SCHOOL OF PHYSICAL SCIENCES

INDIAN INSTITUTE OF TECHNOLOGY MANDI

ABSTRACT BOOKLET

National Science Day

CELEBRATING NATIONAL SCIENCE DAY 2023
WITH ONE DAY WORKSHOP IN PHYSICS

One Day Workshop on National Science Day

Feb 28, 2023
School of Physical Sciences, IIT Mandi

Programme

Inaugural Session	Chair: Ajay Soni
9:20 am – 9:25 am	*Lamp lighting and Felicitation*
9:25am – 9:35 am	*Address by the Chair of SPS, IIT Mandi*
9:35 am – 9:45 am	*Address by Director, IIT Mandi*
9:45 am – 10: 35 am *Plenary Lecture*	***Prof. P K Raina**, IIT Ropar.* *Recalling some contribution of Physical Sciences in evolution of Today's Society*
10:35 am – 11:00 am	*High Tea (A1 ground floor)*
Session – I	**Chair: Nirmalya Kajuri**
11:00 am – 11:25 am **I1**	**Krishnamohan Parattu** *Enhanced power on small scales and evolution of quantum state of perturbations in single and two-field inflationary models.*
11:25 am – 11:50 am **I2**	**Rahul Kothari** *Superhorizon Perturbation Modes and Hubble Tension.*
11:50 am – 12:02 pm **O1**	**Sonika** *Low temperature Raman and X-ray diffraction studies on Fe intercalated VSe2.*
12:02 pm – 12: 14 pm **O2**	**Keshav Thakur** *Dynamics of Local density and its relationship with structural local density, cavity forming, FENE polymer via Lennard jones interaction.*
12:14 pm – 12:26 pm **O3**	**Bharat** *Crystal and electronic structure studies of doped barium bismuthates.*
12:26 pm – 12:38 pm **O4**	**Jaskirat Brar** *Lattice effects on the physical properties of half-doped perovskite ruthenates.*
12:38 pm – 12:50 pm **O5**	**Yogesh Khatri** *Prediction of magnetic moment and formation energy per atom of Iron-based compounds using a data-driven machine learning approach.*

12:50 pm – 1:02 pm **O6**	**Anjali** *Realistic model for photoinduced heterogeneous electron transfer.*
1:02 pm – 2:00 pm	Lunch (Recreation Centre, South Campus)
Session – II	Chair: Prabhakar
2:00 pm – 2:25 pm **I3**	**Arko Roy** *A tale of two condensates.*
2:25 pm – 2:50 pm **I4**	**C S Yadav** *Exotic phases in frustrated magnetic systems.*
2:50 pm – 3:02 pm **O7**	**Rashid Shaik** *Plasmonic resonant intercluster Coulombic decay.*
3:02 pm – 3:14 pm **O8**	**Shivani Bharadwaj** *Finding a suitable theoretical approach for better quantification of electronic and magnetic properties correlated electron systems.*
3:14 pm – 3:26 pm **O9**	**Dheeraj** *Evidence of the novel three-dimensional quantum spin liquid state in HoVO4.*
3:26 pm – 3:38 pm **O10**	**Divya** *Many Body Phenomena in Bismuth Chalcogenides Using Light-Matter Interactions.*
3:38 pm – 3:50 pm **O11**	**Vivek Pandey** *PY-Nodes: An ab-initio python code for searching nodes in a material using Nelder-Mead's simplex approach.*
3:50 pm – 4:02 pm **O12**	**Sonu Chillar** *Magnetodielectric coupling as a manifestation of metamagnetic transition and structural distortion in Ba3RRu2O9 (R = Gd, Dy).*
4:02 pm – 5:12 pm	Tea & Poster Evaluation
5:12 pm – 5:40 pm	Vote of Thanks & Prize distribution

One Day Workshop on National Science Day

Feb 28, 2023
School of Physical Sciences, IIT Mandi

Plenary Talk

Recalling some contribution of Physical Sciences in evolution of Today's Society

Abstract: Starting with history of science and the acceptance of natural sciences as the important aspect for societal growth. Recalling the great contributions in last few centuries and Indian contribution to science for last century. I would try to take through the landmark contributions of Physical sciences especially in last more than one century that has changed the society by making S&T as the driving force of development. How we are observing the transition from sharp disciplines to interdisciplinary S&T. Global concerns on science and wellbeing.

Brief bio P. K. Raina is a professor of Physics at IIT Ropar. He finished his Ph. D. from IIT Kanpur, 1987 and has over 30 years of experience in physics teaching and research at IIT Kharagpur and subsequently at IIT Ropar from 2010. He has been a stalwart researcher in the field of Neutrino Physics and Double Beta Decay, Nuclear structure and interactions. He has several national and international collaborations on Double Beta Decay (DBD) Studies from the last 10-15 years with institutions such as TIFR, India and LNGS, Gran Sasso world class Italian Lab. He has authored over 150 articles in journals, invited talks and conferences, supervised eleven PhD students, and completed over ten sponsored R&D projects. In the past he has held several esteemed administrative and research posts at IIT Ropar, NIT Jalandhar, NIT Kurukshetra, PTU, IIT Roorkee. He is the Board of Governors Member, IIT Ropar from 2010. He served as Dean (Academics), IIT Ropar from 2015-19, was Prof. In charge/ Dean (Academics, Research & Faculty) IIT Ropar August 2011-15, and served as the Head of the Physics and Chemistry Departments, IIT Ropar July 2010-15.

Invited Talks

Feb 28, 2023
School of Physical Sciences, IIT Mandi

Enhanced power on small scales and evolution of quantum state of perturbations in single and two-field inflationary models

Rathul Nath Raveendran[1*], **Krishnamohan Parattu[2*]** and L. Sriramkumar[3]

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Abstract: With the detection of gravitational waves from merging binary black holes, over the last few years, there has been a considerable interest in the literature to understand if these black holes could have originated in the early universe. If the primordial scalar power over small scales is boosted considerably when compared to the COBE normalized amplitude over large scales, such an increased power can lead to a copious production of primordial black holes that can constitute a significant fraction of the cold dark matter density today. Recently, many models of inflation involving single or two scalar fields have been constructed which lead to enhanced power on small scales. I shall present results from the work [1], where we examined the evolution of the quantum state of the curvature perturbations in such single and two field models of inflation using the measures of squeezing, entanglement entropy or quantum discord. We found that, in the single as well as the two-field models, the extent of squeezing of the modes is enhanced to a certain extent (when compared to the scenarios involving only slow roll) over modes which exhibit increased scalar power. Moreover, in the two field models, we showed that the entanglement entropy associated with the curvature perturbation, arrived at when the isocurvature perturbation has been traced out, is also enhanced over the small scales. We also took the opportunity to discuss the relation between entanglement entropy and quantum discord in the case of the two field model. I shall end with a brief discussion on the wider implications of the results.

References:

[1] Rathul Nath Raveendran, Krishnamohan Parattu, L. Sriramkumar, General Relativity and Gravitation, 91, 54 (2022).

Dr. K. Parattu,
SPS, IIT Mandi

About the speaker: Dr. Krishnamohan Parattu has completed his bachelor's in science from Christ College, Bangalore, India. He pursued his master's from IIT Bombay. Dr. Parattu has started his research career at IUCAA, Pune, India. During his Ph.D. he worked with renowned physicist Prof. Thanu Padmanabhan. He worked as postdoctoral fellow at IIT Madras, Chennai; UNAM, Mexico City, Mexico; and PUCV, Valparaiso, Chile. Dr. Parattu is currently working as an assistant professor at IIT Mandi, Himachal Pradesh. His primary research includes gravitation and cosmology, quantum information, and mathematical physics. Currently, he is working on the structure of the actions for various theories of gravity and on the application of quantum information theory to cosmological scenarios.

Superhorizon Perturbation Modes and Hubble Tension

Rahul Kothari[1*]

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Cosmology as a discipline of Physics studies the Universe at its largest length scales. The Hubble parameter governs the expansion dynamics of the Universe. Current cosmological observations point to a serious discrepancy between the values of Hubble parameter obtained from CMB measurements and local Universe. We suggest that this anomaly can be explained by invoking the superhorizon modes. Surprisingly, many other observations that imply a violation of cosmological principle, can also be explained by these modes. The superhorizon modes also predict a significant redshift dependence of the dipole signal. I will also discuss how that can be nicely tested using SKAO.

References:

[1] Prabhakar Tiwari, Rahul Kothari, Pankaj Jain, Superhorizon Perturbations: A Possible Explanation of the Hubble Lemaitre Tension and the Large Scale Anisotropy of the Universe, Astrophysical Journal Letters, 924:L36 (5pp) 2022

[2] Shamik Ghosh, Pankaj Jain, Rahul Kothari, Mohit Panwar, Gurmeet Singh, Prabhakar Tiwari, Probing Cosmology beyond LCDM using SKA, to be published in JoAA special edition, Indian participation in the SKA

Dr. Rahul Kothari,
SPS, IIT Mandi

About the speaker: Dr. Rahul Kothari has completed his graduation in science from Indian Institute of Technology, Kanpur. Dr. Kothari has started his research career at Indian Institute of Technology, Kanpur. He worked as postdoctoral fellow at IIT Madras, Chennai; and University of the Western Cape, South Africa. He worked as an assistant professor at Jamia Millia Islamia University, New Delhi, India Dr. Rahul Kothari is currently working as an assistant professor at IIT Mandi, Himachal Pradesh. Currently, his research interests are focused on 21cm Cosmology. Apart from this, he has worked on a wide variety of topics in theoretical physics – Cosmic Microwave Background, Poincaré Gauge Theory, Bouncing cosmology, Hubble tension, etc.

A Tale of Two Condensates

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Cooled to nano-Kelvin temperatures, ultracold dilute atomic gases manifest as macroscopic quantum systems. Observable in experiments, atomic quantum gases give direct access to the physics of quantum phenomena. Pertinent to observations, we shall discuss the effects of non-zero temperature on condensates of dilute atomic gases.

References:
[1] Roy et al., arXiv: 2212.12253
[2] Rajat et al., Phys. Rev. A 106, 013304 (2022)

Dr. Arko Roy,
SPS, IIT Mandi

About the speaker: Dr. Arko Roy completed his Bachelors' in Physics (Hons.), from Jadavpur University, Kolkata and Masters' from IIT Madras. He did his PhD from Physical Research Laboratory (PRL), Ahmedabad. Dr. Roy then worked as a postdoctoral fellow at PRL, Ahmedabad; Max Planck Institute for the Physics of Complex Systems Dresden, Germany; and Pitaevskii Center for Bose-Einstein Condensation, Trento, Italy. He is currently working as an assistant professor at IIT Mandi, Himachal Pradesh. His primary research interests include “Interacting mixtures of quantum gases at finite temperatures”, “Strongly correlated quantum gases in optical lattices”, and “Quantum devices with cold atoms”. Dr. Roy is a referee of international journals, and was recognized as an Outstanding Reviewer of the Year 2020 for Journal of Physics A, and an Institute of Physics (IOP) trusted reviewer in 2020.

Exotic phases in Frustrated Magnetic systems

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The geometrically frustrated magnetic systems exhibit a variety of interesting quantum phases, non-trivial magnetic ordering and excitations originating from the competing ferromagnetic and antiferromagnetic interactions. In pyrochlores systems of the type A2B2O7 (A = rare earth metal, B = transition metal), the exotic magnetic ground state is achieved by three competing interactions: antiferromagnetic exchange interaction, ferromagnetic dipolar interactions and crystal electric field. In some of the pyrochlores, the dominant effect of crystal electric field forces the spin to point either directly towards or away from the center of the tetrahedra and induces spin anisotropy in the system. In this talk, I shall elaborate on the concept of spin glass, spin liquid, spin ice, and magnetic monopole followed by our studies on the effect of magnetic field and dilution of magnetism on the spin freezing state of the Dy2Zr2O7 system.

References:

[1] A. P. Ramirez, A. Hayashi, et al., Nature 399, 333 (1999).
[2] C. Castelnovo, R. Moessner, and S. L. Sondhi, Nature 451, 42 (2008).
[3] T. Fennell, P. Deen, A. Wildes,et al. Science 326, 415 (2009).
[4] Sheetal, A.Ali, S. Rajput et al., J. Phys: Cond. Matt. 32,365804 (2020).
[5] Sheetal and C. S. Yadav, Scientific Report (2021).

Dr. C. S. Yadav,
SPS, IIT Mandi

About the speaker: Dr. C. S. Yadav has started his research career at School of Physical Sciences, Jawaharlal Nehru University New Delhi. He worked as postdoctoral fellow in Tata Institute of Fundamental Research Mumbai; Argonne National Laboratory USA; and University of Geneva, Switzerland. His primary research includes experimental condensed matter physics, strongly correlated electron systems, superconductivity, topological phases of matter, thermoelectricity, quantum magnetism, and multiferroics. Dr. Yadav is currently working as an associate professor at IIT Mandi, Himachal Pradesh. Dr. Yadav has published many articles in reputed international journals.

Oral Presentations

Low temperature Raman and X-ray diffraction studies on Fe intercalated VSe2

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Layered transition metal dichalcogenides (TMDs) and their intercalation complexes have attracted tremendous engrossment during past few years due to their remarkable physical properties [1,2]. VSe_2 is a group-V TMD and well-known charge density wave (CDW) system at ~ 110 K [3]. Yadav *et al.* reported the suppression of CDW and emergence of a new type of hysteretic anomaly in electrical resistivity of Fe intercalated VSe_2 compounds [4]. We have explored the low temperature structural and Raman studies on the Fe_xVSe_2 (x = 0, 0.10, 0.25) compounds, besides the electronic and thermal transport studies to understand the nature of this anomaly. The low temperature X-ray diffraction patterns of $Fe_{0.25}VSe_2$ compound show a distinct change in c-parameter of the unit cell and the Raman spectroscopic studies shows a shift in E_g mode (~ 24600 – 25200 m^{-1}) in the same temperature range in which hysteresis is observed in electrical resistivity. These observations suggest the presence of structural distortion in the electronic properties of the $Fe_{0.25}VSe_2$. Our low temperature Raman study in the temperature range 80 – 300 K, highlights the fact that A_{1g} mode (at ~ 20500 m^{-1}) and E_g mode (at ~ 25500 m^{-1}) are not related to the CDW state of 1T-VSe_2 and are observed for the Fe_xVSe_2 as well [5].

References:

[1] S. Krishnamurthi, G. Brocks, Phys. Rev. B 102, 161106 (2020).
[2] N.H. Jo *et al.*, Proc. Natl. Acad. Sci. USA 116, 25524 (2019).
[3] C.S. Yadav, A.K. Rastogi, Solid State Commun. 150, 648 (2010).
[4] C.S. Yadav, A.K. Rastogi, J. Phys.: Condens. Matter 20, 465219 (2008).
[5] Sonika, Y. Singh and C. S. Yadav, Journal of Alloys and Compounds 897, 163220 (2022).

Dynamics of Local density and its relationship with structural local density, cavity forming, FENE polymer via Lennard jones interaction

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Fluids undergo glass transition when cooled at faster rate than structural relaxation. As structure is not relaxed transient caging happens which results in slow relaxation. Vander wall's model on Lennard jones(LJ) interaction shows that structure does not play much role in understanding the glass transition as structure remains mostly invariant whereas change in dynamics is very large comparatively. Studies also show that the relaxation dynamics becomes identical when the range of interaction include the whole first coordination shell(2)(3).identical cage potential will produce identical density relaxation irrespective of types of potential .Another research paper indicates that small change in structure g(r) is accompanied by change in dynamics it asserts the importance of g(r) to understand the change in dynamics .Another studies(4) on Kob Anderson binary mixture with LJ interaction, show a direct correlation between the growth of the highest peak of the radial distribution function g(r) which is interpreted as local density $\rho_l oc$ and density relaxation. From the available free-volume of a neighbouring pairs for string-like motion, we derive a relation between local density or surface density of first coordination shell $\rho_l oc$ around a reference particle with density relaxation τ_α , i.e. $\tau_\alpha \propto exp(\rho_0/(\rho_0\rho_l oc))$,Polymers are also prone to glass transition, because of their complex structure and slow rate of relaxation. Usage of polymer in in mankind is widely understood but its dynamics and structure are still not clear. we studied finitely extensible nonlinear elastic (FENE) polymer which consist of monomers connected via FENE potential, for inter-chain LJ potential is used. convergence of local density relaxation τ_α with change in structure's g(r) local density $\rho_l oc$ is also proved in low density cavity forming systems. low density system are very important to study as they get phase separated faster . it is show that indeed change in structure is small but it influences change in dynamics on wide scale ,also in system having cavities or low density systems, where surface and core has different thermodynamic averages , $\tau_\alpha \propto exp(\rho_0/(\rho_0\rho_l oc))$ this relation works perfectly and captures small change in structure with respect to change in dynamics.

References:

[1]. U. R. Pedersen, T. B. Schroder, and J. C. Dyre, Phys. Rev. Lett. 105, 157801 (2010).
[2]. S. Toxvaerd and J. C. Dyre, J. Chem. Phys. 135, 134501 (2011).
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[4]. D. C. Thakur, J. Singh, and P. P. Jose, AIP Conference Proceedings 2265, 030224 (2020)

O3

Crystal and electronic structure studies of doped barium bismuthates

Bharath M[1], Priyamedha Sharma[1], Jaskirat Brar[1], R K Maurya[1], Asif Ali[2], Sakshi Bansal[2], Pankaj R Sagdeo[3], Ravi Shankar Singh[2], Bindu R[1]

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One of the major challenges in condensed matter physics is the quest towards realizing room temperature superconductivity and understanding its underlying mechanism. One of the keys to understand the behaviour of high-T_C superconductivity lies in the understanding of the nature of non-superconducting phase as the superconducting phases are observed in the proximity of more interesting phenomena like charge density waves, spin density waves, etc. Towards this goal, we have investigated the crystal and electronic structure of $BaBiO_3$[1], 10% Y-doped $BaBiO_3$[2], and 75% Pb-doped $BaBiO_3$[3] using various techniques.We have carried out the investigation of the crystal structure of $BaBiO_3$, and 10% Y-doped $BaBiO_3$ using x-ray diffraction (XRD) measurements. To identify the possible relation between the crystal structure and the electronic structure, we have probed the the core level and valence band spectra of the two compounds using x-ray photoemission spectroscopy (XPS) and band structure calculations. The XRD studies reveal a change in the crystal structure upon doping from the monoclinic *I2/m* space group to the *P2/n* space group of the same crystal structure. The valence band spectrum obtained from the XPS measurements of the parent compound displays a gap at the Fermi edge, which widens upon doping with 10% yttrium. High-resolution x-ray photoemission spectroscopy (XPS) measurements close to the Fermi edge reveal the presence of fine structures which are modified significantly upon Y-doping. Band structure calculations reveal the presence of holes in the oxygen 2*p* states due an unequal transfer of electrons from O 2*p* to Bi1 and Bi2 ions, in the parent compound. Upon Y-doping, we not only observe the persistence of the unequal transfer of electrons from O 2*p* to Bi ions, but also observe additional charge transfer to Y states, revealing the importance of Y ions in the doped compound.On the other hand, 75% Pb-doping in Bi-site of $BaBiO_3$ brings about both crystal structure and electronic structure changes. The compound is diphasic, exhibiting both tetragonal and orthorhombic crystal structures. Furthermore, the compound exhibits superconductivity with a $T_C \approx 11$ K. To understand the evolution of the crystal structure, transport properties and electronic states of the compound with temperature, we have performed temperature-dependent XRD, XPS and resistivity measurement studies. In the temperature range (10 K – 25 K) *i.e.* above T_C, our results show an increase in both the orthorhombic and tetragonal strain. The well screened features observed in Bi and Pb $4f_{7/2}$ core levels are indicative of the metallic nature of the sample. The compound exhibits finite intensity at the Fermi level at 300 K and this intensity decreases with decrease in temperature and develops into a pseudogap; the energy dependence of the spectral density of states suggests disordered metallic state. Furthermore, our band structure calculations reveal that the structural transition upon Pb doping results in the closing of the band gap at the Fermi level.

[1]. Bharath M, *et. al.,* Journal of Physics: Condensed Matter 32 (5), 055504, **2019**
[2]. Bharath M, *et. al.*, The European Physical Journal B 94, 1-8, **2021**
[3]. Bharath M, *et. al.*, Journal of Physics: Condensed Matter 35 (9), 095701, **2022**

Lattice effects on the physical properties of half-doped perovskite ruthenates

Jaskirat Brar[1*], Saurabh Singh[2,3], Kentaro Kuga[2,3], Priyamedha Sharma[1], Bharath M[1], Tsunehiro Takeuchi[2,3], and R. Bindu[1]

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We investigate the unusual phase transitions in $SrRuO_3$ and $Sr_{0.5}Ca_{0.5}Ru_{1-x}Cr_xO_3$ (x=0, 0.05 and 0.1) employing x-ray diffraction, resistivity, magnetic studies and x-ray photoemission spectroscopy. Our results show the compounds undergo a crossover from itinerant ferromagnetism to localized ferromagnetism. The combined studies suggest Ru and Cr be in the 4+ valence state. A Griffith phase and an enhancement in Curie temperature (Tc) from 38 K to 107 K are observed with Cr doping. A shift in the chemical potential towards the valence band is observed with Cr doping. In the metallic samples, interestingly, a direct link between the resistivity and orthorhombic strain is observed. We also observe a connection between orthorhombic strain and Tc in all the samples. Detailed studies in this direction will be helpful to choose suitable substrate materials for thin-film/device fabrication and hence manoeuvre its properties. In the non-metallic samples, the resistivity is mainly governed due to disorder, electron-electron correlation effects and a reduction in the number of electrons at the Fermi level. The value of the resistivity for the 5% Cr doped sample suggests semi-metallic behaviour. Understanding its nature in detail using electron spectroscopic techniques could unravel the possibility of its utility in high-mobility transistors at room temperature and its combined property with ferromagnetism will be helpful in making spintronic devices.

Prediction of magnetic moment and formation energy per atom of Iron-based compounds using a data-driven machine learning approach

Yogesh Khatri and Arti Kashyap*

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Iron is well known element for its superior magnetic properties. Most of the Iron based compounds are magnetic in nature, so we developed a model to predict the magnetic moment of iron-based compounds using machine learning (ML) techniques. The open Materials Application Programming Interface (API) [1] and the open-source Python Materials Genomics (pymatgen) materials analysis package [2] were used to collect the data of 11545 Fe-based compounds from the Materials project repository [3]. This data consists of total magnetization, crystal structure and formation energy per atom of all compounds. Using the orbital-field matrix (OFM) representation purposed by Pham et al. [4], which is based on the distribution of the valence cell electrons, the structure of the compounds is turned into a 32*32 matrix corresponding to 1024 features, known as descriptor. Out of various ML algorithms, random forest provides best results for our dataset with a 5-fold cross-validation. so, we used it for our further modelling. Our data is further classified based on magnetic ordering, with ferromagnetic compounds having the best performance in terms of predicting magnetic moment per atom, with a mean absolute error (MAE) of 0.14 μ_B /atom. Formation energy per atom of Fe-based compounds can be predicted with MAE of 0.168. To better comprehend the model, we used SHAP interpretability analysis. Density plots for predicted vs actual values of magnetic moment per atom and formation energy per atom is shown in figure 1.

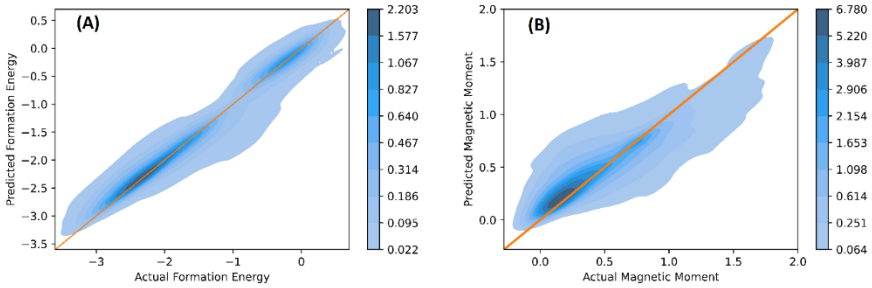

Figure 1: Density plots for predicted vs actual values of formation energy per atom (A) and magnetic moment per atom (B).

References:

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Realistic model for Photoinduced heterogeneous electron transfer

Anjali* and Aniruddha Chakraborty

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The electron transfer from an electronically excited state of an adsorbed dye molecule to the conduction band of a semiconductor has been an interesting topic of research for many years [1-7]. While there has been significant progress in the theoretical modelling of this process, most existing models do not fully account for the effects of the electron image charge, which arises from the interaction between the transferred electron and the surface of the electrode. The electron image effect can have a significant impact on the rate and efficiency of the electron transfer process and neglecting it can lead to inaccurate predictions of the behaviour of the system.

The survival probability of the electron in the excited state is calculated using Green's function approach, and compared with already existing results [1,2]. We found that image effect plays a significant role in the results. We believe that such a model can have important implications for a wide range of applications, including photocatalysis, photovoltaics, and biosensing. By developing a more accurate understanding of the mechanisms and factors that control photoinduced heterogeneous electron transfer, researchers can develop new technologies for harnessing the energy of light to drive chemical reactions and for controlling the transfer of electrons in chemical systems.

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O7. Plasmonic Resonant Intercluster Coulombic Decay

Rasheed Shaik[1*] **,** Hari R. Varma[1] and Himadri S. Chakraborty[2]

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Interatomic/intermolecular Coulombic Decay (ICD) is a process when a weakly-bonded system absorbs a photon in the extreme ultraviolet (XUV) to x-ray range which can cause innershell excitations in one atom, molecule, or cluster leading to outershell ionization of another atom, molecule, or cluster of the bonded system, with the coulomb interaction between excited and ionized electrons being the intermediary of the process. These ICD processes have been the subject of a vast range of studies [1] since its discovery by Cederbaum and collaborators [2] more than two decades ago. Remarkably, no evidence of plasmon resonance decay across an ICD channel has yet been discovered. However, owing to its unique extreme light confinement and control abilities at the nanoscale size, the plasmonic ICD will not only be a fundamental process, but will also significantly broaden the scopes of the huge ICD landscape and associated applications in physics, chemistry, and biology. We found an efficient prototype of spherically nested dimer $\underline{Na_{20}@C_{240}}$ to investigate the Intercluster Coulombic Decay of a plasmon excitation and found the first evidence of this fundamental phenomena [3].

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O8. Finding a suitable theoretical approach for better quantification of electronic and magnetic properties correlated electron systems

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In this talk we will look at the complexity in studying strongly correlated materials, with as particular emphasis on transition metals. Subsequently, the hunt for suitable computational method using DFT, GW, and DFT+DMFT based state-of -the-art techniques, through a comparative quantitative analysis of electronic and magnetic properties of Nickel (Ni) will be discussed. In this work we explore the best suited computational method through a comparative quantitative analysis of electronic and magnetic properties of Nickel (Ni). In this direction DFT, GW, and DFT+DMFT based state-of -the-art techniques are used. The Coulomb interaction parameters, $U_{full} = 5.78\ eV$ and $J = 1.1\ eV$ computed using cRPA and Yukawa screening method, respectively, along with Full type of Coulomb interaction within DFT+DMFT prove to be a suitable choice for studying occupied & unoccupied electronic structures, and temperature dependent magnetization of Ni. The calculated spin resolved values of imaginary part of the self-energy ($Im\Sigma(\omega)$) using DFT+DMFT are found to be important for the best description of experimental electronic excitation spectra. This study shows the equal contribution of correlation effects and plasmon excitation to the intensity of famous *6 eV* satellite and hence paving way for its reinterpretation.

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O9. Evidence of the novel three-dimensional quantum spin liquid state in $HoVO_4$

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Quantum spin liquids (QSL) are considered as "dynamic quantum disordered" ground states in which zero-point quantum fluctuations are so strong that conventional long-range magnetic ordering is prevented down to the lowest temperatures. These QSL exhibit massive many-body entanglement which gives rise to unique physical aspects such as topological properties, non-local and fractional excitations and many more [1]. For a QSL, magnetic frustration acts as an important ingredient as it can result in strong quantum fluctuations. Strong magnetic frustration in a system leads to a strong competition between spin-spin interactions and results in a plethora of exotic ground states, such as spin glass, spin ice and QSL [2, 3]. In this work, we have investigated the signatures of 3D QSL state in a rare-earth orthovanadate $HoVO_4$ via the means of structural, magnetic susceptibility, heat capacity measurements, along with density functional theory calculations. In this compound, the presence of a distorted kind of HoO_8 polyhedral leads to multiple magnetic interaction paths. The 2nd and 3rd near neighbour (NN) Ho atoms form the network of frustrated geometries and can result in magnetic frustration in $HoVO_4$. The observed broad maximum centered at 5 K in the temperature response of DC susceptibility curve implies the presence of short-range correlations. AC susceptibility rules out the possibility of any kind of spin freezing. Temperature dependent heat capacity at zero field indicate towards the absence of long-range ordering, along with the presence of a broad maximum centered around 14 K. The residual heat capacity exhibits a characteristic power-law (T^{α}) behavior below 5 K, with the exponent α nearly equal to 2, which is analogous to that observed for other 3D quantum spin liquid systems. The density functional theory calculations signify the presence of dominant second and third NN interactions, which in turn lead to magnetic frustration in our system. Our investigations suggest that $HoVO_4$ is a promising candidate for realizing a 3D quantum spin liquid state [4].

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O10. Many Body Phenomena in Bismuth Chalcogenides Using Light-Matter Interactions

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The layered transition metal chalcogenides such as $NbSe_2$, TaS_2, Bi_2Se_3, Bi-Ge-Te(Se) are an interesting material which got scientific attention for studying the fundamental physics related to electron-phonon interactions [1]. Recently, the compounds like Bi_2Se_3, Bi_2Te_3 and Bi_2GeTe_4 has been explored for multi-body phenomena using low temperature Raman studies [2-4]. With the understanding of electron-phonon coupling and crystalline anharmonicity, the crystallographic orientations of single crystal can be related with the polarization of light. Bismuth Selenide is a well-known topological insulator as well as thermoelectric material, however, the understanding of the underlying physics of its layered nature is scarcely report [5]. The unit cell has an enormous crystallographic anisotropy along c-axis. Here, we will present the iso-(aniso-) tropic interaction of light with the crystallographic orientation of Bi_2Se_3 [6].

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O11. PY-Nodes: An *ab-initio* python code for searching nodes in a material using *Nelder-Mead's* simplex approach.

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With the discovery of topological semimetals, it has been found that the band touching points near the Fermi level are of great importance. They give rise to many exciting phenomena in these materials. Moreover, these points, commonly known as nodes, are related to several properties of these semimetals. Thus, the proper estimation of their coordinates is extremely needed for better understanding of the properties of these materials. We have designed a Python 3 based code named *PY-Nodes* for efficiently finding the nodes present in a given material using *first-principle* approach. The present version of the code is interfaced with the WIEN2k package. For benchmarking the code, it has been tested on some famous materials that possess characteristic nodes. These include – TaAs, a well-known Weyl semimetal[1], Na_3Bi, which is categorized as Dirac semimetal[2], CaAgAs, classified as a nodal-line semimetal[3] and YAuPb, which is claimed to be non-trivial topological semimetal[4]. In the case of TaAs, 24 nodes are obtained from our calculations. On computing their chiralities, it is found that 12 pairs of nodes having equal and opposite chirality are obtained. Furthermore, for Na_3Bi, a pair of nodes are obtained on either side of the Γ-point in the $\boldsymbol{k_3}$ direction. In the case of CaAgAs, several nodes are obtained in the k_z=0 plane. These nodes, when plotted in the k_x-k_y plane, form a closed loop which is generally referred to as a nodal-line. Finally, in the case of YAuPb, large number of nodes are obtained in the vicinity of Γ-point. The results obtained for these materials are in good match with the previous works carried out by different research groups. This assures the reliability and efficiency of the *PY-Nodes* code for estimating the nodes present in a given material.

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O12. Magnetodielectric coupling as a manifestation of metamagnetic transition and structural distortion in Ba3RRu2O9 (R = Gd, Dy)

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The 6H-perovskites Ba3RRu2O9 (R = Rare Earth) exhibit complex magnetism and have been extensively studied recently for their magnetodielectric (MD) properties [1,2]. Here, we present a detailed study of structural, magnetic, thermodynamic and MD properties of 6H-perovskites Ba3RRu2O9 (R = Gd, Dy) [3,4]. Long range Antiferromagnetic (AFM) ordering sets at ~ 14.8 K and ~ 5.8 K for Gd and Dy compounds respectively, which is evident from the magnetization and heat capacity studies. The AFM ordering for Ba3GdRu2O9 shift towards low temperature besides showing the splitting of peak on the application of magnetic field. Low temperature magnetic isotherms for Ba3GdRu2O9 exhibit three metamagnetic transitions with opening of small hysteresis in different regions which are attributed to spin reorientation of AFM magnetic lattice. Entropy change corresponding to AFM ordering indicates the simultaneous alignment of both Ru and Gd moments. On the other hand Ba3DyRu2O9 shows two additional field dependent anomalies at ~ 28 K (T1) and ~ 33 K (T2) besides AFM ordering at ~5.8 K in the heat capacity. These anomalies are feebly reflected in the derivative of magnetization curve and dielectric response as well. Low temperature crystal structures of the compound show distortion of Ru2O9 octahedra near T2. Our investigation suggest that Ru2O9 is distorted at T2 which in turn forces Ru moments to exhibit magnetic correlations. Dielectric response recorded at zero and 80 kOe field exhibits the development of MD coupling well above TN due to presence of short-range magnetic correlations. These compounds show a large value of MD coupling in comparison to other counterparts in 6H- perovskite family. Our studies suggest that the metamagnetic transition and structural distortion in Ru2O9 octahedra play an important role in inducing large magnetodielectric coupling in these compounds.

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Posters

P1. A possible coexistence of spin semimetal and Weyl semimetal in Ti2MnAl

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Discovery of various new classes of materials like half metal, semimetal, and spin gapless semiconductor (SGS) has generated a lot of interest in the field of spintronics [1]. Recently, a new class of spintronic material, namely spin semimetal (SSM) was predicted [2]. SSMs are unique class of materials in which one spin bands exhibit semiconducting/ insulating nature while the other is semimetallic. The identification of potential half metals, Weyl semimetals (WSM), and SGS in the Heusler family of compounds has renewed interest in examination of different Heusler compounds. Ti_2MnAl is one such compound with inverse Heusler lattice structure (F43m, space group 216). It is predicted to be a compensated ferrimagnet hosting Weyl semimetallic state [3]. Our experimental findings suggest the possibility of coexistence of spin semimetal and Weyl semimetallic state in this compound. Ti_2MnAl was synthesized by arc melting the stoichiometric amount of constituent elements in a highly pure Argon atmosphere. Phase purity and structural analysis of the sample were done using x-ray diffraction (XRD) technique. Electrical resistivity and heat capacity measurements were carried out using physical property measurement system (PPMS) from Quantum design. The Rietveld profile refinement of the XRD data shows that the sample is in single phase. The resistivity vs temperature curve implies negative coefficient of resistivity which hints toward the possibility of either a semiconductor or a semimetal. Further, the deviation of resistivity curve from exponential behavior in the measured temperature range rules out the gapped semiconducting nature. This suggests the possibility of SGS or semimetallic state in Ti_2MnAl. The conductivity data can be fitted with a two-carrier model which indicates the possibility of the presence of two types of carriers. The specific heat vs temperature graph is plotted. The electronic contribution to specific heat in a SGS or a simple semiconductor is small as compared to metals or semimetals due to vanishing density of states (DOS) at the Fermi level. The linear fit of C/T vs T^2 plot gives the Sommerfeld constant, γ which is found to be 8.09 mJ/mole K^2. Using free electron gas model, the DOS at Fermi level is estimated to be ~ 3.5 states/ eV f.u which is expected for semimetals [4]. Further, origin of anomalous Hall resistivity and careful analysis of band structure, magnetic properties are required to validate the coexistence of SSM and WSM states.

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P2. Cluster spin glass and discrete energy states in disordered $LiCoVO_4$

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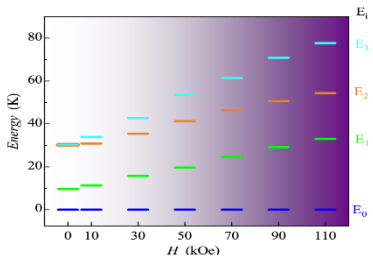
The presence of mixed Co^{2+} and Co^{3+} in Co-based compounds leads to novel magnetic ground state due to spin state degree of freedom and competing interactions [1,2]. In this context, $LiCoVO_4$ is investigated by the means of structural, magnetic and transport measurements. Structural investigations show the presence of anti-site disorder between Li and Co ions give rise to Co^{3+} state along with the expected Co^{2+} state. The disorder arises due to presence of small fraction of Co on tetrahedral sites. Magnetic susceptibility studies along with the dynamic scaling of AC susceptibility reveal the presence of cluster spin glass state at 2.8 K in our sample. The proposed outcome is further established by probing the relaxation dynamics i.e., aging effect, memory effect and relaxation measurements. This glassy behaviour arises possibly due to competing interaction between Co^{2+} and Co^{3+} [3]. The Curie Weiss behaviour of inverse susceptibility indicates the high moment (~ 5.37 μ_{eff}) due to unquenched orbital angular moment contribution of high spin of Co^{2+} [4]. The heat capacity measurements display low temperature Schottky anomaly which reveal the presence of persistent discrete energy state of Co^{3+}, as shown in Fig. 1, which appears due to the octahedral distortion and spin-orbit coupling (i.e., unquenched orbital angular momentum) [5]. This anomaly shifts to higher temperature with increasing field and the calculated value of Landé g-factor yield the presence of high spin state Co^{3+} ions lying energetically near to low spin state. We believe that our investigations provide legitimate evidence against the well-established hypothesis of complete quenching of orbital angular moment in 3*d* complexes owing to discretisation of energy states.



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P3. Interplay of Physical strain, Tilt of the Weyl cone and Intervalley scattering on Longitudinal magnetoconductance in Weyl Semimetals

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Elastic deformations (strain) couple to the electronic degrees of freedom in Weyl semimetals as an axial magnetic field (chiral gauge field), which in turn affects their impurity dominated diffusive transport. Here we study the longitudinal magnetoconductance (LMC) in the presence of strain, Weyl cone tilt, and finite intervalley scattering, taking into account the momentum dependence of the scattering processes (both internode and intranode), as well as charge conservation. We show that strain induced chiral gauge field results in 'strong sign-reversal' of the LMC, which is characterized by the reversal of orientation of the magnetoconductance parabola with respect to the magnetic field. On the other hand, external magnetic field results in 'strong sign-reversal', only for sufficiently strong intervalley scattering. When both external and chiral gauge fields are present, we observe both strong and weak sign-reversal, where in the case of weak sign-reversal, the rise and fall of magnetoconductivity depends on the direction of the magnetic field and/or the chiral gauge field, and is not correlated with the orientation of the LMC parabola. The combination of the two fields is shown to generate striking features in the LMC phase diagram as a function of various parameters such as tilt, strain, and intervalley scattering. We also study the effect of strain induced chiral gauge field on the planar Hall conductance and highlight its distinct features that can be probed experimentally.

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P4. Local Structure Study Around Mn Atom of Co_2MnAl Compound

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The Co based Full Heusler alloys are of particular interest due to their high T_c value, half metallicnature and giant anomalous Hall conductivity, thus making it suitable for spintronics devices [1]. We have prepared polycrystalline sample of Co_2MnAl by arc melting method. The sample was characterized by X-ray diffraction, field dependent magnetic measurements, and Extended X-ray absorption fine structure measurements (EXAFS). The compound can be stabilized in $L2_1$ or B2 (Mn/Al antisite disorder) structure. Our XRD result shows that compound stabilize in B2 cubic structure with lattice parameter 5.76 Å. In addition, X- ray absorption near edge structure also shows the signature of the B2 phase of the compound. The field dependent magnetic measurement gives a saturation magnetic moment of 4.20 μB/f.u. which is nearer to the expected value for the B2 phase[2]. The physical properties are closely associated with the local structure. Therefore, we have investigated the local structure around the Mn site in Co_2MnAl Heusler alloy using EXAFS technique. Our EXAFS result shows the local environment around the Mn atom is different from the global structure as revealed by XRD (shown in Fig. 1).

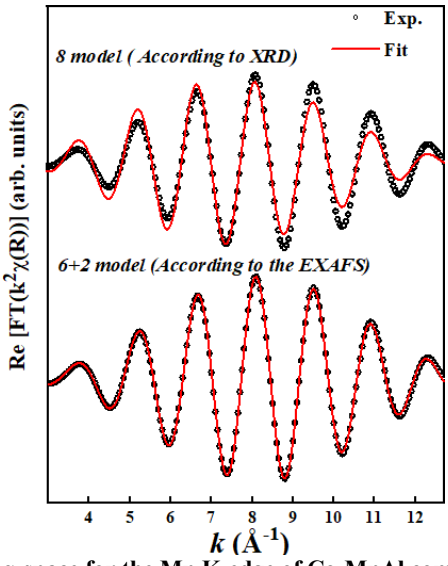

Fig.1. First co-ordination shell fit in q-space for the Mn K-edge of Co_2MnAl compound.

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P5. Chemically transformed Ag_2Te nanowires for thermoelectric energy conversion applications

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Harvesting electricity from waste heat is an important technology because of the fast depletion of fossil fuels and growing energy demand. Thermoelectricity is a capable phenomenon which can provide a direct conversion of heat into electricity and visa-versa.[1]For better efficiency of the materials, a high figure of merit (ZT) is required to compete existing technologies.[1] Metal chalcogenides have been extensively used as TE materials because of their high conversion efficiency.[2,3] To take the technology to the device level, a large quantity of materials is necessary. In this regard, solution-based preparation methods can give better control of composition and morphologies while they also can be scaled up. We will present an effective approach to produce metal chalcogenides nanomaterials using chemical transformation of chalcogens (Se and Te) as a precursor.[4]

We will show the surfactant free chemical transformation of Te nanowires into silver telluride nanowires.

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P6. Fabrication of MoS_2/WS_2 heterostructure as vertical p-n junction diode for optoelectronics applications

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Recently van der Waals heterostructures based on transition metal dichalcogenides have emerged as a promising material for novel optoelectronic and photovoltaic applications since they can have a wide range of optical bandgap from near-infrared to visible spectral range and is a good platform to investigate strong light-matter interactions. [1,2] Vertical van der Waal junctions composed of p and n-type semiconductors. [3] Among the transition metal dichalcogenides, MoS_2 is an n-type semiconductor while WS_2 is a p-type semiconductor. We have fabricated the MoS_2/WS_2 heterostructure by the mechanical exfoliation and dry transfer technique.[4,5] I will present the Raman and photoluminescence characterization of the MoS_2/WS_2 heterostructure.

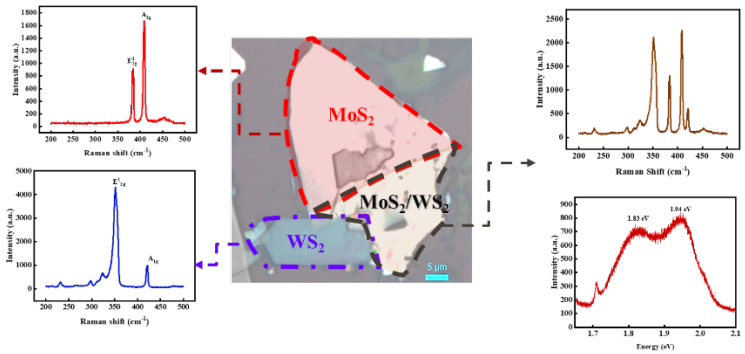

Figure 1: Optical image of heterostructure of MoS_2/WS_2 and corresponding Raman and photoluminescence spectra.

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P7. Third-order optical nonlinearity and charge carrier dynamics in Tin(II) monosulfide

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Tin(II) monosulfide (SnS) is a layered material with low crystal symmetry, large absorption coefficient, high carrier mobility and long-time stability [1, 2]. The presence of unique anisotropic linear and nonlinear optical properties in SnS owing to their distorted-NaCl (*d*-NaCl) structure have prompted their use in photodetectors, photovoltaics, thermoelectrics, and sensing applications [3-5]. Here, we report single photon absorption saturation and self-focussing effect in SnS quantum dots (QDs) using femtosecond z-scan measurements. The nonlinear absorption coefficient and nonlinear refraction coefficient were extracted from open-aperture (OA) and closed-aperture (CA) z-scan measurements, respectively. Furthermore, charge carrier dynamics is explored using ultrafast pump-probe spectroscopy to understand the origin of the observed optical nonlinearity. TA studies infer the presence of mid-gap defect states which not only governs carrier dynamics but also give rise to optical nonlinearity in SnS QDs. Our results also suggest that photogenerated charge carriers in SnS QDs relax through a number of processes like carrier cooling, carrier trapping, defect mediated and band-to-band carrier recombinations. Because of saturable absorption property, SnS QDs could be used as a saturable absorber for mode-locking and Q-switching.

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P8. Optical probing of ultrafast charge transfer in van der Waals WS_2/Ruddlesden–popper perovskite heterojunction

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Two-dimensional (2D) van der Waals (vdW) heterostructures based on transition metal dichalcogenides (TMDCs) and 2D perovskite open up new possibilities for a wide range of optoelectronic applications. These heterostructures enable us to improve device efficiency by combining the properties of constituent materials. [1, 2] TMDCs possess engrossing physical phenomena like exceptionally large binding energy, spin or valley degree of freedom, exciton hall effect, etc. [3] A deep understanding of the dynamical behaviour of charge species (electron, hole, excitons, etc.) within the heterostructure is crucial to improve the performance of optoelectronic devices. There is type-II band alignment between the WS_2 and 2D perovskite ($(TEA)_2PbI_2$) which could be favourable for transfer of charges and interlayer exciton formation. We have utilized the ultrafast transient absorption spectroscopy to study the charge carrier dynamics in WS_2/$(TEA)_2PbI_2$ heterojunction (figure 1). Our results suggested that efficient electron transfer takes from WS_2 to $(TEA)_2PbI_2$.

Keywords. Ultrafast optics, monolayer WS_2, CVD, 2D perovskite, transition metal dichalcogenides (TMDs), 2D materials, type-II heterostructure.

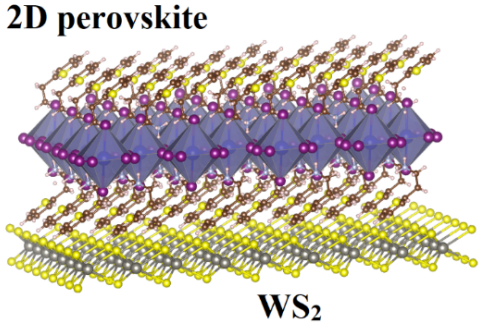

Figure 1 Structural representation of $(TEA)_2PbI_2$ perovskite coated on monolayer WS_2.

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P9. Transport and optical properties of single crystals of Bi_2Se_3 and Bi_2Te_3

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Bi_2Se_3 and Bi_2Te_3 have harnessed the attention of the scientists owing to the coexistence of two phenomenon of Topological Insulators (TI) at low temperature as well as room temperature thermoelectricity.[1, 2] Synthesis of single crystals are favored over polycrystals as they offer numerous advantages such as uniformity, anisotropy, absence of grain boundaries. In this work, we have synthesized high quality single crystals of Bi_2Se_3 and Bi_2Te_3 using vertical Bridgman furnace. Characterisation measurements such as X-ray diffraction and SEM reveal the phase purity as well as layered nature of the synthesized crystals. Linear fitting of heat capacity gives the characteristic constants related to electronic contributions and lattice contributions. In order to probe the phonons in these compounds Raman spectroscopy measurements have been carried out on both the sample which reveal the presence of characteristic Raman modes.[3-5]

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P10. Role of repulsive and attractive interactions in glass forming liquids

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We have performed the molecular dynamics simulations of glass forming pure Lenard-Jones particles using two models i.e., KA(Kob-Anderson) and WCA(Weeks, Chandler and Anderson) models. The potential used in KA model contains both attractive as well as repulsive part while WCA model contains only the repulsive part. We then compare all the statistical and dynamical properties to find the qualitative and quantitative differences that arise due to the different parts of the potential. There is not much difference observed in static properties of the liquids. Difference in dynamical properties is noticed due to the difference in the potential used.

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P11. Surface Passivation by Sulfur-based 2D $(TEA)_2PbI_4$ for Stable and Efficient Perovskite Solar Cells

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Organic-inorganic perovskite solar cells (PSCs) have been recognized as a potential candidate in photovoltaic technologies. The power conversion efficiency (PCE) of three-dimensional (3D) PSCs has improved to 25.7% in the early few years, which is close to silicon-based solar cells.[1] However, poor device stability under humid, bright, and hot conditions is a major obstacle for practical implementation.[2,3] Surface passivation is one of the significant strategies to improve the efficiency and stability of PSCs. The two-dimensional (2D) perovskite on 3D perovskite combines the benefits of the stability of 2D perovskite with the high performance of 3D perovskite.[4] Here, 2-thiopheneethylamine iodide (TEAI) spacer cation is synthesized as a passivation layer to construct a 2D/3D perovskite heterostructure. TEAI-passivated PSCs possess a significantly greater efficiency (20.06%) than the 3D perovskite ($MAFAPbI_3$) devices (17.42%). To investigate the effect of surface passivation on the charge carrier dynamics of 3D perovskite, femtosecond transient absorption (TA) spectroscopy and time-resolved photoluminescence (TRPL) are employed. The stability test of 2D/3D PSCs also demonstrates a considerable improvement in humid (RH ~ 56%) and thermal conditions. Our findings provide a reliable strategy to enhance

device performance and stability successively, paving the way for the commercialization of PSCs.

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P12. Detection of Transients using Light Curve

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Our universe is filled with a large number of strange objects one of them being transients. Transients refer to the sources whose intensity or the flux emission varies as a function of time. A few of the transients include supernovae, Active Galactic Nuclei (AGN), gamma-ray bursts, etc. My current research project deals with the identification of supernovae by plotting a light curve, i.e., a plot between the flux/intensity and time. If we observe a variable intensity of the source as a function of time, we can say that we have found a transient. But we will need further verifications to conclude whether the observed source is a supernova.
The data on which I am working is the Extended Chandra Deep Field South (ECDFS) data obtained from the Chandra X-Ray observatory. The plotting of the light curve begins by identifying the same sources from different catalogs. For this, I ran a script based on Astropy for catalog cross-matching. Then the flux from the same sources was arranged in a table as a function of time. The script involves first locating the closest source to a particular source in some other catalog. Then a threshold radius in units of arcseconds is set depending on the distance of the source from Earth. If the detected closest source lies within the threshold radius, it is the same source and we add its flux to the table, else we check for the other source matches. This is required as the coordinates the telescope returns for a particular source might vary by a few arcseconds due to the radius of the observed source. The observations from the light curve will further be verified using software like Vizier, Simbad, etc., developed by some space-based telescopes, which have their own catalogs.

P13. Imaging of sources and studying its physical properties

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There are a lot of astrophysical phenomena going on in our universe. Gravitational wave multi messenger astronomy allows us to observe these phenomena across multiple wavelengths. Radio waves play an important role in multi-messenger astronomy, as they can be used to study objects and events that emit synchrotron radiation, such as relativistic jets and supernova remnants. Radio interferometry techniques, used by the Very Large Array (VLA) and the Very Long Baseline Array (VLBA), allow astronomers to observe these objects with high angular resolution and sensitivity, providing valuable information about the physical processes at work. Similarly GMRT(Giant Metrewave Radio Telescope) , a radio telescope array located near Pune, India. It is one of the largest and most sensitive radio telescopes in the world, the 30 dishes spanning over 25 kilometers, giving the array an effective collecting area of about 45,000 square meters. It is based on the double-slit experiment and interferometry. My ongoing research project is about getting a hands on with the procedure for calibrating a phase-referenced VLBA observation of the radio galaxy J1203+6031 (IVS 1200+608, ICRF3 J120303.5+603119) to study a distant radio galaxy located in the constellation Ursa Major. My aim of the project is to create high-resolution images of the galaxy and study its physical properties, including its size, shape, and brightness. For this CASA, a software package developed by NRAO is being used. First step involves creating a CASA measurement set as the data was available in the FITS-IDI file. Then inspecting the data to identify a good reference antenna, and finding a good time range to use for calibrating the instrumental delay. Then comes the flagging of the bad data through quacking and even using methods for doing the flagging by hand. Here starts the calibration of the data by correcting the amplitude from the autocorrelations followed by priori , instrumental delay calibration, global fringe fitting, bandpass and final amplitude scaling and flux calibration. Since a technique called phase referencing is being used, self-calibration of the phase reference calibrator is an important step. This involves imaging the calibrator , tracking the improvement followed by phase and amplitude self calibration and applying the calibration on the target. Now after getting a fully calibrated target comes the imaging of the target. After obtaining the images it is clearly visible J1203+6031 has a jet that extends nearly due south of the core. As the calibration improves , a longer and longer jet appears. All these steps are being done using the tasks present in CASA.

P14. Second Harmonic Generation and experimental observation

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Second Harmonic Generation (SHG) is one of the most fundamental processes in the realm of nonlinear optics. In the Second Harmonic Generation, when laser light with typical high intensity interacts with matter, due to the nonlinear interaction a coherent beam emerges with frequency double of the fundamental beam. It has broad applications from the studies of solid-state material properties to biological microscopy or imaging. Here in this work, we tried to generate second harmonics experimentally using BBO ($\beta-BaB_2O_4$) as the nonlinear crystal (beside of being nonlinear, it's uniaxial as well). Then I have measured some optical properties of second harmonics (for example, power dependency of Second Harmonics on the fundamental beam power, Polarization dependent study on SHG etc.) and tried to see whether they are in agreement with the theory or not. I tried to get some ideas about crystal symmetry by observing experimental data. We have understood it doesn't matter in which polarization direction the incident fundamental beam is, when it is falling on the BBO crystal surface, the Second Harmonic beam intensity will depend on how much fundamental ordinary ray component is present inside the crystal while propagating through it.

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P15. Rotational- Translational decoupling and signature of glass transition.

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We are using a tunable diode laser to carry out spectroscopic studies of the rubidium atom. We Rotational- Translation de coupling as signified by the Debye Einstein and Debye Stoke violation is the key for characterizing glass transition of liquids in super cooled regime. Our presentation is about significance of this phenomenon and connecting it to larger glass problem.

P16. Multi-photon lasing in a single quantum dot coupled to photonic crystal cavity

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Lasing is observed in quantum systems when the emission rate is greater than absorption and other decay rates. Lasing can be realized with or without population inversion between the transition levels. Single photon lasing in single quantum dot (QD) cavity system [1] is already observed and single, multi-photon probe gain is detected in strongly coupled atomic systems [2]. In our present work we consider a coherently driven single QD strongly coupled to single mode photonic crystal cavity.

We developed a model to include the QD exciton-phonon interactions using polaron transformation approach [3] and Born-Markov approximations to obtain the master equation for the QD-cavity system. Using the master equation we studied the steady-state populations, cavity field statistics by calculating mean cavity photon number, zero-time delay second order photon correlation function and Fano factor. We constructed a simplified master equation (SME) to clearly see the various coherent and incoherent processes involved. Following the Scully-Lamb procedure [4], steady-state cavity field density matrix rate equation is derived. Thereby calculated the single, multi-photon emission and absorption rates. We compared the results to the atomic system to study the effect of exciton-photon interactions on emission and absorption rates. It is observed in off-resonantly driven QD-cavity system, the exciton-phonon interactions are fruitful in realizing multi-photon lasing. We analyzed this phenomenon by using dressed state picture showing various transitions involved between the manifolds satisfying single and multi-photon conditions. We did numerical calculations for two temperatures, 5K and 20K to see the effect of temperature on the system's steady-state properties, emission and absorption rates since with increase in temperature exction-phonon scattering rates are varied.

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P17. Thermoelectricity in $Cu_{26}Nb_2Sn_6Se_{32}$ with Complex Unit Cell

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From the past few decades, chalcogen-rich minerals are considered as good thermoelectric materials due to ultralow lattice thermal conductivity.[1][2] Minerals such as Argyrodites, Tetrahedrites, Colusites, Skutterudites, Clathrates are the complex materials which have inherently low (glass-like) lattice thermal conductivity due to large number of atoms in the primitive cell and high crystal anharmonicity.[1, 3] I will present our work on series of selenium based complex compound $Cu_{26}Nb_2Sn_6Se_{32}$, where the soft bonded crystal framework results to several compressed low frequency optical branches with low sound velocity and large Gruneisen parameter.[4] In alloy $Cu_{26}Nb_2Sn_6Se_{30}Te_2$, the heavier Te atom results to significant softening of optical modes towards lower frequency (red shift) and high Gruneisen parameter (~2.1) results to lowest lattice thermal conductivity ~ 0.70 W/mK.[5]

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P18. Structural, magnetic and transport studies on oxygen deficient double perovskite NdBaCo2O5.75

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We report here, the temperature dependent structural, transport and thermoelectric studies carried out on oxygen-deficient double perovskite $NdBaCo_2O_{5+\delta}$ (δ~0.75). The samples were

characterized using x-ray diffraction (XRD), dc magnetization, scanning electron microscopy (SEM) and energy dispersive x-ray analysis (EDAX) techniques. At room temperature (RT) the compound stabilizes in tetragonal structure with space group P4/mmm. Careful diffraction studies reveal the signature of superlattice peaks having the lattice parameters $2a_p x 2a_p x 2c_p$ where a_p and c_p are lattice parameters of its basic perovskite structure. The magnetic measurements show transitions at ~110 K and ~45 K, which correspond to paramagnetic to ferromagnetic and ferromagnetic to antiferromagnetic transitions, respectively. Our detailed structural studies reveal signature of these transitions thereby suggesting significant connectivity between magnetism and crystal structure. The compound shows signatures of Griffith's phase in the temperature range 250 K - 125 K. Careful analysis of resistivity data also ,shows the change in transport mechanism in the sample with temperature, around the above discussed magnetic transitions. A metal to insulator transition at ~ 370 K can be clearly seen in the high temperature resistivity data. We have also done high temperature thermoelectric studies (300 – 560 K), which show signatures of metal to insulator transitions in the sample. Interestingly, value of figure of merit (ZT) for our sample at RT (~0.1) is almost ten times higher, compared to the previously reported ZT values of related single and double perovskite oxides[1].

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P19. Saturation absorption spectroscopy of Rb atom

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We are using a tunable diode laser to carry out spectroscopic studies of the rubidium atom. We will found the Doppler-broadened absorption profiles of the D2 transitions at 780 nm. Then use the technique of saturated absorption spectroscopy to improve the resolution beyond the Doppler limit and measure the nuclear hyperfine splittings of the 780 nm 52s1/2 → 52p3/2 (D2 line) transition in 37 Rb. Natural linewidth of the transition has been measured using saturated absorption spectroscopy technique.

P20. Short-range order and canted antiferromagnetism in an inverse spinel $LiNiVO_4$

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Frustration driven short-range magnetic correlations/fluctuations in quantum materials usually host exotic ground states like spin glass, low dimensional magnetism and quantum spin liquid [1]. In this context, different members of spinel (both normal and inverse) family have gained enormous interest and an inverse spinel vanadate, $LiNiVO_4$, seems to be an interesting candidate [2]. Structural investigations reveal that unlike usual cation ordering, Ni and Li ions are randomly distributed at octahedral sites and results in reduced magnetic frustration. Further, an additional anti-site disorder is present, as a small fraction of Ni ions occupies tetrahedral sites. This extra anti-site disorder induces an extra magnetic exchange interaction in the system. Magnetic susceptibility deviates from Curie-Wiess behaviour below 30 K indicating that short-range magnetic correlations develop below this temperature. The presence of these correlations result in a broad maximum, followed by a cusp at 2.2 K in temperature dependent susceptibility curve. Heat capacity verses temperature curve is also manifested by a broad maximum and an anomaly. The frequency independent nature of the peak at 2.2 K discards the possibility of spin glass state. Isothermal magnetization curve indicate towards the presence of small ferromagnetic component at low temperatures. These features confirm that the cusp at 2.2 K is indicating towards a canted antiferromagnetic state below this temperature. Different competing magnetic interactions due to the presence of disorder and reduced magnetic frustration result in the short-range ordering and canted antiferromagnetism in $LiNiVO_4$, respectively [3].

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P21. Ultrafast valley depolarization in TMDC alloys

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Thin film transition metal dichalcogenides (TMDCs) are promising material for, flexible optoelectronics devices and investigating the many-body interactions among quasiparticles (like exciton)[1, 2]. But the most significant property that TMDCs possess is valley degree of freedom, and by using helicity resolved circularly polarised light, one can selectively controls the electrons population of valleys (k or k')[3]. The valley degree of freedom arises due to mainly two reasons; one is the presence of strong spin orbit coupling that leads to splitting of valance and conduction band and second is the time reversal symmetry [3]. Furthermore, previous studies have shown that, at room temperature, the depolarisation (within fs) of valley is faster due to the presence of intervalley scattering [3]. This is the main difficulty for using valley degree of freedom in logic gate operation and low power storage devices [3]. Now, the problem of faster intervalley scattering can solved by alloying the TMDCs with suitable dopant. Instead of single excitonic level, alloy possess the mixed excitonic states (bright and dark) which reduce the intervalley scattering and valley depolarization time increases [3]. Using helicity resolved transient absorption (HRTA) spectroscopy, we have studied the valley depolarisation dynamics of vanadium (V) and selenium (Se) doped monolayer MoS2 alloys. We found that, in case of MoS2 and MoSSe valley polarisation lasts for ~ 1ps and ~ 15 ps respectively, but VMoSSe possesses long lived valley polarisation.

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