National Conference on Electronic Structure

NCES –2019

27th–29th November 2019

Organized by

S. N. Bose National Centre for Basic Sciences

J. D. Block, Sector III, Salt Lake,

Kolkata, West Bengal, India

In Association with the National Convening Institutes

Novel magnetic and transport anomalies in AlB_2-derived ternary rare-earth intermetallics

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We have been working on AlB_2-derived hexagonal (honey-comb type) ternary rare-earth compounds of the type, R_2TX_3 (T= Transition metal ions, X= Si, Ge) for the past 25 years, making pioneering contributions to various aspects in condensed matter physics (Kondo lattice and heavy-fermion phenomena, valence fluctuations, giant magnetocaloric effect, large magnetoresistance, geometrically frustrated magnetism, superconductivity, low-dimensional magnetism etc). In this talk, I will briefly focus on two unexpected findings: (i) Ferromagnetism in Nd_2PdSi_3, unlike in other members of this rare-earth family and the role of Nd 4f hybridization (relatively less known) on this magnetic anomaly, and (ii) anomalous transport behavior including non-monotonous Hall resistivity (as a function of magnetic field) reported by us two decades ago on Gd_2PdSi_3, which is being interpreted in terms of 'magnetic skyrmions' by Tokura's group recently; we therefore stress that, ex post-facto, our work two decades may serve as the first experimental demonstration of 'Topological Hall Effect' in the context of 'magnetic skyrmions'.

Ballistic transport in topological materials

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In this talk, we shall discuss ballistic transport of junctions made out of topological materials such as Weyl and multi-Weyl semimetals and those which hosts effective pseudo-spin one fermions as their low-energy quasiparticles. For junctions made out of Weyl and multi-Weyl materials, we shall show that the junction conductance G can be independent of the barrier potential in the thin barrier limit. This constitutes qualitatively different behaviour of G for conventional or 2D Dirac junctions. For junctions made out of materials hosting pseudospin one fermions, we demonstrate perfect collimated transport for special values barrier potential. All of these properties are shown to be consequences of topological properties of quasiparticles controlling transport in such junctions.

Wigner Lattice or Charge Density Wave formation in low-dimensional materials

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Electron ordering can be observed particularly in low dimensional materials either due to Wigner lattice (WL) formation when long-range coulomb repulsion dominate over kinetic energy or due to charge density wave (CDW) formation as a result of electron-phonon and electron-electron interaction in crystals. Such ordering give rise to the fascinating fundamental physics [1-4] that can be applied in the development of variety of technologies including energy storage devices. Although formation of WL and CDW arise from different physics, the resultant characteristics including resistance switching transition giving Metal-Insulator transformation is similar in both ordering as electron modulation period in WL coincides with $4k_f$ CDW for crystalline materials [3,4]. Fascinating ARPES studies are being done on low-dimensional crystalline materials to differentiate between WL and CDW formation [4,5]. Non crystalline materials like polymer nanowires have exhibited electron ordering and associated switching transition of resistivity similar to insulator-to-metal sliding transition with CDW gap in crystalline materials [6,7]. Here we discuss that CDW gap can be tuned continuously by tuning the electron density in these nanowires with optical excitation. Observed linear dependence of CDW-gap with optical intensity provide further evidence of one-dimensional WL formation in these nanowires as predicted in Hartree-Fock theory of Wigner crystals [8].

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Debates on Excitonic Magnetism in spin-orbit coupled *J*=0 Iridates

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Investigation of elementary excitations has advanced our understanding of many-body physics governing most physical properties of matter. Recently spin-orbit excitons have drawn much attention, whose condensates near phase transitions exhibit exotic physical phenomenon [Nat. Phys. 13, 633 (2017)]. These critical transition points resulting from competing spin-orbit coupling (SOC), local crystalline symmetry and exchange interactions, are not obvious in Iridium based materials, where SOC prevails in general. Here, we present results of resonant inelastic x-ray scattering (RIXS) on a spin-orbital liquid $Ba_3ZnIr_2O_9$ and three other 6H-hexagonal perovskite iridates which show magnetism, contrary to non-magnetic singlet J=0 ground state expected due to strong SOC. Our results show that substantial hopping between closely placed Ir^{5+} ions within Ir_2O_9 dimers in these 6H-iridates, modifies spin-orbit coupled states and reduces spin-orbit excitation energies. Here, we are forced to use at least a two-site model, to match the excitation spectrum going in line with the strong intra-dimer hopping. Apart from SOC, low energy physics of iridates is thus critically dependent on hopping, and may not be ignored even for systems having moderate hopping, where the excitation spectra can be explained using an atomic model. SOC which is generally found to be 0.4-0.5 eV in iridates, is scaled in effect down to ~0.26 eV for the 6H-systems, sustaining the hope to achieve quantum criticality by tuning Ir-Ir separation.

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Machine-learning Assisted Prediction of Magnetic Double Perovskites

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Magnetism is an important property of materials that plays key role in many different applications. In the present study,[1] we used a combination of computational tools; machine learning technique for screening of stable candidates, evolutionary algorithm for crystal structure determination, and first-principles calculations for characterization of electronic and magnetic properties, to make predictions on magnetic double-perovskites, which are yet-to-be synthesized. Out of 412 scanned candidates of $A_2BB'O_6$ composition with 3*d* and 4*d* or 5*d* transition metals at B and B' sites, we found 33 compounds to form in stable double-perovskite structure, 25 of which were further considered for characterization of their structure and properties. Our exercise predicted 21 double-perovskites of varying magnetic and electronic properties, ranging from ferromagnetic half-metals to ferri- and antiferro-magnetic insulators to ferromagnetic metals and rare example of antiferromagnetic metals. Our computational study is expected to help in discovering new magnetic double perovskites.

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Antiferromagnetism in Cubic Antiperovskites

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ABSTRACT

Magnetic spins arranged in a triangular lattice with antiferromagnetic interactions of equal strength between them is a recipe for frustration. A compromise order is achieved with magnetic spins aligning non collinearly at 120^{o} with respect to each other. In cubic antiperovskites like X_3AB, where X is a transition metal like Mn, A are main group elements like Ga, Ge, Sn, etc. and B are nonmetals like C, N, etc. Here even though the Mn atoms occupy the face-centred sites of a cube, antiferromagnetic order is stabilized via a cubic-cubic volume expanding first-order magnetic transition. Through a series of experiments exploring magnetism, structure and especially local structure around metal atoms in Mn-based antiperovskites like Mn_3GaC, Mn_3SnC, Mn_3InC, we attempt to understand the mechanism of the magnetostructural transition that leads to stabilization of collinear antiferromagnetic order. Our results show that the magnetic ground state of these antiperovskites is therefore dependent on the structural distortion of Mn_6C octahedra. Such distortions of the Mn sub-lattice in these antiperovskites results in short and long Mn–Mn bonds. The Mn-Mn bond distances shorter than 2.75 Å aid in antiferromagnetic order while those longer than 2.75 Å support ferromagnetic order. Further, the magnitude of distortion seems to depend on the available free space for the Mn6C octahedra within the cubic cage formed by A-site atoms.

First principles molecular dynamics simulations of pressure and temperature induced structural transitions in $MAPbBr_3$

Recently, there has been a growing interest in a new class of solar cells based on organo-halide lead perovskite due to their superior photovoltaic performances [1]. Methylamine lead bromide perovskite ($MAPbBr_3$) is one of them, having different stable phases (*Pm-3m, Im-3, Pnma,* etc.) at different temperature and pressure [2-4]. In this work, we employ *ab initio* molecular dynamics to obtain equilibrium structural and dynamical properties of different phases at different temperature and pressure conditions. In particular, the focus of the present talk is on the pressure driven structural transitions at 300 K observed in this system. We have explored the nature of ordering of methylamine dipoles in different phases by defining suitable order parameters and show that rotational degrees of freedom of the cations get restricted by applying pressure. Our atomistic simulations allow us to directly capture the correlations between the MA ordering and lattice distortions, characterize the nature and dynamics of the hydrogen-bonds between MA and the halide sublattice, as well as describe electronic changes that are induced along the transitions, thereby yielding insights into the driving force behind the structural transitions. Our work demonstrates that the complete temperature-pressure phase diagram of $MAPbBr_3$ can, in principle, be obtained from *ab initio* molecular dynamics.

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Carbon Allotropes as Anode Material for Lithium-Ion Batteries

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Abstract:

Anode materials that exhibit high energy density, high power density, long life cycle, and better safety profile for lithium-ion batteries are necessary for the development of electric vehicles. The novel morphology (different ring type) and mixed hybridization (sp, sp^2, and sp^3) have paved a way to the design and fabrication of suitable nanostructured new carbon allotropes based anode materials for high energy density and power density LiBs. These structures contain mixed Pentagon(5), Hexagon(6), Heptagon(7), Octogon(8) carbon ring with mixed hybridizations that exhibit the highest capacity at the cost of relatively moderate volume expansion. For the past decade, the unique mixed (s and p orbital) hybridized design of new carbon-based anode materials, including the above examples, has been the talk to advance the electric vehicle application. I will address about the need of new host materials in Li-S batteries.

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Extreme sensitivity of the hexatic vortex fluid in **a** *a*-MoGe films to radio-frequency electromagnetic perturbation

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Recently, detailed scanning spectroscopic imaging revealed that the vortex lattice in a very weakly pinned *a*-MoGe thin film melts in two steps, first from a vortex solid to a hexatic vortex fluid and then from a hexatic vortex fluid to an isotropic vortex liquid. In this talk, I will show that this that, the resistance in the hexatic vortex fluid state is extremely sensitive to extremely radio-frequency electromagnetic perturbation. In the presence of very low-amplitude excitation above few kilohertz, the resistance increases by several orders of magnitude and eventually reaches a value close to the Bardeen-Steffen limit. On the other hand when the superconductor is well shielded from external electromagnetic radiation, the dissipation in the sample is very small and the resistance is below our detection limit.

Strain induced Electronic Patterns on Graphite Surface

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Abstract: An STM's topographic image is composed of the electronic as well as the topographic variations. While various topographic patterns on different scales can be conceived easily, the electronic patterns of sub-micron length scales arise mainly from chemical inhomogenieties, lattice deformation, strong correlation effects or quantum effects. We have observed a variety of large scale patterns on HOPG surface. I plan to review a few of these patterns such as Moirè patterns with spatial variations, and buckling of a layer originating from a defect. Both exist because of defect induced strain and give rise to both topographic and electronic contrast in STM and STS maps, respectively. We have also taken some local spectra that correlate well with the observed patterns. While the origin of the patterns is fairly clear, the detailed spatial variation of the measured spectra is yet to be modeled and understood.

Half-metallicity versus Symmetry in Pt, Ni and Co-based Half Heusler Alloys: An ab-initio study

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Using first principles calculations based on density functional theory, we study the geometric, electronic, and magnetic properties of Pt, Ni and Co-based half Heusler alloys, namely, PtBC, NiBC and CoBC (B = Cr, Mn and Fe; C = Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te). We calculate the formation energy of these alloys in various crystal symmetries, which include, the cubic C1_b (F-43m), orthorhombic (Pnma), as well as hexagonal (P-62m and P6_3/mmc) structures. It has been observed that out of the alloys studied, only 18 are energetically stable in cubic lowest energy structure. These alloys are primarily having either a C atom or an A atom with a high atomic number. We also observe that along with the alloys with C atoms from group IIIA, IVA and VA -- alloys with C atoms from group VIA are also found to be, by and large, energetically stable. Further, among energetically the most stable cubic alloys, only CoMnSb, CoMnTe and NiMnSb show half-metallic property. From the theoretical calculations, many of the half Heusler alloys are reported to be half-metals in cubic phase, but these are synthesized in non-cubic structures. We analyze the magnetic moment, the electronic density of states and the spin polarization at the Fermi level, in detail to find whether a material in the non-cubic lowest energy structure exhibits half-metallicity or not. Based on these analyses, the possibility of existence of a one-to-one relationship between the cubic symmetry and the half-metallicity in these half Heusler alloys is explored. We predict about the existence of a new non-cubic half Heusler alloy with a substantially low density of states at one of the spin channels and subsequently a reasonably high spin polarization at the Fermi level. However, it is found that for alloys in the lowest energy structure, cubic symmetry is necessary for 100 % spin polarization.

Electronic structure of topological materials

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The discovery of topological materials has created tremendous attention in the scientific community and beyond because these materials can exhibit a novel state of matter in which topologically protected gapless states on their edges or surfaces are present. Such states are protected from scattering by impurities and thus have important technological applications. The rare-earth monopnictide LaBi, LaSb exhibits very large, unusual magnetoresistance which stimulates the interest in directly observing any topological surface states. Although band inversions have been postulated to induce a topological phase in LaBi but there was no experimental evidence for topological surface states in this compound. By using angle-resolved photoemission spectroscopy (ARPES) and *ab-initio* calculations, we have revealed the existence of topological surface states of LaBi through the observation of three Dirac cones: two coexist at the corners and one appears at the centre of the Brillouin zone[1]. The odd number of surface Dirac cones is a direct proof of the topological nature of LaBi compound. In my recent work, six fold degeneracy has been observed at the crossing point in PdSb2 compound in contrast to Dirac and Weyl semimetals.

Helical anomaly in symmetry-broken topological phases

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Symmetry breakings in topological phases lead to novel anomalies, such as chiral anomaly in Weyl semimetals, axion anomaly in topological antiferromagnets and so on. More importantly, such anomalies govern novel physical properties including negative magnetoresistance, electromagnetic response with unique applications. In this talk, I will introduce another novel anomaly, namely, helical anomaly in 2D topological insulators with various time-reversal breaking perturbations. The helical anomaly arises from the survival of the Z_2 topological phase in the parent time-reversal invariant system despite the loss of this symmetry. As a result, external electromagnetic fields introduce anomaly in the helical charge and helical current – an analog of chiral charge and chiral current in chiral anomaly cases. I will discuss these results in the context of apparent breakdown of the *ten-fold way* classification of the topological phases and introduce a novel CPT (where C = charge conjugation, P = parity, and T = time-reversal symmetries) invariance criterion to describe the topological phases with broken symmetries.

Spin-resolved Spectroscopic Imaging in Antiferromagnetic Mott Insulator

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A Mott insulator characterized by localization of electrons due to strong electron–electron interactions, is typically accompanied by magnetic ordering. The antiferromagnetic Mott insulator has been of particular interest as the low-temperature ground state of numerous transition metal oxides, most notably cuprate high temperature superconductors. Charge carrier doping can gradually suppress this insulating state, a process theoretically expected to lead to inherent phase separation. Understanding the relationship between the insulating state with a charge gap and the magnetic order in an antiferromagnetic Mott insulator remains difficult due to inherent phase separation as the Mott state is perturbed. Up to now, most information on the magnetic structure of strongly correlated electron systems has been obtained by bulk sensitive neutron scattering. Measuring magnetic and electronic properties at atomic length scales would provide crucial insight, but this is yet to be experimentally achieved. Here, we use spin-polarized scanning tunnelling microscopy (SP-STM) to visualize the periodic spin-resolved modulations originating from the antiferromagnetic order in a relativistic Mott insulator and how they change as a function of doping. We find that near the insulator-to-metal transition (IMT), the long-range antiferromagnetic order melts into a fragmented state with short-range correlations. Crucially, we discover that the short-range antiferromagnetic order is locally uncorrelated with the observed spectral gap magnitude. This suggests that static short-range antiferromagnetic correlations are unlikely to be the cause of the inhomogeneous closing of the spectral gap and the emergence of pseudogap regions near the IMT.

Research in collaboration with H. Zhao & I. Zeljkovic, supported by SRG-SERB, DST and JTF Foundation.

Theoretical modelling of low-dimensional spin systems

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In low-dimensional spin systems, the magnetic interactions are confined to one and two dimensions. In such systems, quantum fluctuations are more pronounced and the interaction of electrons with each other and with other degrees of freedoms gives rise to new phenomena that are very different from those familiar in three-dimensional systems. These systems give unique possibility to study ground and excited states of quantum models, possible new phases of matter and the interplay of quantum fluctuations and thermal fluctuations. A combination of first-principles based simulations and model calculations has the capability to provide deep physical understanding of the nature of electronic and magnetic states of such spin-systems.

In this talk, I will present the results of our theoretical investigations for various real materials compromising spin trimers, weakly coupled spin dimers and frustrated spin chains. The available experimental results will be compared in order to emphasize the significance of various interaction-terms of the model Spin-Hamiltonian. Our focus will also remain on finding a minimal model to understand the physics of such novel spin systems with regard to their physical properties in reduced dimensions.

Hard X-ray photoemission to study surface-bulk differences in electronic structure

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Understanding exotic solids is a difficult task as interactions are often hidden by the symmetry of the system. Here, we study the electronic properties of a noncentrosymmetric solid, BiPd, which is a rare material exhibiting both superconductivity and topological phase of matter. Employing high resolution photoemission spectroscopy with photon energies ranging from hard x-ray to extreme ultraviolet regime, we show that hard x-ray spectroscopy alone is not enough to reveal surface-bulk differences in the electronic structure. We derived the escape depths close to the extreme surface sensitivity and find that the photon energies used for high resolution measurements such as ARPES fall in the surface sensitive regime. In addition, we discover deviation of the branching ratio of Bi core level features derived from conventional quantum theories of the core hole final states. Such paradigm shift in core level spectroscopy can be attributed to the absence of center of symmetry and spin-orbit interactions.

Electronic Structure of Mo and W based transition metal dichalcogenides

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The ability to isolate a monolayer of graphene has led to a flurry of interest in layered materials. Subsequently artificially formed heterostructures of these solids where the coupling is a weak van der Waals interaction between the layers have been examined. Unusual phenomena have been found in the heterostructures which are absent in the monolayers comprising them. In this talk I will consider the transition metal dichalcogenides, and examine the electronic structure of the bilayers cut out of the structure which is favoured in the bulk. This sets up the model for the description of the electronic structure of these systems[1]. We will then examine the modifications in the electronic structure when we allow for rotations of the top layer with respect to the lower layer. Considering arbitrary angles of rotation, we find certain 'symmetries' emerging [2]. The origin of these as well as their consequences will be discussed.

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2. Poonam Kumari, Joydeep Chatterjee and Priya Mahadevan, (submitted).

Quantum Phase Transitions in Magnets, Ferroelectrics and Beyond

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Abstract: Phase transitions are ubiquitous in nature -- water turning to steam is an everyday example. A special kind of phase transition can occur at zero temperature by changing a non-thermal control parameter. Such a quantum phase transition is the driver for exotic quantum critical physics that extends to elevated temperatures [1]. In this talk, I will begin by introducing quantum phase transitions in magnets, which have been widely explored [2]. I will next discuss, the very recently established, ferroelectric quantum critical behavior [3]. Finally, I will present the concept of multiferroic quantum criticality -- in which both magnetic and ferroelectric quantum criticality occur in the same system -- that we have recently proposed [4]. I will describe the associated experimental signatures and material systems to realize it, and highlight possible future directions.

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Interplay of lattice distortion and electronic structure in $BaBiO_3$

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In this talk, I will present the investigation done on room temperature core level and valence band spectra of $BaBiO_3$ using x-ray photoemission spectroscopy and band structure calculations. The features in the valence band spectrum were studied using Density functional theory (DFT) under local density approximation (LDA) and Tran Blaha Modified Becke Johnson (TB mBJ) exchange potential. The calculations were performed for three different structural parameters; monoclinic, cubic and monoclinic (M'). Our results of the core level spectrum and DFT calculations rule out charge disproportionation of the Bi ions. The valence band spectrum displays gap at the Fermi edge and fine structures in the region close to the Fermi edge. The DFT calculation under TB mBJ for the monoclinic structure is able to generate gap and match the energy positions of the fine structure in a better way. Our calculation results show that there are holes in the O $2p$ states and unequal transfer of electrons to the states of the Bi ions. Such mechanism could lead to bond disproportionation and its association with the fine structures in the valence band. The current results reveal the significance of strong link between the lattice distortion and electronic structure and hence to its physical properties.

Influence of orbital selective Mott phase on electronic structure and ordered phase

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Orbital selective Mott transition (OSMT) are shown by certain strongly correlated electronic systems where electron correlations lead to a larger suppresion of quasiparticle weight for certain orbital symmetries. Materials showing this property are characterized by strong but anisotropic band renormalizations and show characteristic incoherent features in experiments such as ARPES. It has been argued that OSMT can be tuned by external strain, and can have profound influence on ordered phases like superconductivity, and density wave transitions. In this talk, I will discuss the influence of orbital selectivity on ordered phases in correlated material systems and present some of our recent theoretical work on modelling the spectroscopic signatures on such systems.

Variable energy photoelectron spectroscopy to study perovskite nanocrystal

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All inorganic cesium lead halide ($CsPbX_3$, X = Cl, Br, and I) perovskite nanocubes (NCs) exhibit fascinating optical and optoelectronic properties [1, 2]. Post-synthesis anion exchange by mixing NCs with reactive anion species have emerged as a unique capability of $CsPbX_3$ perovskite NCs to fine control their composition and bandgap. Understanding such anion exchange reactions is essential for both fundamental understanding and optimized applications. However, the internal structure of the anion exchanged NCs are not probed. It is largely believed that the anion exchanged NCs possess a homogeneous composition.

In this talk, we will first discuss about the surface of $CsPbBr_3$ NCs and the internal heterostructure that exists inside the anion exchanged $CsPbX_3$ (X = Br/I, and I) NCs probed by variable energy hard X-ray photoelectron spectroscopy. Our results show that for pure $CsPbBr_3$ NCs, there is an excess of bromide ion on the surface of the NCs. We further probed how the ligands replace the Cs ions from the surface of the NCs to stabilize the system. Whereas the anion exchange process makes the $CsPbX_3$ NCs as a gradient alloy with higher concentration of the exchanged anion at the surface of the NCs. A significant amount of native anions are present at the core of the NCs even optical studies suggest a complete anion conversion. The insights from this study provide important directions in future understanding about the electronic properties of the anion exchanged $CsPbX_3$ NCs.

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Zero-Field Room-Temperature Skyrmions in Magnetic Multilayers

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Magnetic skyrmions are topologically nontrivial spin textures which we believe can be created in any chiral magnet as a general phenomenon under applied magnetic field. However, there is no guaranty that the required magnetic field exists in reality and one therefore needs alternative routes. Starting with a prototype example of chiral magnet one monolayer Mn on W(001) driven by Dzyaloshinskii-Moriya interaction we show the thermodynamically stabile skyrmion phase by means of calculating magnetic phase diagram. An abruptly high external magnetic field range where skyrmions exist as stable lattice phase and/or metastable isolated phase motivates us to propose supplanting the external magnetic field by inter-layer exchange coupling (IEC) between a reference magnet and a free magnet. The proposed route provides a perspective direction to extend the number of multilayers as a host of zero-field skyrmion even at room temperatures. The tunability of IEC strength in magnetic multilayers allows us to tailor the properties of magnetic skyrmions at room temperature.

Electronic Structure of Low Dimensional Ruthenates

Two-dimensional honeycomb lattice, Li_2RuO_3, undergoes structural transition due to the dimerization of Ru-Ru bond at T_c = 540 K from nearly honeycomb lattice with C2/m monoclinic structure to distorted honeycomb lattice with $P2_1/m$ monoclinic structure with decrease in temperature [1,2]. Results of room temperature photoemission spectroscopy on in-situ fractured samples will be presented. Strong unscreened feature in Ru 3*d* core level is commensurate with the absence of intensity at E_F in the valence band spectra indicating the insulating nature. Ru 4*d* bands extracted from high and low energy photoemission spectra, having different bulk sensitivities, reveal that the surface and bulk electronic structures are very similar in this system. Comparison of Ru 4*d* band with various band structure calculations [3,4] suggests strong correlation among 4*d* electrons leading the system towards Mott insulating ground state.

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Posters

CDW and piezoelectricity in Re-doped $MoTe_2$

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The transition metal dichalcogenides (TMDs) have attracted attention of the condensed matter community due to their exotic quantum properties. $MoTe_2$, the type-II Weyl semimetal is a unique example among TMDs which exhibits various structural forms. The superconducting transition temperature gets enhanced upto 4.1 K upon Re doping in Mo sites. Based on bulk transport and local scanning tunneling microscopy (STM) we will show that Re doping also leads to the emergence of a charge density wave (CDW) phase in $Re_{0.2}Mo_{0.8}Te_2$. In addition, the tunneling I - V characteristics display non-linearity and hysteresis which is commensurate with a hysteresis observed in the change in tip-height (z) as a function of applied voltage . The observations indicate an electric field induced hysteretic switching consistent with piezoelectricity accompanied by the possibility of ferroelectricity in $Re_{0.2}Mo_{0.8}Te_2$.

ABSTRACT

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Interface effects between superconductors and normal or magnetic metals can reveal interesting effects that provide useful information not only about the superconducting state but also lead to new exotic states of matter. For example, at the interface between a superconductor and ferromagnetic metal, proximity effect can cause the cooper pairs to penetrate into the ferromagnetic layer. This results in many interesting effects such as, spatial oscillation of electron density of states, spin valve effect, superconducting critical temperature dependence on the ferromagnetic layer thickness etc. In our work we have studied theoretically a S/F superlattice consists of a d-wave superconductor $YBa_2Cu_3O_{7-\delta}$ and a half metallic ferromagnetic material $La_{1/3}Ca_{2/3}MnO_3$ where a strong penetration of superconductivity has been argued to be the result of formation of equal sin pairing triplet gap. We have found that due to proximity effect a subdominant spin triplet superconducting order penetrates inside LCMO near the interface and also gets induced inside YBCO due to inverse proximity effect. Proximity and inverse proximity effect strongly depend on the thickness of YBCO and LCMO layers. We also found that the triplet superconducting order parameter is likely to be quasi one dimensional due to the four fold symmetry breaking induced by the YBCO chain layers.

Magnetism in Sr_2CrMoO_6 : A Combined Ab-initio and Model Study

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Double perovskites (A_2BBO_6) have drawn enough attention due to their half metallic behaviour which opens up the possibility of designing spintronics materials. We here carried out a microscopic analysis using a combination of first-principles calculation and exact diagonalization study of first-principle derived model to calculate the magnetic properties of the well known half-metallic double perovskite compound, Sr_2CrMoO_6(SCMO) having cubic structure with space group *Fm-3m*, which is a sister compound of the much discussed material Sr_2FeMoO_6(SFMO) . The electronic structure of SCMO , which appears similar to SFMO at first glance, shows non trivial differences. The shift of Cr *d* states with respect to Fe *d* suppresses the hybridization between Cr t_{2g} and Mo t_{2g} driven by the change in charge transfer energy between Cr and Mo sites. This suppressed hybridization in SCMO makes Mo t_{2g} electrons more localized comapre to SFMO. This opens an additional superexchange contribution to magnetism. To explain the high value of the magnetic transition temperature of SCMO in spite of the dehybridization, additional super-exchange contribution has to be taken into account which arises due to the finite intrinsic moment developing at Mo site. We also examine the effect of correlation beyond DFT, through dynamical mean field theory (DMFT) calculations carried out in the Wannier function basis derived from DFT. The DMFT calculations confirm the half-metallicity of SCMO , implying its robustness against correlation effect.

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LEED and ARPES Study of Oxygen Induced Surface Reconstruction and Electronic Structure of Mo(110)

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Abstract: The adsorption of oxygen on Mo(110) surface is studied by a combination of Low Energy Electron Diffraction (LEED) and Angle-Resolved Photoemission Spectroscopy (ARPES) measurements with fine coverage dependence. Oxygen adsorption at Mo(110) surface corresponds to ordering in a single-phase region p(2×2) and in a two-phase coexistence region p(2×1) structure at low and medium coverage respectively. Energy degeneracy of adsorption sites plays a significant role in the occurrence of two-domain structure. For moderately higher coverage, we observe the occurrence of a single-phase p(2×6) structure. Higher temperature oxygen annealing forms Molybdenum oxide (MoO_2) on top of Mo(110) substrate surface. Band structure of clean Mo(110) surface exhibits the presence of *d*-derived surface states in the mid-region of the $\bar{\Gamma}$ to $\bar{N}$ symmetry line. We also observe dispersive bands, including both positive and negative curvature due to adsorption of oxygen on Mo(110) surface. Curvature of the Oxygen induced surface band gets reversed along $\bar{\Gamma}$ to $\bar{N}$ symmetry direction. Dispersive nature of oxygen-induced band increases at $\bar{\Gamma}$ point with increasing oxygen coverage on the Mo(110) surface.

Short-range and long-range order in AFM – FM exchange coupled compound $LiCu_2(VO_4)(OH)_2$

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The presence of both strong interchain and intrachain interactions of an antiferromagnetic as well as an ferromagnetic nature may lead to the appearance of a gap in the magnetic excitation spectrum of $LiCu_2(VO_4)(OH)_2$ as evidenced by the hump in magnetic susceptibility χ at $T^* \approx 30$ K. The temperature range of short-range magnetic order is terminated by the onset of long-range magnetic order at $T_N = 10$ K, which is triggered by substantial interchain exchange interactions. This observation is corroborated by the specific heat, C_p, singularity, electron spin resonance, and nuclear magnetic resonance measurements. The latter reveals a broad distribution of the resonance fields ascribed to the formation of a helix magnetic structure. First-principles calculations allow estimations of both intrachain and interchain exchange interaction parameters, suggesting the implementation of a strongly coupled scenario with competing inter- and intrachain interactions.

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Magnetic Linear Dichroism Studies of CoO/NiO/MgO(001) System

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Antiferromagnetic (AFM) CoO/NiO thin films are grown epitaxially on MgO(001) substrate and investigated by x-ray linear dichroism (XLD). Temperature-dependent measurement confirms that the observed XLD effect in this system originates entirely from the magnetic ordering. The temperature-dependent XMLD measurement indicates that the exchange coupling at the CoO/NiO interface can greatly enhance the Néel temperature of the CoO layer. The XAS of NiL_2 edge shows the spin of the NiO in the system is in-plane.

ABSTRACT

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2H-$NbSe_2$ forms a charge density wave order when cooled below 33.5 K and undergoes a transition to a superconducting state below Tc 7K. Formation of the charge density wave in 2H-$NbSe_2$ has been argued to be the result of strong momentum dependent electron- phonon coupling. Experiments also find that there is a transition from 3Q to 1Q charge ordered phase when the material is subjected to uniaxial strain. The superconducting transition temperature starts decreasing under the application of strain and there is evidence of a non-trivial competition between superconductivity and different charge ordered states. Here we study the competition between charge density wave order and superconductivity in 2H-$NbSe_2$.

Facet Modulation In Perovskite Nanocrystal

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II-VI semiconductor nanocrystals have been extensively studied by soft chemistry method. In addition to a control on the size, one has found modulation of the shape under various experimental conditions. This increases the surface area for similar sized objects and facilitates use in various applications such as catalysis where the increased surface area would imply more active sites. While experiments on hybrid perovskites have found only cubic facets , recently it was shown for CsPbX3 (X= Br,Cl) under certain experimental conditions one found a faceted polyhedron which could be transformed into a hexapod. We will present our recent theoretical studies which examine the stability of different facet and shown how a shape modulation possible [1].

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J. Am. Chem. Soc. , 141, 40, 16160-16168 (2019).

Theoretical identification of Silicene/Graphene heterostructure as anode material for Li-ion batteries

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Anode materials require a basic property such as fast and easy insertion (diffusion) of Li-ion and very low redox potential vs. Li-ion. According to the Li-ion storing mechanism, anode materials can be classified into three categories: (i) alloying (Li alloys with Si, Sn, Ge and Al), (ii) insertion (layered structure e.g. graphite) and (iii) conversion (CoO_2, FeO_2). Current technology is towards the development of composite or heterostructures utilizing same/different categories of materials. The graphite as base materials is common to design composite based anode materials for Li-ion batteries because of its good electronic conductivity and better rate capability (charging and discharging process) and the target is to overcome its limitation of 372 mAh/g theoretical specific capacity.

Using First-principles based calculation we have studied the Li storage properties of Silicon/Graphite and Silicon/Graphene bulk hetrostructures. Three bulk hetrostructures are considered in this work, (i) Si-ML/Graphene (ii) Si-ML/BL-Graphene and (iii) Si-ML/Graphite In case of Si-ML/Graphite hetrostructures the layer staking is in the format of A-B-Si-B-A-B-Si-B, here A and B represent the stacking of Graphite. Whereas, in case of Si-ML/BL-Graphene we follow A-B-Si-A-B-Si-A-B stacking. The specific capacity is estimated to be about 750 mAh/g for SiML/Graphene hetrostructure. For Si-ML/BL-graphene and Si-ML/Graphite the estimated capacity of 529 mAh/g and 476 mAh/g respectively. All the hetrostructures are stable during Li intercalation and de-intercalation process with low diffusion barrier energy of 0.6 - 0.7 eV. We estimated the open circuit voltage, formation energy and volume expansion during Li intercalation and de-intercalation process to understand the structural distortion.

Keywords: Storage, Battery, Anode, Carbon, DFT, LIB's

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Metal-chalcogen bond-length induced electronic phase transition from semiconductor to topological semimetal in ZrX_2 (X = Se and Te)

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Using angle resolved photoemission spectroscopy (ARPES) and density functional theory (DFT) calculations we studied the low-energy electronic structure of bulk $ZrTe_2$, an early transition metal dichalcogenide (TMDC). ARPES studies on $ZrTe_2$ demonstrate free charge carriers at the Fermi level, which is further confirmed by the DFT calculations. An equal number of hole and electron carrier density estimated from the ARPES data, points $ZrTe_2$ to a semimetal. The DFT calculations further suggest a band inversion between Te p and Zr d states at the Γ point, hinting at the non-trivial band topology in $ZrTe_2$. Thus, our studies for the first time unambiguously demonstrate that $ZrTe_2$ is a topological semimetal. Also, a comparative band structure study is done on $ZrSe_2$ which shows a semiconducting nature of the electronic structure with an indirect band gap of 0.9 eV between Γ(A) and M(L) high symmetry points. These observations are in good agreement with earlier ARPES studies on this system, i.e., $ZrSe_2$ is a semiconductor with an indirect band gap [1-4]. In agreement with a previous ARPES report on $ZrSe_2$ [4], a tiny spectral feature near the M(L)-point at a binding of 0.3 eV has been observed. Moreover, an earlier ARPES study on $ZrSe_2$ showed Fermi level lying in between valence and conduction band [5], whereas from our study we found that the Fermi level is moved to the conduction band. Here we show that the metal-chalcogen bond-length plays a critical role in the electronic phase transition from semiconductor to a topological semimetal ingoing from $ZrSe_2$ to $ZrTe_2$.

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arxiv: 1907.03987

Magnetic ground state of distorted $6H$ perovskite $Ba_3CdIr_2O_9$

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(Dated: October 25, 2019)

Perovskite iridates of $6H$ hexagonal structure present a plethora of possibilities in terms of the variety of ground states resulting from a competition between spin-orbit coupling (SOC), hopping, non-cubic crystal field ($\Delta_{\rm CFE}^{\rm NC}$) and superexchange energy scales within the Ir_2O_9 dimers. Here we have investigated one such compound $Ba_3CdIr_2O_9$ by x-ray diffraction, *dc* magnetic susceptibility(χ), heat capacity(C_p) and also ^{113}Cd nuclear magnetic resonance (NMR) spectroscopy. We have established that the magnetic ground state has a small but finite magnetic moment on Ir^{5+} in this system, which likely arises from intradimer Ir-Ir hopping and local crystal distortions. Our heat capacity, NMR, and *dc* magnetic susceptibility measurements further rule out any kind of magnetic long-/short range ordering among the Ir moments down to at least 2K . In addition, the magnetic heat capacity data shows linear temperature dependence at low temperatures under applied high fields ($>$ 30 kOe), suggesting gapless spin-density of states in the compound.

First-principle study on collinear magnetism of Mn_2PtSn Heusler compound

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At the present time, the demand for new advanced materials with different magnetic properties is constantly increasing. Non-collinear magnetism in some alloys and compounds have large probability for applications in spintronic devices. Heusler alloys are famous for their tunable electronic and magnetic properties and according to many experimental reports Mn_2-based Heusler compound shows non-collinear magnetism. Before studying this type of magnetic properties we need to know about collinear magnetic behaviour in these systems. So, this work focuses on different collinear magnetic structures of Mn_2PtSn Heusler compound. We carry out the calculations using first-principle method based on Density functional theory using the software Vienna Ab-initio Simulation Package (VASP).

Keywords: Density fuctional theory, Collinear magnetism, Heusler alloy, VASP

Exploring Spin Valley Physics in Bilayers of MoS_2

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Abstract

Bilayers of MoS_2 in the stacking that is found in the bulk have their valence band maximum at Γ point as well as have no net spin splitting at the K point. The former is attributed to the interaction between the out of plane orbitals of the two layers. One way to bring the valance band maximum back to K point in bilayers is by applying bi-axial compressive strain. This increases the interaction between the in plane orbitals. We determined the amount of strain required to shift the valence band maximum from Γ point back to K point. This was found to be 3.5%. Alternate strategies to reduce the strain will be presented. As the presence of inversion symmetry results in a vanishing spin splitting, we will use twisted bilayers to arrive at a net spin splitting.

f-wave pairing symmetry in YBCO cuprates

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D-wave nature of (superconducting) order parameter is observed in YBCO and other family of cuprate superconductors. In cuprate family, superconductivity is mostly governed by the CuO2 plane. However there exist a metallic CuO chain like one dimensional structure in YBCO. This layer couples to the CuO2 plane via both non-interacting hopping as well as Coulomb interaction. In this work we study the effect of chain state on the pairing symmetry and pairing strength on the plane states. We numerically calculate linearized superconducting gap equation within spin-fluctuation mechanism. We find that above a critical value of the chain-state's doping, keeping all others parameters fixed, the pairing symmetry in the CuO2 plane changes from the *d*-wave to a *f*-wave pairing symmetry. The proposed doping range is within the experimental reach, and thus the observation of f-wave pairing in cuprate setup can add a new feature to the many unique properties of cuprates.

An *ab initio* molecular dynamics approach to determine the low energy structures of titanium nitride (TiN) nanoclusters

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Titanium nitride (TiN) is a promising material in the field of plasmonic activities nowadays. There is already a lot of reports on bulk TiN through experiment and theoretical approaches, but none with detailed investigation on small nanocluster systems to the best of our knowledge. In this work we are predicting the low energy structures of TiN nanoclusters with the help of *ab initio* molecular dynamics. Here we are starting with $(TiN)_n$ where $n = 2, 3$. In future we will go for higher values of n depending upon the computational feasibility. All the calculations are taken at room temperature i.e. 300 K. We have also done simulated annealing to determine the global minima in these systems.

Keywords: nanocluster, ab initio molecular dynamics, titanium nitride, low energy structures

Covalency driven stereochemical lone pair activity and consequent multiferroicity in Pb based langasite compound

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We have investigated the structural, magnetic and dielectric properties of Pb-based langasite compound $Pb_3TeMn_3P_2O_{14}$ both experimentally and theoretically in the light of Pb lone pair activity driven generation of spontaneous polarization. We find that large covalency within Mn - O tetrahedra helps to redistribute the charges among the other cation-oxygen bonds, which in turn induces crucial electronic changes and consequently, the individual elemental magnetic moment gets altered in the system. The Mn-O covalency eventually facilitates the lone pair activity within Pb, which further manipulates the magnetic Mn motif to some extent in order to develop a finite magneto dielectric effect in the system. Our Density functional calculation shows that the covalency within Pb - O assists Pb 6*s* to hybridize with Pb 6*p* as well as O 2*p*, and as a result Pb lone pair takes lobe like structure. Further, the covalency effect within Te-O causes a nonuniform distribution of Te-O bond lengths within TeO_6 octahedra. This charge disproportionation in Pb and Te creates a polar geometry at room temperature. As a result of stereochemical active lone pair in the polar geometry, spontaneous polarization along with magneto dielectric effect are evident in this compound.

Keywords: Covalency, Stereochemical activity, Multiferroic.

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Deposition of superconducting thin films of tungsten using DC magnetron sputtering

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Abstract

Tungsten commonly exists in two forms, α-W and β-W. α-W is bulk superconducting at 15mK and β-W films have been reported superconducting in 1-4 K. It has been shown in the literature that the formation of β-W is aided by the presence of oxygen and nitrogen impurities. In addition, amorphous films of W grown through focused ion beam aided deposition have also been shown to exhibit superconductivity with T_c ranging between 2-4 K.

Here, we will present the synthesis of superconducting W films using d.c. magnetron sputtering. When W films (with thickness ~ 200 nm) are deposited using pure Ar as the sputtering gas, the films either do not show any superconductivity down to 300 mK or occasionally exhibit superconductivity with Tc < 2 K. However, when we introduce ~ 1-3 % N_2 in the Ar/N_2 gas mixture we obtain reproducible T_c in the range 3 – 4.4 K. Higher amounts of N_2, results in the formation of non-superconducting W_2N and a resultant drop in T_c. Structural analysis of the films indicate that these films are not simply β-W but contain a mixture of and β-W, α-W as well an amorphous component. It is unclear at this stage whether the origin of superconductivity is due to β-W or amorphous W or strain in the α-W phase.

Magnetization reversal through vortex nucleation in a single magnetic nano-particle probed using Nb μ-SQUIDs in hysteresis free mode

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Abstract:

The magnetization reversal of an individual magnetic nano-particle (MNP) has been best studied using a μ-SQUID. An optimum inductive shunt helps in eliminating the hysteresis in μ-SQUID's current voltage characteristics, giving thus a direct voltage readout of magnetic flux with high bandwidth and sensitivity. We briefly present a new μ-SQUID magnetometry setup to study the magnetism of individual MNP and techniques to place a single MNP on a μ-SQUID loop. The switching field anisotropy of a single Permalloy ($Ni_{80}Fe_{20}$) nano-needle and single Fe_3O_4 nano-particle was studied. The observed anisotropy in permalloy is described well by magnetization reversal through a curling mode under the Néel-Brown model as well as by micro-magnetic simulations. In both the nano-particles magnetization reversal happens through the vortex nucleation and annihilation which we observe through minor hysteresis loops in experiments supported by micro-magnetic simulations. We also observe multiple pathways of vortex nucleation in switching field histograms and switching probability-vs-time obtained from switching time histograms at a fixed field below the switching field. Intriguingly, the switching time histograms for Fe_3O_4 follow a log-normal distribution which is understood assuming a stepped barrier between two magnetization states. A stretched exponential function that generally describes the lifetimes in relaxation processes does not hold for a stepped single barrier in a single nano-magnet. Many other thermal relaxation processes in different systems may fall under same category, i.e. a stepped barrier due to pinning at defects.

Electronic descriptors and design principles of graphene based electrocatalyst for ORR using QM/ML approach

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The oxygen reduction reaction (ORR) is an important reaction that takes place in the cathode of a fuel cell, wherein molecular oxygen is reduced to water. A descriptor-based approach to identify the best catalysts will simplify the tedious task of experimentally synthesizing and testing all possible combinations of catalysts. With a rising interest in sp2-based carbon materials as catalysts for ORR, it is desirable to understand their chemical activity and its dependence on various configurations of substitutional doping and develop simple predictive models.

Using QM/ML approach, we proposed π–electronic descriptors and developed predictive models using simple fits, multiple linear regression, and random forest regression to identify the best active site. As a model structure, we have considered heteroatom (S, P, SO2, PO2) edge-doped graphene nanoribbons. In DFT analysis, the activity of 112 sites of the 14 structures is considered. Further 26 models, i.e. (4-, 5-, …to 20-) AGNR and (4-, 6-, …to 20-) ZGNR is taken to understand the effect of nanoribbon width. We have shown that the QM/ML approach is more efficient towards the searching of highly active catalysts for ORR, through reducing the computational cost and improving the prediction capability.

Keywords: ORR, carbon, adsorption, fuel cell, electrocatalyst, DFT

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Domain structure dynamics in the ferromagnetic Kagome-lattice semimetal $Co_3Sn_2S_2$

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$Co_3Sn_2S_2$, a Weyl semimetal that consists of layers of Kagome lattices, transitions from a high temperature paramagnetic phase to a low temperature ferromagnetic phase below 177 K. The phase transition occurs through an intermediate non-trivial magnetic phase just below the Curie temperature. The intermediate phase was earlier linked with a competing anti-ferromagnetic phase, a spin-glass phase and certain indirect measurements indicated the possibility of magnetic Skyrmions in this phase. We have imaged the magnetic domain structure in a single crystal of $Co_3Sn_2S_2$ at different temperatures, magnetic fields and field-angles by magnetic force microscopy. At low temperatures, we observed stripy domains indicating presence of uniaxial anisotropy. Above 130 K, the domain walls become mobile and they tend to align relatively easily when the magnetic field is increased in the $a-b$ plane than along the c-axis. Our detailed study of field-dependent domain dynamics reveals that the anomalous nature of the phase transition just below T_c is dominantly governed by domain wall motion. We also observed significant decrease in the fraction of ferromagnetic domains above 160 K which might indicate the emergence of local anti-ferromagnetic puddles as indicated by previous μSR experiments.

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Polymerization of acrylamide under pressure: A first principles study

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Abstract:

Polymerization of acrylamide, a hydrogen bonded molecular crystal, induced by pressure has been reported previously indicating onset of possible polymerization at ~20 GPa [1]. However, there exists controversy in literature about changes of hydrogen bonded network with pressure [2]. The modes and mechanism of polymerization are still unknown. In this presentation, we employ Density Functional Theory (DFT) to investigate the process of polymerization. We clarify that subtle reorientation of hydrogen bonding occurs at ~4 GPa. For a defect-free crystal, static compression and dynamic compression lead to occurrences of polymerization at higher pressure, for instances, at ~67 GPa and ~98 GPa. These two different modes of polymerization occur through different pathways in potential energy surface. The phonon study explains the dynamical stability of various polymers. Good agreement is found between pressure dependent experimental IR-Raman frequencies and calculated phonon frequencies from density functional perturbation theory (DFPT). The changes in various phonon modes with pressure in both types of compression are correlated with structural changes. The thermodynamic stability and thermal stability of polymers are compared and it is shown that both type of polymerisations could be achievable by modelling experimental conditions using *ab initio* molecular dynamics.

References:

[1] Sharma et al. J. Raman Spectrosc. 2013, 44, 785–790

[2] Bhatt et al. Spectrochim. Acta A. 2017,185, 45–51

Title: Flourination of Oxygen deficient compound $CaMnO_{2.5}$: A Possible route to Multiferroicity

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Abstract:
Perovskite materials are being studied since years due to their wide variety of physical, chemical and magnetic properties. In recent time, mixed anion compounds along with oxygen deficient compounds of the perovskites are drawing attention in Solid State Physics due to their unique properties and a range of new structures.

In this work, we chose the oxygen deficient compound, $CaMnO_{2.5}$ with square pyramidal environment of Mn, and studied its properties upon flourination. Our first-principles density-functional theory calculations, established stabilization of a unique up-up-down-down magnetic configuration in the un-flourinated compound with strong magneto-structural coupling, akin to that found in compounds like $HoMnO_3$[1]. This establishes promise of these compounds as possible materials showing coupling between electron, spin and lattice degrees of freedom. Upon flourination, we found that F occupies both the interstitial site of the missing oxygen position of metal-oxygen octahedra, driven by the tendency of Mn to be in octahedral environment instead of square pyramidal environment as well as the substitutional oxygen site in the square pyramid. This results in Mn valency in flourinated compound close to 3+. The resultant structure of the flourinated compound breaks the inversion symmetry of the crystal, through off-centric movement of F atom in the interstitial, which makes the compound polar with finite polarization. This together with strong magneto-structural coupling holds promise of the compound to be high temperature multiferroic.

Work carried out in experimental collaboration with Prof. Sugata Ray.

Reference:
1. S.Picozzi,K.Yamauchi,B.Sanyal,I.A.Sergienko and E. Dagotto,PRL,2007,99,227201.

Low Energy Electron Microscopy Investigation of First Order Phase Transition on Si(111) Surface

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Abstract. The surface phase transition from the low temperature reconstructed (7x7) phase to the high temperature (1x1) phase of the Si(111) has been studied by Low Energy Electron Microscopy (LEEM) and Low Energy Electron Diffraction (LEED) technique. The phase transition is found to be reversible and is of first order. Furthermore, in the LEEM, we detect the nucleation of triangular (7x7) domains from the terrace edges and these domains almost cover the whole surface when the temperature is reduced from transition temperature. We observe that upon quenching surface from very high temperature, it does not completely transform to (7x7) structure because of the destruction of mechanical stress on the surface.

Event : NCES 2019 Poster Presentation

Title : Spectroscopic Signature of two Superconducting Gaps and Their Unusual Field Dependence in RuB_2

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Abstract : Recently, RuB_2 was reported to be a possible two-gap, type-I superconductor. Temperature dependent heat capacity measurements revealed a two-gap superconducting ground state while magnetic field dependent magnetization measurements indicated surprising type-I superconductivity with a very low experimental critical field H_C=120 G. Here, we present direct spectroscopic evidence of two superconducting energy gaps in RuB_2. We have measured scanning tunnelling spectra exhibiting signature of two gaps on different grains of polycrystalline RuB_2, possibly originating from multiple bands. Analysis of the temperature dependent tunnelling spectra revealed that the gaps from different bands evolve differently with temperature before disappearing simultaneously at a single T_C. Interestingly, our experiments also reveal that the gaps in quasiparticle density of states survive up to magnetic fields much higher than the bulk H_C and they evolve smoothly with field, unlike what is expected for a type-I superconductor, indicating the existence of a “mixed state”.

Antiferromagnetic Ordering and Kondo Lattice Behavior in Heavy Fermion System Ce_3NiSi_3

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Abstract

We report the low-temperature physical properties of polycrystalline R_3NiSi_3 (R = La and Ce), which crystallizes in orthorhombic (Space group Immm) structure. A detailed study has been performed using electrical resistivity ρ(T), magnetic measurements, and heat capacity measurements, which suggest that Ce_3NiSi_3 orders antiferromagnetically below T_N ~6 K. Electrical resistivity data of Ce_3NiSi_3 resembles with that observed in usual Ce based Kondo lattice/ heavy-fermion(HF) compounds. Electrical resistivity and heat capacity are significantly influenced by the crystal electric field (CEF) effect. The enhanced value of the Sommerfeld coefficient (~118.5 mJ/mol K^2) strongly indicates the HF behavior of Ce_3NiSi_3.

Reference: S Malick *et. al*; JMMM 482 (2019) 108–112

Wannier pairs in the superconducting twisted bilayer graphene and related systems

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The twisted bilayer graphene (TBG) presents a new setting where superconductivity emerges on the flat bands whoseWannier wavefunctions spread over many graphene unit cells, forming the so-called Moir´e pattern. To unravel how Wannier states form Cooper pairs, we study the interplay between electronic, structural, and pairing instabilities in TBG. For comparisons, we also study graphene on boron-nitride (GBN) possessing a different Moir´e pattern, and single-layer graphene (SLG) without a Moir´e pattern. We compute the pairing eigenvalues and eigenfunctions by solving a linearized superconducting gap equation, where the spin-fluctuation mediated pairing potential is evaluated from materials specific tight-binding band structures. We find an extended s-wave as the leading pairing symmetry in TBG. In contrast, GBN assumes a p + ip-wave and SLG has the d + id-wave symmetry. Moreover, while p + ip, and d+id pairings are chiral, and nodeless, but the extended s-wave channel possesses accidental nodes.

[1] S. Ray, J. Jung, and T. Das, Wannier pairs in the superconducting twisted bilayer graphene and related systems, Phys. Rev. B **99**, 134515 (2019)

Interlayer coupling of twisted bilayer $MoSe_2$

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Twisted bilayers of various van der Waals materials have been generated by rotating the upper layer with respect to the lower layer. These have resulted in structures with properties very different from either of the constituent layers. We will present our recent results to understand the evolution of the electronic structure as a function of the twist angle. For large twist angles we find that the low energy electronic structure is very similar to what one has for the 2H stacking.

Starting with bilayers of $MoSe_2$ in its most favoured stacking (2H), one finds that interlayer interactions determine the changes in the electronic structure from what one has for the monolayer. These interactions affect the valence band extrema at Gamma and K points inducing a splitting of this band. However, inspite of large variations in the Se-Se distances in the twisted bilayers, one finds that at large twist angles, the coupling strength between the layers at Gamma point remains invariant, while that at K point goes to 0. The origin of this will be discussed by complementing the results obtained within ab-initio calculations with appropriate tight-binding calculations.

Angle Resolved Photoemission Spectroscopy Study on Electronic Band Structure of Topological Insulator Bi_2Se_3 in the Presence of Magnetic Impurities

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As magnetic ordering in topological insulators (TIs) can break the time reversal symmetry (TRS), the TIs are predicted to open up a band gap at the Dirac point in presence of magnetic impurities. To experimentally observe the effect of magnetic impurities on the electronic structure, we have performed high-resolution angle-resolved photoemission spectroscopy (ARPES) experiments on 3D TI Bi_2Se_3 along with various magnetically doped compounds such as $Co_{0.1}Bi_2Se_3$, $Mn_{0.1}Bi_2Se_3$ and $Eu_{0.1}Bi_{1.9}Se_3$. Though no band gap opening at the Dirac point was observed due to very small amount of doping, a clear shift of Dirac point to higher binding energy was observed. Our measurements show the presence of conducting surface and insulating bulk states for all the compounds and also indicate that all the magnetic elements we doped in Bi_2Se_3 provide additional electrons to the compound which eventually causes shift of the Dirac point.

Growth and Characterization of amorphous MoGe thin films

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We report growth and characterization of MoGe thin films, deposited on thermally oxidized Si substrate using Pulsed Laser Deposition technique (*PLD*) at room temperature. High resolution Transmission Electron Microscopy (HR-*TEM*) studies showed that films are amorphous in nature. Superconducting transition temperature (T_c), sheet resistance (R_s), superfluid stiffness (J_s) are measured as a function of thickness of the film and compared to several theoretical models for disordered superconducting films. Scanning tunneling spectroscopy (*STS*) reveals that films are conventional *BCS* type superconductor for moderate disorder. In addition, it also shows that the suppression of superconducting energy gap (Δ) is much slower as compared to T_c with increasing disorder. This leads to pseudo gap phase in ultra-thin film (thickness ~ 2 nm). Moreover, in the ultra-thin film, we have observed that vortices are in fluid state down to lowest temperature, 280 mK and it is confirmed through electrical resistance measurement as a function of temperature at different magnetic fields where resistance remains finite at the lowest temperature.

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