in the gross estimation of Fe trapped in nanosilicates along various lines of sight in the cold interstellar medium.

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Poster 14

Electric field induced Rashba state in topological layered intermetallics

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Emergence of composite phenomena in a quantum material is always fascinating from the perspective of the interplay of different degrees of freedom. In the same line of thought, we have investigated using the DFT based electronic structure method, a newly synthesized layered ABX type intermetallic compound where A=K, B=Cd, X=Bi, in contrast to the previously reported same class of structure KZnBi. Going from Zn to Cd, hexagonal to tetragonal structural change can be understood from the radius of B site elements. Electronic structure calculation reveals that in absence of spin orbit coupling (SOC) gapless metallic band structure that has 2-types of crossing: C_{2v} symmetry protected band crossing close to the Fermi energy and non-symmorphic symmetry protected 4 fold-Dirac crossing. Incorporation of SOC leads to open up a gap ~ 17-146 meV close to Fermi energy and produced electron-hole-like pockets, whereas non-symmorphic symmetry enforced gapless-crossing still remain gapless close to the energy ~0.7eV below Fermi level. Topological study concludes the compound to be a strong topological Z_2 semimetal hosting linear crossed surface state. We have extended our inquisition with the 2D monolayer of the easily cleavable layered structure. The 2D structure is also metallic in absence of SOC similar to that of bulk 3D, but having completely gapped bands with SOC throughout the brillouin zone around the Fermi level. The 2D monolayer is completely gapped in contrast to that of bulk because there is an enhancement of anisotropy in going from bulk 3D to monolayer 2D structure, which is magnified more in presence of SOC along the direction of dimensional confinement. The 2D monolayer structure also retains its non-triviality hosting non-trivial edge state. On application of electric field in the 2D monolayer, Rashba states appear and there is an enhancement of Rashba coefficient with increasing applied electric field. In topological perspective, there is a transition from topologically non-trivial insulating Rashba state below the critical field to nontrivial metallic state without Rashba above the critical field.

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Poster 15

Magnetic anisotropy and magnetotransport in the distorted kagome antiferromagnet DyAgGe

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The kagome lattice, characterized by a network of corner-sharing triangles, provides a fertile platform for exploring geometric frustration and nontrivial electronic properties. In particular, distortion in the kagome lattice breaks inversion symmetry and can enhance topological properties. Here, we present a detailed investigation of DyAgGe, a frustrated antiferromagnet crystallizing in the hexagonal P-62m structure, featuring a distorted kagome bilayer of Dy atoms. Through combined structural, magnetic, transport, and thermodynamic measurements, we uncover pronounced magnetic anisotropy both in-plane and out-of-plane, complex field induced metamagnetic phase transitions, and signatures of strong magnetic frustration along with anisotropic magnetotransport responses. Our results reveal an intricate interplay between lattice symmetry, magnetic ordering, and electronic behavior in this frustrated kagome compound.

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Poster 16

Machine Learning–Accelerated Discovery of Intrinsic Magnetic Two-Dimensional Materials

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Intrinsic magnetism in two-dimensional (2D) materials remains challenging because magnetic ordering is strongly suppressed by thermal fluctuations, as described by the Mermin–Wagner theorem [1]. However, in recent years, room-temperature 2D magnets [2] have been realized experimentally, where magnetic anisotropy stabilizes long-range magnetic ordering. These materials are promising for future low-power spintronic devices such as magnetic tunnel junctions, a building block in magnetoresistive random-access memory (MRAM) and hard disk drives because of their reduced dimensionality and the ease of exfoliation enabled by van der Waals gaps. Nevertheless, identifying magnetic 2D materials through trial-and-error experimental synthesis or first-principles calculations remains time-consuming, computationally demanding, and expensive.

In this work, we propose a data-driven workflow to accelerate the discovery of magnetic 2D materials. A hierarchical screening framework is developed based on multiple target properties, including thermodynamic and dynamical stability, followed by classification into magnetic and non-magnetic categories. The models used in this framework are trained on data obtained from the Computational 2D Materials Database (C2DB) [3]. Initially, we restrict our exploration to binary compositions that are not present in C2DB. Since our machine-learning models rely heavily on crystal-structure features, we employ the M3GNet universal machine-learning interatomic potential [4] to search for ground-state structures among possible prototypes of binary 2D materials. Finally, our multistep machine-learning models predict new magnetic 2D compounds with both thermodynamic and dynamical stability. Such screening can guide future experiments and support the development of 2D materials for spintronic applications.

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Poster 17

Computational Exploration of Mo_2C: New Phases and Properties

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The family of transition-metal carbides (TMCs) has emerged as an important class of multifunctional materials, offering promising applications in hard and refractory materials, coatings, superconductivity and catalysis [1]. The unique combination of a robust metal sub-lattice with carbon atoms occupying interstitial sites endows these materials with high thermal and chemical stability, mechanical stiffness and good conductivity [2]. These remarkable properties originate from strong metal-metal and metal-carbon covalent bonding. However, these strong bonds also make high-temperature synthesis challenging (1200-1800 °C) [3]. Motivated by this exceptional potential and synthesis difficulties, most experimental and theoretical investigations have focused on the experimentally realized phases: (a) MC with an FCC structure and (b) M_2C with α-orthorhombic, β-hexagonal and δ-trigonal phases. Despite this progress, exploration of new Mo_2C phases remains relatively unexplored with only a few recent studies [4].

In this work, we undertake an unbiased exploration of the M_2C phase space to identify new candidates, taking Mo_2C as a representative system. We combine structural templates with a high-throughput screening methodology [5], curating a dataset from M_2X structure files in material databases [6] and implementing a multistep workflow to filter promising candidates. Relaxed structures were obtained via density functional theory calculations [7], and duplicates were removed using the Valle-Oganov fingerprint [8]. Applying a thermodynamic stability criterion (ΔE_f < 100 meV/atom) yielded ~15 new Mo_2C phases. Analysis of their local chemical environments reveals atomic organization distinct from known phases. Their calculated properties span a wide range of mechanical stability and electronic behaviour. These findings reveal a far richer structural landscape of Mo_2C, highlighting candidates for experimental realization under suitable synthesis conditions.

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Poster 18

Emergent SU(4) Symmetry and Gapless Spin-Orbital Liquid in α-$ZrCl_3$ inspired model

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Quantum Spin Liquids (QSLs) are the exotic phases of matter characterized by fractionalised excitations and the absence of long-range magnetic order. One intriguing route to realizing a nontrivial QSL is by generalizing conventional SU(2) spin systems to SU(N) spin systems with N > 2 [1]. Recent theoretical studies[2] have suggested an emergent SU(4) symmetry in honeycomb lattice α-$ZrCl_3$ by considering an indirect Zr-Zr hopping mechanism through the intermediate Cl p states. In contrast, our first-principles calculations[3] reveal dominance of direct metal-metal d-d hopping, which modifies the underlying model.

Building on this input, we derive an effective spin Hamiltonian for J = 3/2 quartets in the infinite SOC and strong-coupling limit (U/t >> 1). Despite the breaking of explicit SU(4) symmetry by hopping and SOC, a gauge transformation restores an effective SU(4)-symmetric Hubbard form. Further, using the fermionic mean-field approach, we compute the dynamical spin-structure factor revealing the gapless-fractionalized excitation. This results in spectral features that can be accessed via inelastic neutron scattering experiments allowing us to distinguish QSLs arising from the indirect and direct hopping mechanism.

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The talk is based on the works [3] and [4]

Poster 19

Electronic Structure of the Mixed Compounds, $Ca_{1-x}La_xFe_{1-x}Mn_xO_3$

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The unusually high valence state of Fe^{4+} ions in $CaFeO_3$, despite their orbital degeneracy (t^3_{2g} – e^1_g), remain free from the Jahn-Teller effect, unlike isoelectronic Mn^{3+} in $LaMnO_3$ [1,2]. In the case of $CaFeO_3$, this orbital degeneracy is overcome by Breathing Mode distortion, resulting in charge disproportionation [3]. To investigate the interplay of these structural and electronic properties, the first-principles density functional theory (DFT) calculations were carried out in the plane-wave basis with projector augmented-wave potentials [4], as implemented in the Vienna Ab initio Simulation Package (VASP) [5]. We explored the mixed compounds $Ca_{1-x}La_xFe_{1-x}Mn_xO_3$ (x = 0.25, 0.50, 0.75) [6, 7, 8, 9], where intersite charge transfer from Mn to Fe results in non-degenerate electronic states for both Mn ions (Mn^{4+}: t^3_{2g}) and Fe ions (Fe^{3+} : t^3_{2g} e^2_g). Our findings reveal a transition from an insulating parent phase to a half-metallic state at x = 0.25 and 0.75 [10], while it remains insulating at x = 0.50. Additionally, a local structural study uncovers atomic-scale phase separation in La, Mn- and Ca, Fe-rich regions driven by strong Fe-O covalency [11]. Magnetic calculations indicate ferromagnetic ordering in the half-metallic state, whereas an A-type antiferromagnetic ordering emerges in the insulating phase[12, 13, 14]. The origin of these magnetic states is attributed to a kinetic energy-driven mechanism, offering insights into the complex electronic and magnetic behavior of these materials.

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Poster 20

Probing Carrier–Lattice Interactions in $CsCuX_3$ via Femtosecond Spectroscopy

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Understanding carrier dynamics in halide perovskites is essential for assessing their suitability for optoelectronic applications. In this work, femtosecond transient absorption (fs-TA) spectroscopy, analyzed through both spectral and temporal domains, is employed to investigate charge carrier kinetics and relaxation pathways in $CsCuBr_3$, $CsCuCl_3$, and mixed-halide $CsCu(Cl_xBr_{1-x})_3$ perovskites. Global analysis of the transient absorption data enables identification of the nature of photoexcited carriers and their relaxation channels. The fs-TA measurements reveal ultrafast cooling of hot excitons followed by intraband relaxation processes. The carrier dynamics in the mixed-halide compositions closely resemble those of $CsCuBr_3$, exhibiting similar spectral signatures and relaxation timescales. In contrast, $CsCuCl_3$ shows a weak periodic modulation in the kinetic traces at probe wavelengths of 460–475 nm. Fourier analysis of the residual oscillations identifies a low-frequency component (~5–6 cm^{-1}), which is attributed to coherent lattice vibrations involving Cs^+ and Cl^- ions. Notably, such oscillatory behaviour is absent in the mixed-halide systems. These results provide important insights into the interplay between excited-state dynamics and lattice degrees of freedom in copper-based halide perovskites, offering guidance for tailoring their properties for optoelectronic applications.

Poster 21

Intrinsic Nonlinear Anomalous Hall Response Induced by Broken C_{3z} Symmetry in Bi_2Se_3|MnTe Heterostructure

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Materials with preserved PT symmetry lead to both the linear anomalous Hall effect and all Berry curvature–dependent extrinsic contributions to the nonlinear Hall response vanishing identically[1]. Nevertheless, a finite intrinsic second-order anomalous Hall (ISAH) response can still occur, arising solely from the quantum-metric properties of the Bloch bands. In the presence of three-fold rotational symmetry (C_{3z}), the ISAH response is forbidden in PT symmetric system[2]. A finite intrinsic Hall response requires the breaking of C_{3z} symmetry. We have found that the Bi_2Se_3|MnTe heterostructure[3], in which the three-fold rotational symmetry C_{3z} is intrinsically broken, provides a natural and highly tunable platform for exploring quan tum geometry-driven electronic responses. Breaking the C_{3z} symmetry at the interface removes important symmetry constraints that typically forbid intrinsic second-order Hall response tensors in PT -symmetric materials. As a consequence, geometric quantities such as the quantum metric dipole and Berry-connection polarizability dipole become finite. These geometric tensors directly contribute to nonlinear phenomena such as ISAH response[4]. The Bi_2Se_3|MnTe interface thus enables the controlled manipulation of the electronic quantum geometry via structural asymmetry, layer thickness, and interfacial exchange strength. This makes the heterostructure a promising experimental platform for realizing quantum geometric responses that are otherwise symmetry forbidden in pristine Bi_2Se_3.

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Poster 22

Title : To be announced

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