AAPALI PSI-K, Pune

19-25 May 2025

International Conference on Electronic-Structure Theory and Applications

ABSTRACTS OF TALKS

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DAY 1 : 19 May 2025

Session 1

Fingerprints of excitonic effects in valence electron spectroscopies

Lucia Reining

LSI, CNRS, CEA/DRF/IRAMIS, École Polytechnique, Institut Polytechnique de Paris,
F-91120 Palaiseau, France, and European Theoretical Spectroscopy Facility (ETSF)

Excitation spectra of valence electrons are often influenced by interaction effects, even in the absence of strong correlation. In particular, excitonic effects are known to dominate absorption spectra. In this talk, we start by reminding how taking into account a screened electron-hole interaction in ab initio calculations allows one to understand excitonic effects in semiconductors and insulators that go beyond textbook exciton models [1]. We compare absorption spectroscopy with electron energy loss and inelastic x-ray scattering, and we show some surprising excitonic effects at large momentum transfer. Finally, we will discuss exotic collective excitations that may be found in low-density metals, in spite of perfect macroscopic screening [2].

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Theoretical Spectroscopy Including Electron-Phonon and Exciton-Phonon Coupling

Claudia Draxl

Physics Department and CSMB, Humboldt-Universität zu Berlin
Zum Großen Windkanal 2, 12489, Berlin, Germany

Treating various excitations in materials on equal footing allows us not only to achieve excellent agreement with experiment, but, importantly, to gain a deeper understanding of complex processes and materials. Prominent examples are organic-inorganic hybrid systems whose building blocks are very different in nature. I will discuss the critical role of both the mutual dynamical screening of the constituents and electron-phonon coupling (EPC) [1] to obtain the correct ground state and excitation spectra. Many-body perturbation theory (MBPT) is the state-of-the-art methodology for such problems. In particular, the Bethe-Salpeter equation (BSE) is the method of choice for computing optical excitations. For polar materials, the dielectric screening of both the electronic and vibrational degrees of freedom must be considered to obtain correct exciton binding energies and spectral features [2]. Finally, I will show, how the BSE together with EPC matrix elements can be used to treat exciton-phonon coupling and thus geometry relaxation in the excited state [3], giving a handle to the description of photoluminescence and exciton dynamics.

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Ab-initio multiparticle excitations in materials

Manish Jain[1]

[1] *Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore*

Experimental studies have observed absorption peaks in low-dimensional materials corresponding to trions, Fermi polarons, and biexcitons. There are limited theoretical studies on multiparticle excitations in materials as the methods to study them have very high computational requirements. We have developed a first-principles many-body theory to study these multiparticle excitations in materials. We show how this method can be used for calculating binding energies of biexcitons. Biexcitons are bound states of two electrons and two holes. To mitigate the computational cost of the calculations, we use two strategies: symmetry for generating finite center-of-mass momentum excitons; and an exciton product basis to describe biexcitons. Using the symmetry of the system, we can reduce the number of finite center-of-mass momentum excitons to be calculated. The exciton basis offers an advantage over the conventional four-particle approach, as it inherently includes strong electron-hole interactions within the exciton, leaving only the weaker exciton-exciton interactions to be addressed. The interactions among the biexciton's constituent fermions are described using an effective many-body Hamiltonian [1], which incorporates screening. We have used the many-body theory of cobosons [2] to construct the biexciton Hamiltonian within the exciton product basis. Using this method, we have calculated biexciton energies for molecules and carbon nanotubes, and our results are in good agreement with other calculations and experiments.

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Variational Calculations of Excited Electronic States by Converging on Saddle Points on the Electronic Energy Surface

Hannes Jónsson

Faculty of Physical Sciences, University of Iceland, Reykjavík, Iceland

Calculations of excited electronic states are important in various contexts such as light harvesting, photocatalysis and molecular motors. They are challenging as commonly used optimization algorithms are based on minimization and thereby converge on the ground state. As a result, a time-dependent formulation of density functional theory (DFT) is frequently used, TD-DFT, especially within the linear response and adiabatic approximations. This approximate approach, however, has several limitations especially when significant charge transfer occurs during the excitation and when states are close in energy. Within configuration interaction (CI) theory, it is evident that excited states correspond to saddle points on the electronic energy surface, with the saddle point order increasing with the excitation level. While CI calculations can be accelerated greatly by using neural networks [1], they are much too computationally demanding for most systems of interest. DFT is used in most electronic structure calculations carried out today, and by using an algorithm for converging on saddle points on the electronic energy surface, the orbitals can be optimised for excited states to provide higher energy solutions to the underlying Kohn-Sham equations [2, 3]. This gives more robust estimates of the excitation energy than TD-DFT with computational effort similar to that of ground state calculations. Several applications of this approach with commonly used density functionals will be presented, as well as calculations using a self-interaction corrected functional that gives improved results. In particular, various excited states of the ethylene molecule, including twisting of the C=C double bond, the active element of various molecular motors, and high energy Rydberg states, have been analysed [4]. Calculated conical intersection between the ground and an excited state as a function of the twist and pyramidalization angles is found to be in close agreement with multireference quantum chemistry calculations [5]. In a solid state application, the various states relevant for the optical preparation of a pure spin state in nitrogen/vacancy defect in diamond have been calculated, a system used in various types of quantum technologies. The results show close agreement with computationally demanding, embedded beyond RPA calculations as well as experiments [6].

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Role of Dimensionality on Excitonic Properties of BiSeI from Many-body Perturbative Approaches

Saswata Bhattacharya

Department of Physics, Indian Institute of Technology Delhi, New Delhi-110016, INDIA

The mechanical exfoliation of two-dimensional (2D) materials has sparked significant interest in the study of low-dimensional structures. In this work, we investigate the bulk and low-dimensional derivatives of BiSeI, a quasi-1D anisotropic crystal known for its remarkable stability and novel electronic properties. Specifically, using the density functional theory and many-body perturbation theory, we examine the influence of dimensionality on their electronic, optical, and excitonic properties. Quasi-particle (QP) $G_0 W_0$ calculations reveal a significant increase in the band gap with reduced dimensionality, driven by quantum confinement effects and reduced dielectric screening. By solving the Bethe-Salpeter equation, we identify a transition from weakly bound Wannier-Mott excitons in bulk BiSeI to strongly bound excitons in its low-dimensional forms. These structures feature band gaps spanning the infrared to the visible spectrum and exhibit large exciton binding energies, making them promising for next-generation optoelectronics and excitonic applications. Our findings[1] provide a theoretical foundation for future experimental studies on BiSeI and its low-dimensional counterparts.

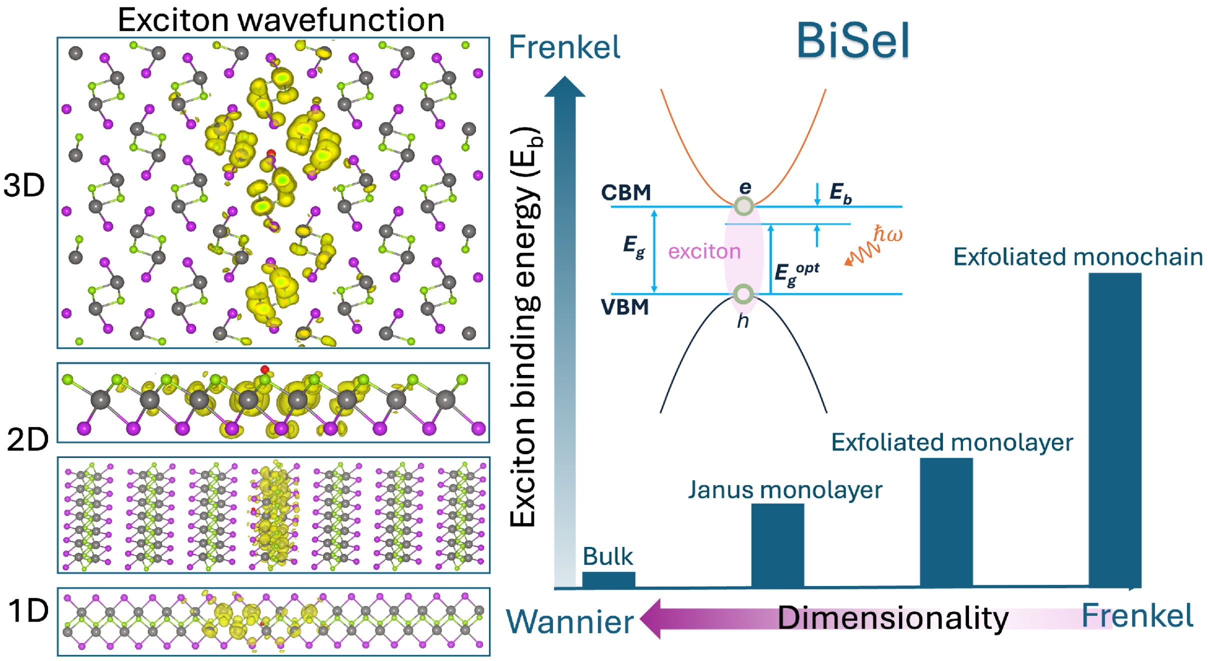

Figure 1: Table of Contents (TOC).

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Abstract for AAPALI PSI-K 2025

Saswata and Roy

Azim Premji University, Bangalore

The objective of resolving the fate of a excited state molecule or matriel has been a challenge for the last few decades. Two main challenges are been addressed are : a) how to model the non-classical nuclear dynamics on a manifold of coupled electronic potential energy surfaces, and b) how to accurately describe the Born-Huang electronic states of the molecule/material with their nonadiabatic couplings. Withing the framework of Kohm Sham Density Functional theory and it's time-dependent variant, some of proprties necessary for nonadiabatic dyamics have been approximately accessible within reasonable accuracy. However, the appromixations pose fundamental contradtions in the quadratic response theory within Density Functional theory[1], and the perpose of the presentation is to discuss the potential improvement within this theory[2].

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Electronic structure in light-element-doped TiO_2 by all-electron *GW* calculation using TOMBO code

Ryoji Sahara[1*], Takashi Ishikawa[2], Kaoru Ohno[1,3],

Kyosuke Ueda[2], and Takayuki Narushima[2]

[1]Research Center for Structural Materials, National Institute for Materials Science, Tsukuba, Japan;
[2]Department of Materials Processing, Tohoku University, Sendai, Japan;
[3]Graduate School of Engineering, Yokohama National University, Yokohama, Japan;

TiO_2 is known as a photocatalytic material, with its band gap corresponding to the UV region[1]. By doping impurity elements such as C and N, photocatalytic functionality of TiO_2 can be extended to respond to visible light, enhancing its potential for technological applications. One example is the TiO_2 coating on Ti dental implants, which imparts antibacterial properties through photocatalytic reactions [2].

To investigate anatase and rutile TiO_2 doped with C and/or N phase stability was first analyszd using density functional theory calculations considering interstitial and substitutional positions and oxygen vacancies at 700K for anatase and at 1,000K for rutile. The stable defect states were found to depend on the oxygen (O_2) pressure conditions or oxygen chemical potential for C and N monodoped and codoped TiO_2 systems. Next, using TOMBO (TOhoku Mixed Basis Orbitals ab initio program) [3], the all-electron *GW* approach based on the many-body perturbation theory was adopted to determine the electronic structures of the stable systems. The program, TOMBO, uses the all-electron mixed basis approach in which the electronic wave function is expressed by a linear combination of plane waves and atomic orbitals. Among various models, C and N codoped anatase TiO_2 under intermediate oxygen pressure shows a band gap of 2.28 eV, while, N doped rutile TiO_2 under high pressure shows a band gap of 1.86 eV. These materials can be used as photocatalyst for visible light [4,5].

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Fast and accurate finite-element based methods for DFT calculations within the projector-augmented wave formalism in the exascale era

Phani Motamarri*, Kartick Ramakrishnan and Nikhil Kodali
Department of Computational and Data Sciences, Indian Institute of Science,
Bangalore, INDIA - 560012
phanim@iisc.ac.in

The predictive capability offered by quantum modelling of materials, especially using density functional theory (DFT), has opened up a gateway for gaining crucial insights into materials' behavior, leading to an accurate prediction of mechanical, transport, chemical, electronic, magnetic and optical properties of materials. However, the stringent accuracy requirements required to compute meaningful material properties and the asymptotic cubic-scaling computational complexity of the underlying DFT problem demand enormous computational resources. Thus, these calculations are routinely limited to periodic simulation domains with material systems containing a few hundred atoms. Additionally, these DFT calculations occupy a sizeable fraction of the world's computational resources today but mostly remain in the high throughput calculation mode as the widely used DFT implementations struggle to keep up pace with evolving heterogeneous architectures in today's exascale era. To this end, the talk first introduces the recent advancements in finite-element (FE) based methods for DFT calculations - via- the DFT-FE code, the workhorse behind the ACM Gordon Bell Prize 2023. These methods provide a systematically convergent, computationally efficient and scalable hybrid CPU-GPU framework for large-scale norm-conserving pseudopotential DFT calculations that overcome the aforementioned limitations while accommodating generic boundary conditions. Subsequently, we will discuss our group's very recent efforts to go a step further in developing a fast and scalable approach combining the efficiency of projector-augmented wave (PAW) formalism involving smooth electronic fields with the ability of systematically improvable higher-order FE basis facilitating substantial reduction in degrees of freedom to achieve significant computational gains (~8x-10x) compared to the current DFT-FE calculations for medium to large-scale material systems (5000-50,000 electrons). Moreover, our approach PAW-DFT-FE demonstrates a considerable computational advantage over state-of-the-art plane-wave codes for system sizes greater than 5000 electrons. Notably, our framework represents the first real-space PAW approach capable of competing with plane-wave methods. Furthermore, extensions of the aforementioned PAW-DFT-FE framework to incorporate noncollinear magnetism and spin-orbit coupling effects will also be discussed. Finally, we illustrate the effectiveness of PAW-DFT-FE in enabling large-scale simulations with generic boundary conditions using few case studies.

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Development and implementation of new features in fully-relativistic DIRAC program package

Malaya K. Nayak

STCS, ChD, BARC, Mumbai - 400085

The matter-antimatter asymmetry of the present-day universe is one of the biggest mysteries to scientists. Many attempts have been made to unravel the physics behind this asymmetry. Sakharov showed that the dominance of matter over antimatter in our universe can only be explained if these conditions are fulfilled- (a) there must be *CP* violation (where *C* and *P* means charge conjugation and parity invariance, respectively), (b) there must be non-conservation of baryon number, and (c) there must be interactions out of thermodynamic equilibrium. My research deals with the first condition of Sakharov's proposal, i.e. searching for CP-violation in atomic and molecular systems. In this context, we developed many new codes/modules which are integrated with the DIRAC program package from time to time. We also interfaced the DIRAC code with many in-house developed codes based on the advanced CI and CC level of theories for the highly accurate/precise calculations of relevant atomic and molecular properties of experimentally promising molecular systems. I will mostly discuss these important developments relevant to the search electron electric dipole moment (eEDM) and other *CP* violating interactions to probe physics beyond the standard model (SM) of particle physics, i.e. so called "New Physics" beyond the SM.

DAY 1 : 19 May 2025

Session 2

Computational Insights in Heterogenous Catalysis: An Industrial Perspective

Sharan Shetty

Shell India Markets Pvt. Ltd, Bangalore

Industriual processes are energy intensive and contribute to large amount of GHG emissions due to the large scale and complex nature of the processes involved in the conversion of carbon based feedstock. Heterogeneous catalysis plays an important role in reducing the energy required to produce the chemicals and hence reducing the CO_2 footprint of the process. Several studies have been dedicated to investigate the role of molecular catalysis in the efficient conversion of the reactants to products with high activaity and selectivity. In recent years, computational methods in conjunction with machine learning algorithms have accelerated the design of novel catalysts that can reduce the time for lab scale experiments and scale-up.[1,2]

In the present work, we will discuss the role of computational catalysis in industrial applications. We will present the work on synthetic fuel production through the Fischer-Tropsch process where conventional DFT has been applied to understand the effect of promoters.[3,4] In another example, we will discuss the development of machine learning based potential approach for investgating the deactivation of the catalyst.[5] We will conclude the presentation on the challenges and opportunities for catalyst technology development to achieve carbon net zero emissions.

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Graphene Based Photocaltalysts for Green Hydrogen Production

P. Ravindran

SCANMAT center, Department of Physics, Central University of Tamil Nadu, Thiruvarur

Designing new functional materials with higher efficiencies beyond current state-of-the-art based on earth abundant nontoxic materials for renewable energy technologies is key to mitigate the climate change and develop prosperous sustainable society. Hydrogen production by photocatalytic water splitting emerges as a potential approach for a clean, green, and sustainable energy source. Graphene based 2D materials offer enormous opportunities to use as higher efficiency photocatalysts due to large surface area as well as short diffusion length for carriers along with easly tuning their optoelectronic properties. With this idea in mind we are designing new high efficiency photocatalysts using graphene monoxide, graphene dioxide, and derivatives of graphene as a promising candidate for visible light photocatalytic water splitting using solar energy [1-5].

We have studied comprehensively the structural, electronic, and optoelectronic properties of monolayer and few layers of graphene monoxide (GMO) graphene dioxide (GDO) and its S substitution at the O site and (B,N) co-substitution at C-sites. The bonding analysis of pure and substituted systems are made after complete structural relaxation. The overall stability of these compositions were analyzed using formation energy calculation, phonon spectra, and AIMD simulations. Further the DFT calculations on the electronic, optical, charge transport, photocatalytic and photovoltaic properties of GMO with respect to the application of electric field, strain and heterostructure with CdX (X=S, Se or Te) are made. From these analyses, we found that band engineering strategies such as isoelectronic substitution, electric field, strain and heterostructure building are giving promising results to use them as visible light photocatalyst or efficient energy harvesting from solar spectrum through solar cells. We have also demonstrated that the influence of molecular adsorbates such as H_2, F_2, Cl_2, Br_2, and I_2 on the electronic properties and photocatalytic activity of the nitrogenated holey graphene (C_2N) using hybrid density functional calculations including van der Waals interaction.

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Modelling of Transition Metal Based Catalyst for Hydrogenation of CO_2 towards Fuel

Krishnakanta Mondal

Department of Physics and Astrophysics, University of Delhi, India-110007

Mankind is living under the growing threat of global warming because of the increasing level of man made greenhouse gases, particularly CO_2, in the environment. The recycling of CO_2 gas from the environment would be a possible way to tackle this problem. The storage of CO_2 through the formation of fuel is a practical way to control the CO_2 level in the environment. This will also help to fight against the crisis of fuel. In this direction a large number of research activities are being carried out around the world [1, 2, 3]. The hydrogenation of CO_2 towards methanol, which can be mixed with gasoline to fuel motor vehicles, is found to be a successful route to recycle CO_2. For optimizing this process the production of hydrogen plays a key role. To this end, I will discuss various models based on the industrially known ZnO/Cu catalyst for CO_2 to methanol conversion[3, 4, 5]. I will focus on the possible configuration of the active sites and the reaction pathways. In addition, I will discuss how incorporating nitrogen can enhance the efficiency of the ZnO/Cu catalyst. I will end my discussion with our findings on the role of d-orbitals for the adsorption & activation of CO_2 and hydrogen production from water[6].

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DFT studies of Fe oxyhydroxide Nanostructures in Water: Structure and OER Activity

Bidisa Das
Research Institute for Sustainable Energy (RISE)
TCG-CREST, Sector V, Salt Lake, Kolkata 700091
Email: bidisa.das@tcgcrest.org

Nanostructured minerals like Fe oxyhydroxides are responsible for geochemical cycling and mobility of numerous nutrients and contaminants in the environment. Such processes involve multinuclear Fe oxyhydroxide clusters in aquatic environments which form during early-stage polymerisation processes.[1] We used these nanostructures as model systems to theoretically study various chemical processes occurring in the environment, for example, surface adsorption of contaminant ions and catalysis.[2,3] Key to these predictions is the microscopic insights of the reactions which starts with understanding the hydrolytic and subsequent polymerization steps of Fe(III) ions in aqueous solutions. We employed electronic structure methods to study the formation of the dimeric Fe oxyhydroxide clusters in an aqueous medium and investigated the mechanistic pathways of formation from the hydrated monomeric ions.[4] We then examined Fe-oxyhydroxides for catalytic applications, specifically for Oxygen Evolution Reaction (OER). Due to poor conductivity, the electrocatalytic performance of lab-synthesized solid Fe oxyhydroxides were reported inferior compared to *in situ* synthesized electrocatalyst for OER in earlier experimental studies. We therefore first explored Fe oxyhydroxide nanoclusters for OER, in aquoeus medium which might form *in-situ* and studied the step-wise reaction mechanism and reaction free energies.[5] We systematically compared the catalytic performances of pure and transition metal doped Fe oxyhydroxide clusters. We then also modelled the layered Fe oxyhydroxide surfaces for OER activity. The overall understanding obtained from these studies spanning different length-scales helps in the strategic development of more effective catalysts for OER from low-cost earth-abundant minerals, contributing to progress in renewable energy technologies.

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Electronic descriptors for metal center catalysts to define C_2 product selectivity during CO_2ER

Ranjit Thapa

Department of Physics & Centre for Computational and Integrative Sciences, SRM University AP, Amaravati 522 240 Andhra Pradesh, India

The industrial era's excessive fossil fuel use has led to a significant rise in CO_2 emissions over the past century, reaching approximately 40 billion tons annually, with a sharp increase from 25 billion tons in 2000 to the 2020 level. To combat this, the development of technology capable of capturing and converting CO_2 into useful products is imperative for achieving a carbon-neutral environment. While CO_2ER predominantly yields single carbon products (C_1 products) with high efficiency, there is a growing interest in producing double carbon products (ethanol, C_2 products) due to their higher energy density and greater industrial significance. However, the complexity of C_2 product formation, involving C-C bond formation, presents challenges as it competes with the hydrogenation of *CO to *CHO, reducing C_2 product efficiency.

We introduce a screening protocol that leverages density functional theory calculations to optimize catalysts across multiple criteria. This approach enables the identification of catalysts with both high selectivity and minimal overpotential towards C_2 product formation. We introduce an innovative graphical method and C_2 vs C_1 parity plot to facilitate this screening process. We believe that this user-friendly graphical screening technique for CO_2 electroreduction catalysts has the potential to gain widespread adoption, possibly becoming as prevalent as 'volcano plots' in other reaction analyses. we have reported the charge disparity index (CDI) as electronic descriptor to explain the fundamental criteria as well as to predict the possibility of ethanol formation by prohibiting competing and parallel pathway of C_1 product or hydrogen formation in CO_2ER.

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Structure and reactivity of fullerenes and their derivatives

Utpal Sarkar

Department of Physics, Assam University, Silchar-788011, Assam, India.
Email: utpalchemiitkgp@yahoo.com

The geometrical structure and stability of fullerenes and their doped derivatives have been a subject of interest for researchers worldwide due to their unique chemical features as well as fascinating physical properties, and are frequently employed in various fields of nano-applications *e.g.* photovoltaic devices, molecular switches, sensing devices, spintronics, drug delivery, radiotherapy, medical imaging *etc*. Different properties of a series of fullerenes (C_{24} to C_{50}) and its endohedral counterpart [1] will be discussed. Their chemical reactivity parameters [2], bonding nature and energy components will be discussed in addition to the absorption spectrum of these systems. We designed a donor−acceptor dual complex where fullerene acts as a donor component. The static and dynamic characteristics of anthracene-fullerene intermolecular complex, in their ground and excited states that provides valuable insights into their respective reactivity behaviors, will be discussed along with the dynamical behavior of the complex for seven trajectories [3]. A combination of *ab initio* molecular dynamics and time-dependent density functional theory is employed to study not only the system's behavior in the excited state but also the temporal evolution of chemical reactivity parameters when it moves in a particular excited state. It shows greater reactivity in the excited state as compared to that in the ground state.

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Thermal expansion in cross-coupled order parameter oxides

Hena Das

Laboratory for Materials and Structures, Institute of Integrated Research (IIR), Institute of Science Tokyo, 4259 Nagatsuta, Midori-ku, Yokohama, Kanagawa 226-8503, Japan

Kanagawa Institute of Industrial Science and Technology (KISTEC), 705-1 Shimoimaizumi, Ebina 243-0435, Japan

e-mail: *das.h.aa@m.titech.ac.jp*

Phase transitions and quantum phenomena in materials with multiple order parameters and cross-coupling between them are of utmost importance. Our research focuses on understanding how the presence and competition among multiple order parameters influence quantum phenomena in materials, like magnetism, magnetoelectricity, non-trivial topological phenomena, and thermal expansion. In this talk, I will delve into the microscopic origin of the uniaxial negative thermal expansion (NTE) observed in the Ca_2RuO_4. This system exhibited a giant volumetric negative thermal expansion of 6.7% within the temperature range of 135 - 345 K [1]. As temperature increased, the system underwent shrinkage and expansion of the crystallographic $\boldsymbol{b}$ and $\boldsymbol{c}$ lattice parameters, respectively, in the low-temperature orthorhombic phase. Notably, the thermal expansion along the crystallographic $\boldsymbol{a}$-axis remained virtually constant throughout this temperature range [2]. In my presentation, I will discuss the mechanism of uniaxial NTE in Ca_2RuO_4. I will explore how the interactions among different order parameters influence the thermal expansion characteristics of this system, highlighting the importance of higher-order anharmonic effects, which deviate from the quasi-harmonic approximation (QHA), in understanding thermal expansion in Ca_2RuO_4 and related systems.

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Exploration of some efficient high temperature thermoelectric materials: a focus on half Heuslers

Prakash Khatri[1, 2], Ashesh Giri[1], Kashi Ram Panday[1], Govinda Gaire[1], Nabin Regmi[1], Hari Krishna Neupane[1], Narayan Prasad Adhikari[1,*]

[1]*Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, 44613, Nepal*

[2]*Department of Physics, Siddhanath Science Campus, Tribhuvan University, Mahendranagar, 10406, Nepal*

*Corresponding Email**: narayan.adhikari@cdp.tu.edu.np

Abstract

Half Heusler (HH) compounds are promising materials for enhanced thermoelectric performance at high temperatures. In this study, we examined the stability, electronic, phonon, and thermoelectric properties of several 18-valence electron count hH compounds, including XFeTe (X = Ti, Hf), XNiAs (X = Sc, Y), NbXBi (X = Ru, Os), and XIrY (X = Nb, Ta; Y = Pb). We used density functional theory (DFT) and semi-classical Boltzmann transport theory to assess these properties. All the compounds studied are thermodynamically, dynamically, and mechanically stable. Spin-orbit interactions were taken into account for compounds containing the heavy elements Pb and Bi. The compounds are non-magnetic semiconductors, each having a band gap of less than 1.00 eV. All the compounds show better stiffness, ductility, hardness, elastic anisotropy, and melting points, except for HfFeTe, which lacks ductility. The compounds with heavier elements like Bi or Pb have lattice thermal conductivity below $11\ \mathrm{Wm^{-1}K^{-1}}$, while the others have higher values. Except for the XNiAs compounds with flat bands, the other compounds exhibit a zT around 1 or higher in the high-temperature range, due to their suitable electronic structure and low lattice thermal conductivity. For XFeTe and XNiAs, electrons demonstrate superior transport properties compared to holes, whereas the opposite is observed in the other compounds. Among the studied compounds, TiFeTe achieves the highest zT of 1.79 at 1200 K for electrons. Our observations indicate that the doped hH compounds are promising candidates for high temperature power generation.

Improved Thermoelectric Properties of Doped and Strained XCaB (X-Li, Na, K) Alloys

Bulumoni Kalita and Geetimallika Das

Department of Physics, Dibrugarh University, Assam 786004, India

Thermoelectric power generators (TEGs) can provide efficient solution by directly converting waste heat into electricity [1]. The efficiency of a thermoelectric material is represented with a dimensionless physical quantity called figure of merit (*ZT*) defined as $(S^2\sigma)T/\kappa_{tot}$. Here S, σ, T and κ_{tot} represent Seebeck coefficient, electrical conductivity, temperature and total thermal conductivity, respectively. κ_{tot} is a combination of electronic (κ_{el}) and lattice (κ_l) thermal conductivities. A good thermoelectric material is characterized by a higher power factor ($PF=S^2\sigma$) and lower κ_{tot}, resulting in higher *ZT* value. Half-Heusler (HH) alloys, a group of potential eco-friendly thermoelectric compounds possessing high *ZT* value and having the advantage of operating in the moderate temperature range [2]. A HH alloy, *LiCaB* with VEC (valence electron count) value of 6 possesses relatively higher structural, dynamical and mechanical stability among *XCaB* (X = Li, Na, K) alloys. *In* doping in *LiCaB* causes significant reduction in κ_l due to increased phonon scattering. The lowest κ_l is recorded to be 1.25 *W/mK* (800K) for 25% doping concentration in *LiCaB* ($Li_{0.75}In_{0.25}CaB$), which is ~79% lower than that of pristine *LiCaB* (5.94 *W/mK*). Ductility increases with isotropic compressive strain (≤10%) in both pristine and *In* doped *LiCaB*, which detests κ_l and favours ZT_{tot}. κ_l value as low as 1.34 *W/mK* could be achieved for *LiCaB* with application of 10% compressive strain and this is even lowered down to 0.45 *W/mK* in $Li_{0.75}In_{0.25}CaB$. This in turn improves ZT_{tot} from ~0.56 to ~0.75 at 800K in strained *LiCaB* retaining ferromagnetic and half-metallic behaviour of the alloy. ZT_{tot} increases slightly to 0.59 in $Li_{0.75}In_{0.25}CaB$ followed by a significant boosting up to 0.80 when introduced with compressive strain of 8%.

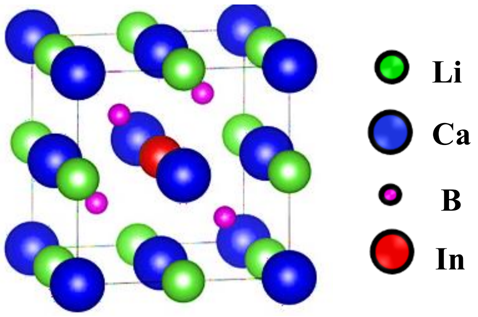

Fig. Crystal Structure of $Li_{0.75}In_{0.25}CaB$

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DAY 1 : 19 May 2025

Session 3

Rashba and Zeeman effects in Non-magnetic MXene

Himangshu Sekhar Sharma[1], Kunal Dutta[2], Indra Dasgupta[2] and Subhradip Ghosh[1]

[1]Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039
[2]School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata-700032

In this work, we have conducted a detailed investigation of possible spin-orbit coupling induced novel physical effects in Ta_2CS_2, a member of MXene family of two-dimensional compounds First-principles calculations, supplemented by a model Hamiltonian, demonstrate the presence of both linear and higher-order Rashba effects at the Brillouin zone center. Additionally, we find valley-dependent Zeeman-type spin splitting at the non-TRIM points. Interestingly, we identify opposite spin-band splitting at these non-TRIM points, which arises from a complex orbital composition that induces an intrinsic orbital moment, influencing the spin splitting. The nontrivial spin splitting observed at high-symmetry points is governed by both local symmetry and orbital composition. Our findings indicate that This Mxene shares key physical properties with transition metal dichalcogenides (TMDs), making it a promising candidate for spintronic and valleytronic applications.

Magnetic skyrmions on the noncollinear ground state

Mathews Benny[1,†], **Moinak Ghosh**[2,†], **Stefan Heinze**[3,4], **Souvik Paul**[1,2]

[1]School of Physics, Indian Institute of Science Education and Research Thiruvananthapuram,
Thiruvananthapuram, Kerala 695551, India

[2]Center for High-Performance Computing, Indian Institute of Science Education and Research
Thiruvananthapuram, Thiruvananthapuram, Kerala 695551, India

[3]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel,
Leibnizstrasse 15, 24098 Kiel, Germany

[4]Kiel Nano, Surface, and Interface Science (KiNSIS), Christian-Albrechts-Universität zu Kiel,
Christian-Albrechts-Platz 4, 24118 Kiel, Germany

[†]These authors contributed equally to this work.

Email: souvikpaul@iisertvm.ac.in

Magnetic skyrmions — topologically protected swirling spin structures — generate enormous interest as potential building blocks for next generation spintronic devices. Their nanoscale size and intrinsic protection against external perturbations make them particularly promising for technological applications.

So far, skyrmions have been observed as metastable states on the ferromagnetic, anitferromagnetic and ferrimagnetic ground state. However, a more general class of topological spin structures can be conceptualized, where skyrmions appear as metastable states on the noncollinear spin configuration rather than on the conventional collinear ones.

In this talk, I will explore the possibility of realizing such skyrmions in transition-metal ultrathin films and discuss their spin structure and stability.

Interplay of SOC and Coulomb Interaction – Route to Unconventional Magnetism

Tanusri Saha-Dasgupta

S.N.Bose National Centre for Basic Sciences, Kolkata

In this talk, I will discuss two examples of SOC driven unconventional magnetism, one on possible realization of Quantum spin Liquid phase in cobaltates [1,2] and another on Multipolar Magnetism in Vacancy-ordered Perovskites [3].

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[2] Anjishnu Bose, Manodip Routh, Sreekar Voleti, Sudip Kumar Saha, Manoranjan Kumar, Tanusri Saha-Dasgupta, and Arun Paramekanti, PRB 108, 174422.
[3] Koushik Pradhan, Arun Paramekanti, and Tanusri Saha-Dasgupta, PRB 109, 184416 (Editor's suggestion).

Complex Chiral Magnetism in Quasi-2D Fe_4GeTe_2

Debjani Karmakar[1,2,3]

[1]Technical Physics Division, Bhabha Atomic Research Centre, Mumbai, 400085, India
[2]Homi Bhabha National Institute, Anushaktinagar, Mumbai, 400094, India
[3]Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120, Uppsala, Sweden

In recent times, the series Fe_nGeTe_2 (n = 3,4,5) (FnGT) were identified with the potential to generate a room-temperature ferromagnetic (FM) order, where, an intralayer 3D-like magnetic network was created after incorporating Fe within a Ge-layer. A few such magnetic layers are encapsulated within the Te-ligand layers. The experimentally obtained T_c for n = 3, 4 and 5 are 220 K, 280 K and 310 K respectively, indicating a monotonous rise of T_c with an increasing Fe content. The middle member of this series, Fe_4GeTe_2 (F4GT), is experimentally known to be the most interesting one, where, the magnetic and magnetothermal measurements revealed a multitude of phase-transformations, indicating an underlying complex interplay of electron correlation, temperature-dependent magnetocrystalline anisotropy, field-induced symmetry breaking, X-ray spectral properties, anisotropic intersite exchange and dynamical magnetism. A complete picture of all these tangled attributes is not yet available in the existing literature leading to a defragmented understanding of the experimental and theoretical analysis of the system.

We have explored the magnetism in the quasi-2D F4GT compounds with a wide range of first-principles methodologies. Treatment of dynamical electronic correlations with DFT+DMFT+SOC reveals a directional dependence of the field-induced symmetry breaking leading to the opening of a pseudo-gap around Γ-point near T_{SRT} and presence of linearly dispersive band-crossing near E_F. The 2D planar Fermi Surface and its spin-polarization map corroborates with this observation. The x-ray spectral properties extracted with DFT+DMFT+MLFT have a good agreement with the experimental data. The ab-initio extracted intersite exchange interactions indicate an RKKY-like oscillatory behaviour for all pairwise interactions between Fe_1 and Fe_2 as well as the presence of significant DM interactions. The calculated phase diagram and the corresponding dynamical magnetic textures show four distinct regions bearing substantial differences of the underlying long range orders for the two inequivalent sites of Fe. The underlying complex chiral spin textures extracted by taking into account the dynamical properties of the spin, explains the experimental observations of multiple phase-transformations quite successfully.

Dynamical electronic correlation and chiral magnetism in van der Waals magnet Fe_4GeTe_2, Md. Nur Hasan, Nastaran Salehi, Felix Sorgenfrei, Anna Delin, Igor Di Marco, Anders Bergman, Manuel Pereiro, Patrik Thunström, Olle Eriksson and Debjani Karmakar. (Under review)

Intriguing Tale of van-der-Waals Magnets: Interplay of Unusual Structural Reconstruction, Exchange Mechanism and Electron Correlation

Sukanya Ghosh

Department of Physics, Central University of Kashmir, Tulmulla Campus, Ganderbal, J & K 191131, India

In recent years, the discovery of van der Waals (vdW) magnets has opened up numerous possibilities in fundamental science and technological applications. Their tunable structural, electronic, and magnetic properties make these materials promising candidates for low-power spintronic devices. Among these, the family of metallic magnets Fe_nGeTe_2 (where n = 3, 4, 5) has garnered significant attention due to their high Curie temperatures and fascinating physical characteristics.

Our research on the Fe_nGeTe systems began with an investigation into the unusual structural reconstructions observed in Fe_5GeTe_2, the most complex member of this family. By conducting density functional theory (DFT) calculations and Monte Carlo simulations, we discovered that the magnetic peculiarities associated with a specific iron (Fe) site are responsible for this structural behavior[1]. Once we resolved this puzzle, we became interested in exploring the entire Fe_nGeTe_2 family. However, we soon realized that the literature lacked a suitable computational approach to accurately capture the site-dependent electronic and magnetic properties, as well as the correct spectral features of these systems. The presence of Fe-site-dependent electron correlation effects further complicated this task. To address this, we employed three different ab initio approaches: (i) standard DFT, (ii) DFT with static electron correlation (DFT + U), and (iii) DFT combined with dynamic electron correlation effects (DFT + DMFT)[2]. Our results indicate that DFT + DMFT is the most accurate technique for capturing the many-body effects present in Fe_nGeTe systems and reproducing the experimentally reported transition temperatures and spectral properties[2]. Additionally, we explored ways to enhance the magnetism of this class of systems beyond room temperature[3]. My talk will cover the intricate story of the FGT family in the monolayer limit, proposing their applicability in spintronic applications[4].

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[2] S. Ghosh et al. npj Comput Mater **9,** 86 (2023)
[3] S. Ghosh et al. 2D Mater. **11**, 035002 (2024)
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Modelling spin-orbitronics effects at inorganic interfaces and through chiral molecules

Poonam Kumari, Cyrille Barreteau and Alexander Smogunov

Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

Spin-orbitronics is an emerging field that leverages not only the spin magnetization but also the generation of orbital angular momentum (OAM) currents in nanoelectronics. In this talk I will present results based on density functional theory (DFT) and the real-time dynamics of electronic wave packets to explore the possibility of generation and propagation of spin and orbital currents.

I will first present the case of the two interfaces $\mathrm{LaAlO_3}$/$\mathrm{SrTiO_3}$[1] and Cu/O[2, 3] where a strong OAM appears at the interface due to the existence of an orbital Rashba effect (ORE). ORE is the orbital counterpart of spin Rashba but that does not require any spin-orbit coupling (SOC). Then I will consider the propagation of this OAM across the interface Cu/O via wave-packet real-time dynamics. Interestingly it comes out that the OAM is very quickly dying away from the interface due to orbital quenching in Cu bulk, but the presence of SOC generate spin-dependent transmission.

In a second part I will present the case of a very different model system: a chiral cumulene molecule connected to two semi-infinite monatomic carbon chains[3]. For this molecular junction, the mixing of the carbon p_x and p_y (degenerate) channels by the chiral molecular orbital gives rise not only to an efficient generation of orbital current but also to its long-range propagation along the carbon chain. This orbital current is not converted to spin current due to very small SOC in carbon. However our calculations strongly suggest that the so-called chiral induced spin selectivity (CISS) effect could in fact be due to the conjunction of chiral-induced orbital selectrivity (CIOS) and SOC as also suggested by a recent work[4].

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[2] Go, D. et al, Phys. Rev. B.. **103**, L121113 (2021).
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[4] Göbel B., Schimpf L., Mertig I., arXiv:2502.04978v1 (2025).

Electronic Structure of Altermagnetic Materials: A Chemical Bonding Perspective

Birabar Ranjit Kumar Nanda

Indian Institute of Technology Madras

In the domain of condensed matter physics, a new buzzword has emerged and it is altermagnetism. While some are claiming it as a new collinear magnetic quantum state, the others are claiming that this quantum state was already known. In the first part of the talk, we will distinguish the altermagnetism from the conventional ferromagnetism and antiferromagnetism. Through a brief literature survey, we will highlight how the group theoretical analysis is a successful tool in designing a binary selection rule to identify probable altermagnetic materials. In the second part of the talk, by examining the strongly correlated electron system, NiS, we will explore the deterministic role of the chemical bonding in developing a quantitative description of altermagnetism. Finally, we will discuss the possible ways of tuning the altermagnetism.

[1] A. Mandal, A. Das, and B. R. K. Nanda, arXiv:2501.00453

Altermagnetism from nonsymmorphic symmetry

Nirmal Ganguli

Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhauri, Bhopal 462066, India

Besides hosting several intriguing physical properties, the recently discovered time-reversal-asymmetric antiferromagnets, known as altermagnets, hold immense promise for technologies based on spintronics, thanks to the possibility of spin-splitter torque and linear dispersion of THz-frequency chiral magnons. Understanding the symmetry conditions leading to the spin-splitting becomes the key to further progress in the field. With examples of hexagonal MnTe [1, 2] and orthorhombic $\mathrm{BiFeO_3}$ and $\mathrm{CaMnO_3}$ [3], we will demonstrate why the manifestation of altermagnetism requires nonsymmorphic symmetry in the crystal system, although it does not guarantee altermagnetism. Further, we will discuss how local symmetry may enforce partial spin degeneracy and how that may impact the chiral magnons. Additionally, spin-orbit interaction induced weak ferromagnetism anomalous Hall effect will be discussed.

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Interplay of altermagnetism and pressure

Awadhesh Narayan

Indian Institute of Science, Bengaluru

Alternative magnetic materials, or “altermagnets,” characterized by their unconventional nonrelativistic, momentum-dependent spin-split states, represent a new direction in the field of collinear magnetism [1]. Among these materials, hexagonal MnTe has emerged as a standout candidate for its substantial spin-splitting [2,3]. In this talk, I will present our investigations into the interplay of altermagnetism and pressure in two main phases of MnTe by means of first-principles electronic structure calculations and spin group symmetry analysis [4]. Our results underscore the pivotal role of pressure as a tuning parameter for the alternative magnetic traits in the system. Furthermore, we identify a second phase of MnTe with orthorhombic structure, namely γ-MnTe, hosting altermagnetic characteristics.

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[2] J. Krempasky et al., Nature 626, 517 (2024).
[3] T. Osumi et al., Phys. Rev. B 109, 115102 (2024).
[4] N. Devaraj, A. Bose, and A. Narayan, Phys. Rev. Materials 8, 104407 (2024).

DAY 2 : 20 May 2025

Session 1

Rapid Exploration of Crystal Chemical Space

Aron Walsh

Department of Materials, Imperial College London, United Kingdom

Traditional materials modelling workflows, even in the form of high-throughput approaches, are limited to small numbers of compositions and structures. I will present progress in materials informatics solutions for navigating a larger crystal chemical space. This includes techniques for compositional screening based on elemental features and mapping from chemical formulae to three-dimensional crystal structures [1,2]. A focus will be placed on hand-built chemical filters to reduce the magnitude of the search space and filters that are learned from data in the form of deep learning models based on crystal graphs. The performance of data-driven and domain knowledge-inspired approaches will be compared. Outstanding challenges in the field including robust synthesisability metrics [4] and generative artificial intelligence models for sampling new materials will also be discussed.

[1] D. W. Davies et al, "Computational Screening of all Stoichiometric Inorganic Materials", Chem **1**, 617 (2016)
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High-Throughput Computational Materials Design

Laalitha Liyanage, University of Kelaniya

Andrew Supka, Central Michigan University

Priya Gopal, Central Michigan University

Luis Agapito, University of North Texas

Gus Hart, Brigham Young University

Marco Fornari, Central Michigan University

Stefano Curtarolo, Duke University

Marco Buongiorno Nardelli, University of North Texas

Abstract: High-throughput (HT) density functional theory (DFT) has become an indispensable tool for rapid computational screening and accelerated discovery of novel materials. However, conventional DFT methods exhibit well-known limitations in treating strongly correlated systems, particularly those containing transition metals, where self-interaction errors lead to inaccurate electronic structure predictions. To address this challenge, corrective approaches such as DFT+U and hybrid functionals are essential, though their empirical parameterization often limits predictive reliability.

The Agapito-Curtarolo-Buongiorno Nardelli (ACBN0) functional—a first-principles, pseudo-hybrid Hubbard extension of DFT+U—which provides a parameter-free framework for first principles methodology derives the Hubbard U parameter without empirical inputs at the computational cost comparable to post-processing tasks in regular DFT. ACBN0 employs a projection onto localized atomic orbitals to self-consistently determine Hubbard U parameters, enabling automated, high-throughput workflows. We demonstrate its efficacy through the derivation of Hubbard U parameter for A, B and O of 3969 cubic perovskites (ABO3) built by permutating 63 different elements in the A and B sites which was carried out within the AFLOWπ computational infrastructure.

To further enhance computational efficiency, a machine learning (ML) model trained on ACBN0-derived U values is developed, enabling rapid estimation of Hubbard corrections for new compositions. This data-driven approach significantly reduces the cost of first-principles screening while retaining accuracy. By integrating HT-DFT, ab initio Hubbard corrections, and ML, this work establishes a robust pipeline for accelerated materials design, bridging the gap between high-fidelity electronic structure theory and large-scale materials informatics.

Ab-initio Temperature Concentration Phase Diagrams

Jan Janssen

Max-Planck-Institute for Sustainable Materials

Starting from the interactions of the electrons the phase stability in dependence of the temperature and chemical concentration is predicted, including thermodynamic vibrations and anharmonicity. This is achieved by fitting machine learned interatomic potentials (MLIP) to a diverse set of Density Functional Theory (DFT) calculation and employing the MLIPs for computationally efficient sampling of the potential energy surface[1]. Achieving qualitative agreement with temperature concentration phase diagrams constructed from experimental measurements. This highlights the impact of ab-initio materials design.

The resulting increase in technical complexity of coupling simulation codes for different scales is addressed by the pyiron workflow framework[2]. pyiron provides a Jupyter notebook interface for rapid prototyping and up-scaling simulation workflows for High Performance Computing (HPC), enabling a data-driven approach to materials design.

The presentation addresses the challenge of calculating temperature concentration phase diagrams with a focus on the impact of exchange correlation functionals, precision in terms of plane wave energy cut-off and k-point mesh, and the computational efficiency. It highlights the impact of automated workflows and demonstrate the qualitative agreement of ab-initio temperature concentration phase diagrams in comparison to experiment.

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Toward General-Purpose Machine Learning Interatomic Potentials

Stefano de Gironcoli

Scuola Internazionale Superiore di Studi Avanzati (SISSA) - Trieste

Machine learning interatomic potentials are transforming atomistic simulations promising to deliver the accuracy of first-principles calculations at a fraction of their cost. It is now established that accurate potentials can be obtained for a specific system if enough accurate data of all the relevant phases are computed and included in the training phase. A number of state-of-the-art architechtures have been proposed to this end. Challenges remain to develop general-purpose ”foundational” models which can deal accurately and efficiently with systems of arbitrary stoichiometry, interpolating in the chemical space, incorporating long-range electrostatics for metals and insulators as well as van der Waals interactions when necessary, and efficiently leveraging the wealth of, not necessarily mutually consistent, ab-initio calculations available, avoiding as much as possible the need to repeat expensive calculations to improve consistency and chemical/structural coverage. I’ll discuss some of these issues and our attempts to address them [1, 2, 3, 4, 5].

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Machine Learning-Assisted Design and DFT Validation of High Entropy Na-Deficient Cathode Materials

Amreen Bano

Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology (TCG CREST), Sector V, Salt Lake, Kolkata 700091, India

This work focuses on the optimization of high entropy (HE) Na-deficient cathode material, $Na_{0.62}Ni_{0.33}Mn_{0.67}O_2$ (NNMO) [1], by incorporating various substituents (Mg, Cu and Ti) in different compositions to enhance its performance. Using MACE-MP0 model [2] of machine learning-based interatomic potentials (MLIP) and Atomic Simulation Environment (ASE) optimization, the energetically favourable compositions were predicted and subsequently validated through density functional theory (DFT) analysis. These compositions underwent rigorous analysis of structural degradation, electronic structure, cation and anion redox activity, changes in bonding environment, and voltage profiles via density functional theory (DFT). Experimental validation of computational predictions revealed excellent agreement with theoretical results, reinforcing the reliability of the approach. This comprehensive study integrates computational and experimental methodologies to pioneer advanced cathode material design, with promising implications for sodium-ion battery innovation.

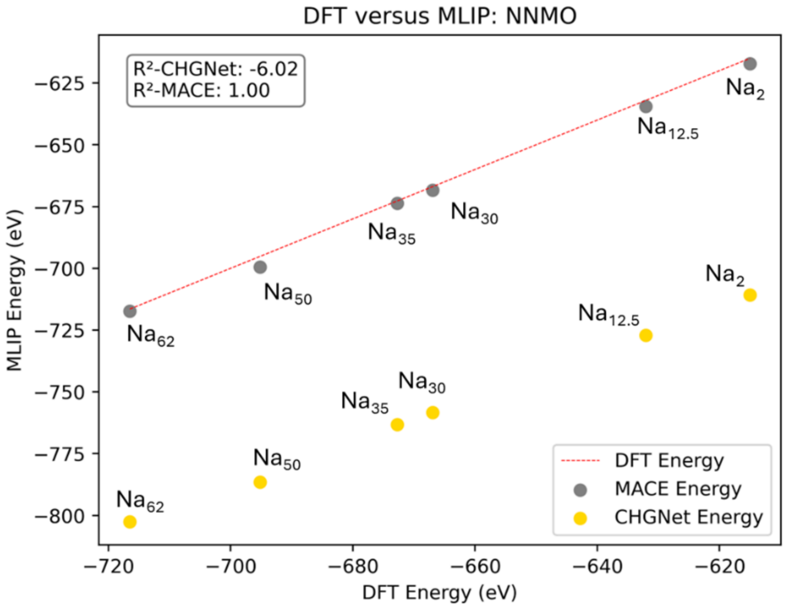

Figure 1: Linear fitting of energies obtained by MLIPs: MACE and ChgNet with DFT. MACE vs DFT are found in good overlapping.

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Machine Learning Guided Exploration of Amorphous Electrodes and Electrolytes

Aqshat Seth, Vijay Choyal, Debsundar Dey, and Sai Gautam Gopalakrishnan

Department of Materials Engineering, Indian Institute of Science, Bengaluru 560012

The state of the art in energy storage technologies, namely lithium-ion and solid-state batteries, are made viable due to the use of robust crystalline materials that are used as electrodes and/or solid electrolytes. However, there are fundamental limitations in the properties that can be accessed within crystalline materials, owing to bonding, symmetry, and ordering constraints. For example, crystalline materials typically do not exhibit good ionic conductivity for multivalent ions (such as Mg, Ca, etc.), which is a critical bottleneck in the development of multivalent batteries. Similarly, the defective regions that form across a metallic anode||crystalline solid electrolyte interfaces typically cause a spike in the electric field, eventually resulting in metal dendrite nucleation and propagation. Such limitations of crystalline materials can be mitigated, to an extent, by the use of (metastable) amorphous materials. Thus, in my talk, I will present some of our recent work on modelling and understanding possible amorphous electrodes, electrolytes, and their interfaces that are relevant for energy storage systems. Using a combination of density functional theory based calculations, ab initio molecular dynamics, and trained machine learned interatomic potentials, I will highlight our work on characterising ionic transport and reaction energies within bulk electrodes, solid electrolytes, and their interfaces, where the bulk materials can also adopt an amorphous form. I hope that our study will kickstart further work on utilising amorphous materials to a greater extent in battery systems.

Predicting thermochemical equilibria with interacting defects:

$Sr_{1-x}Ce_xMnO_{3-\delta}$ alloys for water splitting

Anuj Goyal[1*], Michael D. Sanders[2], Ryan P. O'Hayre[2], Stephan Lany[3]

[1] Department of Materials Science and Metallurgical Engineering, IIT Hyderabad
Sangareddy, Kandi, Telangana 502284, India

[2]Metallurgical and Materials Engineering, Colorado School of Mines
1500 Illinois St, Golden CO 80401, USA

[3]National Renewable Energy Laboratory
Golden CO 80401, USA

[*]E-Mail: anujgoyal@msme.iith.ac.in

Solar thermochemical hydrogen is one of the few potential routes toward direct fuel production from renewable energy sources, but the thermodynamic boundary conditions for efficient and economic energy conversion are challenging. Success or failure of a given oxide working material depends on the subtle balance between enthalpy and entropy contributions in the redox processes. Developing a mechanistic understanding of materials behavior on the basis of atomistic models and first-principles calculations is an important part of advancing the technology. One challenge is to quantitatively predict thermochemical equilibria at high concentrations when the redox active defects start to interact with each other, thereby impeding the formation of additional defects. This problem is of more general importance to applications that rely on high levels of off-stoichiometry or doping, including, e.g., batteries, thermos-electrics, and ceramic fuel cells. To account for such repulsive defect interactions, we introduce here a statistical mechanics approach, defining an expression for the free energy of defect interaction based on a limited sampling of defect configurations in density functional theory supercell calculations. The parameterization of this energy contribution as function of defect concentration and temperature allows for on-the-fly simulation of thermo-chemical equilibria. We demonstrate the capability and utility of the approach by simulating the water-splitting redox processes for $Sr_{1-x}Ce_xMnO_{3-\delta}$ alloys.

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Isotopes as proxies to understand earth system processes: The role of first-principles calculations

Swastika Chatterjee

*National Centre for High-Pressure studies and Department of Earth Sciences,
IISER-Kolkata, Nadia, West Bengal, India.*

Isotopes of different elements are known to partition/fractionate between co-existing phases in natural systems. Such ‘isotopic fractionation’ data can not only be utilized to understand the pressure and temperature conditions experienced by the rocks and minerals but also gain insight into the history of time-scales involved. As a result it offers a powerful tool to interrogate a range of scientific problems from the origin of the terrestrial planets, the past climate change, to igneous processes and the source of elements in a variety geological reservoirs. Isotopic fractionation may occur either due to an equilibrium or a kinetic process. In this talk I am going to take up one example of each [1,2] and discuss the pivotal role played by first-principles calculations in understanding the processes involved and also decrypt the isotopic signature.

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Metal Organic Frameworks for the detection and storage of small gases

D. Adhikari, R. Karki, K. Adhikari and **N. Pantha**

Central Department of Physics, Tribhuvan University , Kathmandu, Nepal

Metal organic frameworks are porous materials where the reactive metal sites are linked with the organic ligends. The materials have exceptionally high surface area and their pore size along with electronic/magnetic properties are tunable via proper selection of linkers and metal atoms [1]. We use Mg-MOF-74 (where Mg acts as metal center) to detect and adsorb small gas molecules which are environmentally significant (toxic and pollutant). Density functional theory based first principles calculations have been employed in Gaussian-09 and Quantum ESPRESSO suites of the programs to study adsorption properties of small gases on MOFs. Change in HOMO-LUMO gap upon the adsorption of gas molecules may refer its relevancy in sensor applications [2]. The adsorption behaviour and change in electronic properties further reveal the nature and strength of binding during the host-guest interaction.

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Computational Studies to Explore Metal Organic Frameworks for Energy Related Applications

Dr. Srinivasu Kancharlapalli

Structural & Theoretical Chemistry Section, Chemistry Division,
Bhabha Atomic Research Centre, Mumbai-400085, India
Email: ksvasu@barc.gov.in

Metal organic frameworks (MOFs) are a new class of inorganic-organic hybrid ordered materials with potential applications for separation and storage of different important gases like H_2, CO_2, CH_4 etc.[1-2] Computational high-throughput screening (HTS) is a powerful tool to screen a large database of materials and identify the top performing candidates for specific application.[4-4] We carried out a systematic computational HTS of computational ready experimental (CoRE)-MOF 2019 database using a multi-scale modeling strategy that includes, machine learning model, density functional theory (DFT) calculations, force field optimization and grand canonical Monte Carlo (GCMC) simulations to identify the top performing MOFs for selective adsorption of CO_2 under wet flue gas conditions. For fast and accurate calculation of atomic charges, we trained and tested a Random Forest machine learning model involving a list of features that represent both the elemental properties and the local bonding environment to predict the partial atomic charges in MOFs accurately.[5] Atomic charges calculated using the machine learning model are used to screen the MOF database using the force field simulations. CO_2 selective MOFs from force field simulations are further screened using the more accurate adsorption energies from DFT calculations. MOFs showing strong affinity towards CO_2 compared to H_2O and N_2 are further studied for their loading capacities and adsorption selectivity by simulating the adsorption isotherms under wet flue gas conditions using GCMC simulations. Our HTS results could find good number of CO_2 selective MOFs and the selectivity is mainly driven by the confinement effects.[6] Entrapment of radioactive noble gases is a challenging issue in nuclear waste management. To address this, we screened a database of around 20,000 MOFs for separation and storage of xenon/krypton mixture. Initial screening using the structural properties were followed by adsorption studied using the GCMC simulations to identify the top 10 MOFs for effective separation of Xe/Kr with high loading capacities and selectivity factors. Shortlisted MOFs are under experimental validation and the preliminary results are consistent with the computational predictions. We have also studied the heavy metal binding in different MOFs and understand the local metal binding environment and selectivity for particular metals. Recently, we have explored the conjugated MOFs for their catalytic activity towards different important reactions like HER, OER and ORR.

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First-Principles Insights into Interstitial–Substitutional Interactions in Titanium Alloys

Dr. N S Harsha Gunda

Indian Institute of Technology Delhi, New Delhi

Titanium's strong affinity for interstitial oxygen dramatically influences its mechanical properties, oxidation resistance, and alloy design potential, particularly in structural and high-temperature environments. Despite its ability to dissolve large amounts of oxygen, titanium exhibits complex behavior when introducing substitutional alloying elements. In this talk, we present a first-principles investigation into the interactions between interstitial oxygen and substitutional solutes in hcp-Ti.

Our calculations reveal a surprising but consistent trend: substitutional solutes that typically form stable oxides in bulk, such as Al and Si, experience strong repulsive interactions with interstitial oxygen when both are dissolved in a Ti matrix[1]. We attribute this repulsion to a combination of localized Coulombic effects arising from charge transfer from the Ti host and electronic hybridization that leads to closed-shell-like repulsion at short distances. To quantify these effects, we employ cluster expansion techniques and Monte Carlo simulations to construct the finite-temperature phase behavior of the Ti-Al-O system[2,3]. Our analysis predicts the stability of a new ternary compound, and reveals how increasing oxygen content lowers the order-disorder transition temperature of α_2-Ti_3Al. The oxygen atoms consistently avoid coordination with Al, enforcing a strong short-range ordering pattern in both disordered solid solutions and ordered intermetallic phases.

These insights offer a mechanistic understanding of oxygen–solute interactions in Ti alloys and demonstrate how targeted alloying strategies can be used to control interstitial behavior, optimize phase stability, and improve oxidation resistance in advanced Ti-based and high-entropy alloy systems.

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Session 2

Excess Electron in Water

Nisanth N. Nair

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, 208016, Uttar Pradesh, India

Solvated electrons play a crucial role in various chemical and biological processes. Here, we study the properties of an excess electron solvated in water under different environments. Accurate modeling of the dynamic behavior of solvated electrons is challenging. To treat solvated excess electron in water, density functional theory (DFT)-based molecular dynamics (MD) with hybrid density functionals is ideal. However, the computational cost of hybrid density functional theory-based MD is about two orders of magnitude higher than Generalized Gradient Approximation (GGA) functional-based MD. To significantly speed up hybrid functional-based MD, and to simulate long trajectories of solvated electrons, we use the Resonance Free Multiple Timestep based Adaptively Compressed Exchange Operator (RF-MTACE) method [1]. Our simulations show that the localization of excess electrons is highly dependent on the structure and dynamics of the immediate hydrogen bonding environment. Most importantly, the spatial arrangements of neighboring water molecules determine the behavior of the solvated electron. Detailed insights into the properties of solvated electrons, as obtained from the long MD simulations of various solvated-electron systems, will be presented during my lecture.

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Ab initio study of point defects in halide solid electrolytes

Tanmoy Paul

Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology, Sector V, Salt Lake, Kolkata 700091, India
and
Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India

Solid-state electrolytes are key component for the development of lithium-all-solid-state batteries. Halide-based solid electrolytes with general formula Li_3ACl_6 (A = Y, Er, In, Sc) have shown high ionic conductivity and oxidative stability. Here excess Li as interstitials, Li deficiencies as vacancies and isovalent/anisovalent substitutions by O and F atoms are treated as defects in halide solid electrolytes and the formation energies have been determined by first principles calculations. The diffusivity of Li, mechanical and thermal stability, and electrochemical windows are studied for the solid electrolytes having monoclinic and trigonal phases respectively. The diffusion pathways along both the c axis and *ab* plane are observed and the activation energies (~ 0.44 eV) and room-temperature Li-ion conductivities for all the structures have been determined. It is found that anisovalent substitution (O_{Cl}) is an effective way to promote Li-ion conductivity for Li_3InCl_6 increasing the ionic conductivity from 1.34 mS/cm to 6.23 mS/cm at room temperature. Whereas isovalent substitution (F_{Cl}) and interstitial (Li_i) defects help to achieve the similar conductivity values as that shown by Li_3YCl_6 and Li_3ErCl_6 solid electrolytes at room temperature. Due to the transition from high symmetry (trigonal) to low symmetry (monoclinic) results a decrease in the bulk modulus. Also, the defect structures have a lower reduction potential compared to sulfide solid electrolytes. The addition of defects also increases the band gaps in all the compounds. These results highlight the importance of defects in halide solid electrolytes for improving all-solid-state batteries.

Unlocking the Thermal Transport in Disordered Solids: A Computational Approach using Wigner Formulation

Anees Pazhedath[1,2]

[1]Defects and Damage Studies Division, Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam 603102, India
[2]Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India

We introduce a theoretical/computational framework that enables us to accurately predict the macroscopic thermal conductivity of compositionally disordered solids from first principles. The framework employs the recently developed Wigner formulation [1] of thermal transport to simulate atomic vibrations in disordered solids; its accuracy is demonstrated by quantitatively rationalizing experiments in the paradigmatic thermal-barrier $LaPO_4$ ceramic, its alloys with $GdPO_4$, and its composites with $La_2Zr_2O_7$; these materials are employed in thermal barrier coatings (TBC) for turbine blades, power production plants, and nuclear industries [2]. We elucidate how the interplay between anharmonicity and compositional disorder determines the thermal properties of these alloys and discuss the fundamental physics underlying the emergence and coexistence of particle-like and wave-like heat-transport mechanisms. Most importantly, we show how the Wigner transport equation correctly describes the thermodynamic limit of a compositionally disordered crystal, while the Boltzmann transport equation does not [3]. The computational scheme introduced here sets the stage for rationalizing thermal transport with quantum accuracy in solids with the compositional-mass disorder, and it will potentially be very useful in developing novel design strategies for TBC materials.

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Accelerating thermal conductivity prediction through machine-learning

Ankit Jain

Mechanical Engineering Department, IIT Bombay

Understanding thermal transport physics in semiconductors is essential for applications like thermoelectric energy conversion, heat dissipation, and microelectronics. Since free electrons are not available, thermal transport in semiconductors occurs through atomic vibrations, which are quantized as phonons. The contribution of phonons to thermal conductivity can be determined by solving the Boltzmann transport equation using ab-initio interatomic force constants. These calculations have demonstrated excellent agreement with experimental results, without the need for fitting parameters when possible. However, calculating interatomic force constants and phonon scattering rates (involving three- and four-phonon processes) remains a significant computational challenge for large-scale applications of this method. In this talk, I will present our group's efforts to overcome this computational bottleneck by using step-wise machine learning for (a) calculating anharmonic interatomic force constants and (b) determining phonon mode scattering rates. When applied to over 200 different materials, these approaches reduced computational time from 480,000 CPU hours to under 12,000 CPU hours.

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Thermal transport in Semiconductors Studied Using a Physics- and Data-Driven Solution of the Peierls-Boltzmann Equation

Navaneetha Krishnan Ravichandran

Department of Mechanical Engineering, Indian Institute of Science Bangalore

Unconventional heat flow regimes such as the wave-like hydrodynamic and Poiseuille phonon flow arise out of strong interactions among phonons in a handful of crystalline insulators. The linearized Peierls-Boltzmann equations (LPBE), which is a set of coupled multi-dimensional first-order partial differential equations, govern the transport of phonons in these systems. Hence, solving the LPBE is the first and important step towards identifying new material candidates that can host these unconventional heat flow phenomena.

However, solving the LPBE from first-principles in a predictive manner including three-phonon, four-phonon and phonon-isotope scattering with the inputs of the interatomic force constants from density functional theory, has been computationally intractable until recently [1, 2]. Even considering these recent advances, the computational cost due to the high dimensionality of the LPBE and the need to resolve the ultrafast (picosecond timescale) coupled dynamics among phonons makes these conventional methods unsuitable for the rapid search of new materials that show exceptional wave-like heat transport.

To address this issue, we have developed a physics- and data-driven approach to solve the LPBE [3], which simultaneously facilitates fast convergence of the LPBE solution under steady-state conditions, and enables high temporal resolution of the coupled dynamics of phonons under transient transport conditions, which is crucial to resolve strongly hydrodynamic phonon flow in materials. We show that, for ultrahigh thermal conductivity materials such as diamond, BAs, graphite and hBN, where hydrodynamic transport is achievable below liquid nitrogen temperatures, the data-driven scheme is significantly faster than the conventional iterative solution of the LPBE under both steady-state and transient conditions. In several situations, where the conventional approach to solve the transient LPBE would take several weeks to converge to the solution, we show that the data-driven approach tracks the transient dynamics of phonons accurately on a single workstation in a timescale of few hours. Our findings highlight the potential of this new data-accelerated first principles framework for the LPBE, which can have drive future materials discovery efforts in a computationally efficient manner.

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Indispensable roles of anharmonic renormalization, high-order scattering and wave-like tunnelling of phonons in ultralow thermal conductivity semiconductors

Koushik Pal

Dept. of Physics, IIT Kanpur, Kanpur UP 208016
koushik@iitk.ac.in

Anharmonic crystalline semiconductors exhibiting ultralow thermal conductivity are both fundamentally and technologically important, where phonon quasiparticles dominate the heat transport. Understanding the microscopic mechanisms that govern phonon heat transport are therefore important to uncover the physics of phonons in the presence of strong anharmonicity and tune them to achieve desired thermal conductivity. Quantum-mechanical investigations of such mechanisms have been enabled by state-of-the-art first-principles calculations based on density functional theory and Peierls Boltzmann transport equation, which in most cases treat phonons within a harmonic approximation, neglecting the renormalization effects that arise at finite temperatures due to anharmonic phonon-phonon interactions. Secondly, most of the theoretical investigations calculate phonon lifetime considering only three-phonon interactions assuming higher-order (e.g., four-phonon) interactions to be negligible. Furthermore, in most of the studies thermal conductivity due to phonons are calculated considering their particle-like propagation (i.e., Peierls picture) where the off-diagonal terms in the phonon group velocity operators are neglected.

In this talk, we present examples of two semiconductors [1, 2] exhibiting ultralow lattice thermal conductivity, where two or more of the above factors become very important. Through detailed and rigorous first-principles calculations and analysis, we demonstrated that an accurate understanding of phonon heat transport mechanisms can only be obtained when we (i) incorporate anharmonic renormalization of phonon quasiparticles at finite temperatures, (ii) consider both third-order and fourth-order phonon scattering processes and (iii) account for the coherence contributions to thermal conductivity that arise from the off-diagonal terms of the phonon group velocity operators. Our unified theoretical approach reproduces the experimental measurements quite well both in terms of magnitude and temperature dependence.

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DFT+DMFT Modeling of Strongly Correlated Electron Systems

N. S. Vidhyadhiraja

JNCASR, Bengaluru

Density-functional theory followed by dynamical mean-field theory (DMFT) has become one of the most employed methods for material-specific investigations of strongly correlated electrons systems [1]. We have been developing interpolating approximations based on finite order perturbation theory for the interacting self-energy of the self-consistent impurity problem arising within DMFT [2]. In this talk, I will discuss the existing approaches, results for a few materials and challenges in subsequent development.

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Distribution of Charge Centers in Matter from Geometric Phases of Electrons

joydeep Bhattahcarjee

School of Physical Sciences
National Institute of Science Education and Research (NISER)
An Autonomous Institute under the Dept. of Atomic Energy, Govt. of India. Bhubaneswar,
PO: Jatani, Dist: Khurda, Odisha, 752050, India

Based on the geometric phases of Bloch electrons, we propose a scheme for the unambiguous spatial partitioning of charge in matter from first-principles, derivable directly from the KohnSham states. Generalizing the fact that geometric phases acquired by electrons, due to the evolution of their crystal momentum in any arbitrary direction throughout the Brillouin zone (BZ), render the location of their spatial localization with net minimum spread along the direction in real space reciprocal to that of the evolution of $\vec{k}$, we find that the total charge can be meaningfully distributed into centers of a class of correlated hermaphrodite Wannier functions simultaneously contributed by electrons with their crystal momenta evolving linearly independently through each unique $\vec{k}$ across the BZ. The resultant map of charge centers[1] readily renders not only the qualitative nature of interatomic as well as intra-atomic hybridization of electrons but also unbiased quantitative estimates of electrons that can be associated with atoms or shared between them, as demonstrated in a selected variety of isolated and periodic systems with varying degrees of sharing of valence electrons among atoms, including variants of multicentered bonds.

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FIRST PRINCIPLES STUDIES ON GREEN ALTERNATIVES TO POPULAR PIEZOELECTRIC AND PHOTOCATALYTIC CERAMICS

Vaishali Shah

Department of Scientific Computing, Modeling and Simulation
Savitribai Phule Pune University, Pune 411007

Green energy technologies based on piezoelectric, photovoltaic and photocatalyst materials are being increasingly pursued as alternatives to fossil fuels. All of these require semiconducting materials with suitable band gaps to facilitate the separation of charges. Piezoelectrics are of interest due to the charges separated under applied stress/electric field and photovoltaics, photocatalysts for charge carriers generated through absorption of solar radiation. Green technologies require these semiconducting materials to be environment friendly while being stable and providing better efficiency. In our work, we have explored a stable, non-toxic alternative, doped barium titanate for the most popular industrially used lead titanate. We demonstrate that all physical properties of lead titanate can be reproduced by doped barium titanate with suitable applied stress, making it a viable replacement for lead based titanates. In photocatalytic materials, we explored ways to induce visible light absorption in titania, the most popular UV light photocatalyst. We characterized the photocatalytic behavior and visible light response of the anatase phase of titania through dopants and adsorbants based on investigations of their structural, electronic, and optical properties. The effect of adsorbants, dopants and dopant concentration on visible light absorption will be discussed. Our studies on an alternative material to titania, a known toxin in its nanomaterial form will be presented.

Ab initio studies of halide perovskites and β-W

Vijay Kumar

Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence
Delhi-NCR, NH-91, Tehsil Dadri, Gautam Buddha Nagar, Uttar Pradesh 201 314
Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon 122001, Haryana

Halide perovskites (HP) have attracted great interest for solar energy and optoelectronic applications due to their low cost and high efficiency while β-W has emerged as an attractive material for developing spintronic devices for low energy consumption. In this talk I shall present our results on 2D inorganic HPs [1], effects of surface ligands on their stability [2] as well as small doping of Cl to enhance the stability of bulk HPs [3]. Further we have studied double halide perovskites [4] to avoid toxic Pb and the doping of rare-earths such as Eu [5] as well as the formation of cubic and platelet forms of quantum dots [6] of inorganic HPs for optoelectronic applications. Our extensive ab initio molecular dynamics studies [7] have helped to understand the effects of oxygen in the formation of the first observation [8] of the A15 (β) phase in W.

Acknowledgements: The work on HPs has been performed in collaboration with Dr. Anu Bala under the DST projects SR/WOS-A/PM-1042/2015 and SR/WOS-A/PM-53/2019 while the work on β-W has been done in collaboration with Prof. A. Kanjilal. The calculations have been performed on Magus high performance computing system of the Shiv Nadar University.

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Computational Modeling of Semiconducting Materials for Their Applications in Transport Properties

Swapan K Pati

Theoretical Sciences Unit, School of Advanced Materials (SAMat)
Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)
Bangalore 560064
E-mail: pati@jncasr.ac.in and swapan.jnc@gmail.com

The Boltzmann transport equations (BTE) for charge carriers and phonons have been developed along with first principles calculations to model and understand the transport processes in semiconductors. Using the BTE methods, we have computed thermoelectric efficiency in a few interesting and unique materials, namely, p-type SnO-PbO superlattice [1], n-type S and Te doped Ag_2Se systems [2] and 9 Bi based half-Heusler compounds XYBi (X: Ti, Zr, Hf; Y: Co, Rh, Ir) [3]. In the second part of my talk, I shall discuss the computational modeling for obtaining thermal conductivity in TlAgSe, which have been synthesized and investigated experimentally [4]. I shall also discuss one of our attempts on finding the reasons behind the contradictory results from the theoretical calculations which predicted orders of magnitudes higher carrier mobility than what was observed experimentally in the transition metal di-chalcogenides (TMDC), $HfSe_2$ [5].

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DAY 2 : 20 May 2025

Session 3

Topological Quantum Hall Phases in Twisted Bilayer Graphene and Orbital Hall Phases in Rhombohedral Multilayer Graphene

Bheema Lingam Chittari

Quantum Theory of Functional Materials Group, Department of Physical Sciences (DPS),
Indian Institute of Science Education and Research (IISER) Kolkata,
Mohanpur 741246, West Bengal, India

The magic angle twisted bilayer graphene (TBG) [1] and rhombohedral trilayer graphene (RTG) have shown the signatures of superconductivity [2]. Followed this discovery, TBG has emerged as a fascinating platform for exploring correlated electron physics due to its moiré-induced flat bands and tunable electronic structure [3]. At the magic angle ($\sim 1.1°$), these flat bands enhance electron interactions, leading to strongly correlated phases, Mott-like insulators, and unconventional quantum Hall effects [4]. Other hand, RTG, has emerged as a versatile platform for exploring rich electronic phenomena, including strong correlations, symmetry-breaking states, spin and orbital magnetism [5]. In this presentation, I aimed to present the topological quantum hall phases in TBG [6] and Orbital Hall Phases in Rhombohedral Multilayer Graphene (RMG) [7]. The isolated electrons in the low energy flat bands in these graphene layers (TBG or RTG) spontaneously break the inversion and time reversal symmetry [8] under the topological proximity or under external fields. In TBG, at small twist angles, under the magnetic field ($B = 1T$), the Hall conductivity transform from a half-integer quantum Hall effect $\sigma_{xy} = \pm\, 4(n + \frac{1}{2})(2e^2/h)$ to an integer quantum Hall effect $\sigma_{xy} = \pm\, 2n(2e^2/h)$ ($n = 0, \pm\, 1, \pm\, 2, \ldots$), around $\theta = 2.005°$, where a well-defined zero-energy Hall plateau appears [6]. It indicates a strong inter-layer effect towards the small twist angles. Further, it is found that the pressure-induced flatbands at large twist angles ($\theta > 1.1°$) exhibit spatial localization similar to magic-angle TBG and transform to an integer quantum Hall effect [6]. Later, I will present the broken symmetries lead non-trival topological bands and non-zero orbital magnetization in RMG [7] under the topological proximity. The orbital magnetization of these isolated bands arise from the Berry curvature, Ω_n^{xy}, and the topological nature of the bands. The orbital magnetic moment (m_z^{SR}) due to the self-rotation of electrons in the orbital show a magnitude equal to $\pm 10\ \mu_B$ for all 2L, 3L and 4L RG/$\tilde{G}$. The carrier doping drives the formation of valley-specific Fermi surfaces, while the polarity of the electric fields determines the dominance of specific carriers, and lead to non-zero orbital magnetization. We conclude that topological proximity in multilayer rhombohedral graphene leads to valley imbalance and diverse Fermi surface topologies.

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Anomalous Hall Effect in Pt-based Heusler alloy

Munima B Sahariah

Institute of Advanced Study in Science and Technology(IASST), Guwahati, Assam, India

The unusual Hall effect that appears in some materials without the application of any magnetic field is termed as Anomalous Hall Effect (AHE) [1]. This effect has importance because of the non-dissipative transport property. The origin of AHE can be splitted into two categories : intrinsic and extrinsic. While the extrinsic contribution comes from impurities present in the material, the electronic band structure has a major role to play in the intrinsic effect. Large non-zero Berry curvature appears due to spin-orbit coupling induced band splitting at the Fermi level [2]. Berry curvature behaves as a fictitious magnetic field in momentum space and gives rise to Anomalous Hall voltage by deflecting electrons. The intrinsic AHE can in many materials be described well by ab-initio calculations based on Density Functional Theory (DFT). In this work, we calculated the Berry curvature induced AHE in Pt_2MnGa using DFT and Wannier interpolation and the AHE value comes out to be higher than the available values for Co-based Heusler alloys [3-6].

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High-Order van Hove Singularities as a Route to Emergent Quantum States

Bahadur Singh

Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai, 400005 India
**Email: bahadur.singh@tifr.res.in*

ABSTRACT: Beyond conventional two-dimensional saddle-point van Hove singularities (VHSs), which exhibit logarithmic divergences in the density of states, recent studies have uncovered *high-order* VHSs that feature faster-than-logarithmic divergences. These high-order VHSs arise from regions of substantial local band flatness in single-particle energy dispersions, leading to the suppression of electronic kinetic energy and the emergence of highly degenerate electronic states with enhanced electron correlation effects. In this talk, I will present our recent work on identifying both the mechanisms and material platforms that host high-order VHSs and discuss their role in driving many-body symmetry-lowering states such as unconventional superconductivity and nematic ordering. I will highlight our work on a kagome material CsTi3Bi5, where their presence suppresses charge ordering while enhancing superconductivity and nematic ordering. I will also show that cuprate high-Tc superconductors harbor high-order VHSs in their electronic structure and reveal a new correlation: cuprates with high-order VHSs tend to exhibit higher Tc's. Our work shows that the order of VHSs can provide an indirect indicator for identifying materials with a higher propensity toward nontrivial quantum states in materials.

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The emerging world of topological semimetals

Abhirup Roy Karmakar [1] Arghya Taraphder [1] and Gour P Das [2]

[1] Department of Physics, Indian Institute of Technology Kharagpur, W.B.721302, India
[2] Research Institute for Sustainable Energy (RISE), TCG Centres for Research and Education in Science and Technology, Sector V, Salt Lake, Kolkata 700091, India.

The emergence of topological order in condensed matter physics marks the beginning of a new era in the world of materials. The tone has been set up by some disruptive discoveries, such as Quantum Hall effect, Graphene etc. More recently, topological semimetals have captivated focus due to their intriguing electronic, transport and optical properties as well as application potential in fabricating topological quantum devices. In this talk, I shall first give a brief overview of the Berry curvature induced phenomena in topological semimetals, which came into limelight after the discovery of Graphene. This will be followed by some recent works carried out in IIT Kharagpur on anomalous thermal transport in Weyl Semimetals (WSM) [1].

We shall discuss a case study on the anomalous thermal Hall effect in $Co_3Sn_2S_2$ a Co-based Shandite material which is ferromagnetic with Curie temperature ~175K. It preserves inversion symmetry, but time reversal symmetry is broken, thereby making it a magnetic WSM [3,4]. Using a Wannier tight-binding Hamiltonian derived from first principles density functional theory calculations, we have identified the material as a tilted type-I magnetic Weyl semimetal [1]. Within the quasi-classical framework of Boltzmann transport theory, a giant anomalous thermal Hall (ATHC) signal appears due to the presence of large Berry curvature at the positions of the Weyl nodes. The thermal Hall current changes and even undergoes a sign-reversal upon varying the chemical potential. Furthermore, a 33% enhancement in the conductivity has been observed on application of uniaxial compressive stress of 5% along z-axis, when the material turns into a non-tilted Weyl semimetal. We have also found the Wiedemann-Franz law to be well satisfied at low temperatures for this system.

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Mapping from fermionic to bosonic topology in incommensurate spin spiral of kagome-lattice YMn_6Sn_6

Banasree Sadhukhan

SRM Institute of Science and Technology, Chennai, India

The vast progress of topological investigation in magnetic quantum materials over the past few years has led to new insights into the topology of the magnetic excitations, called magnon. A magnon band structure can exhibit topological insulators and semimetals as a result of magnetic couplings due to Berry phases associated with magnetization dynamics. Therefore, topology in magnon provides fresh air into the old physics of magnetism. Unlike topological properties in electronic structures, magnon topology in kagome lattice is rarely studied. We report that the magnetic ground state of a kagome magnet YMn_6Sn_6 is an incommensurate spin spiral which switches into ferromagnetic phase with correlation due to antiferromagntic spin exchange. YMn_6Sn_6 has been the subject of several experimental investigations in the past few years, but no detailed theoretical research has been conducted so far. We explore magnon topology in spin spiral phase of YMn_6Sn_6. We additionally, employed a model Hamiltonian to find deep insight into the physics behind spin spiral - ferromagnetic crossover. Our results of YMn_6Sn_6 are illustrated by highlighting the experimental features.

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Unveiling the Device Applications of Emerging Topological Materials

V. KANCHANA

Department of Physics,
Indian Institute of Technology Hyderabad,
Kandi, 502285, Sangareddy, Telangana, India

Abstract: The development of next-generation quantum technologies relies heavily on quantum topological materials, which offer energy-efficient processing, high-speed operation, and robust quantum storage capabilities. These functionalities arise from the complex interplay between magnetism, topology, electronic correlations, and superconductivity, especially in materials exhibiting topological features in both electronic and phononic spectra. BeAu exemplifies this class, hosting an array of exotic topological excitations including Weyl, Rarita-Schwinger-Weyl, and fourfold fermions, as well as degenerate nodal surface states in its electronic structure. Its phonon spectrum further reveals threefold and fourfold degenerate phonons and two-dimensional nodal surfaces. Combined with its strong spin Hall conductivity and large transverse magnetoresistance, BeAu is a strong candidate for spintronics, quantum computing, data storage, and sensing applications [1]. GdCuSn, a C-type antiferromagnet with a Néel temperature of 27 K, features symmetry-protected nodal surfaces and Dirac points near the Fermi level, which correlate with observed positive magnetoresistance. Its significant spin Hall effect enhances spin transport, positioning it as a promising antiferromagnetic spintronic material [2]. MnRuAs, built on a distorted kagome lattice, displays complex structural, magnetic, and electronic behavior. The inclusion of correlation effects through DFT+U stabilizes a ferromagnetic ground state and unveils a quasi-one-dimensional Fermi surface and a nodal sphere [3]. MnGaGe is investigated as a two-terminal quantum transport device model [4], while the MnAlGe/TiO_2 (001) heterostructure demonstrates proximity-induced spintronic behavior, where electron transfer metallized TiO_2 and forms an Ohmic contact, achieving a spin injection efficiency of 43% under a 0.2 V bias [5]. These findings collectively underscore the promise of topological materials in advancing quantum computing, energy-efficient electronics, and next-generation spintronic technologies.

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Unveiling Novel Topological Phases: Theoretical Insights and Predictions

Poorva Singh[1], Shivendra Kumar Gupta[1], Ashish Kore[1], and Saurabh Kumar Sen[1]

[1]Department of Physics, Visvesvaraya National Institute of Technology, Nagpur, 440010, India

The study of topology in condensed matter physics has garnered significant attention in the past decade, with topological insulators and Dirac/Weyl semimetals taking centre stage [1]. Among these, topological insulators (TIs) hold great promise for next-generation nano-electronic devices due to the unique spin-momentum locking of their topological surface states. Our recent research has identified materials (XSnBi, X = Rb, Cs) that exhibit both giant Rashba splitting and topologically nontrivial states within a single crystalline system [2]. The coexistence of Rashba spin physics and topological nontriviality in these materials opens avenues for discovering novel physical phenomena. Furthermore, the topological insulating state in these systems arises from multiple band inversions and the presence of multiple Dirac surface states. In a separate investigation, we found that XCdP compounds exhibit a pressure-induced Dirac semi-metallic phase, which remains robust due to crystal symmetry protection. The tunability of these materials under external pressure suggests their potential utility in next-generation electronic devices and quantum technologies.

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Examining the ground state of the Slater insulator NaOsO$_3$

Priya Mahadevan

Department of Condensed Matter and Material Physics,
S.N. Bose National Centre for Basic Sciences, Kolkata , India

Email: priya.mahadevan@gmail.com

Metal insulator transitions(MIT) have been widely studied in condensed matter physics as a suitable platform to understand the effects of correlations between electrons. In the Mott Hubbard picture, such transitions, driven by electron electron interactions, are usually accompanied by structural distortions. However, Slater put forward a different scenario where electron localization is caused by emergent antiferromagnetic ordering that opens up a band gap. There is no role for structural distortions in this transition. However, finding a material realization of a Slater insulator has been difficult as most materials that show a MIT have also been found to go through structural changes and symmetry lowering. NaOsO$_3$ was considered to be an exception to this when it was found that the MIT in this material is also accompanied by a long-range, collinear G-type antiferromagnetic (AFM) ordering setting in. Although NaOsO$_3$ is usually accepted as an example of Slater insulator, some studies have put forward the idea of spin-orbit driven Lifshitz transition being responsible for the MIT in NaOsO$_3$ I will discuss aspects of the ground state found in NaOsO$_3$ and the phase diagram that one finds under pressure [1].

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Hidden Magnetic Order and Engineering of Non-Relativistic Spin Splitting

Sayantika Bhowal

Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Non-relativistic spin splitting in collinear antiferromagnets has recently recieved significant interest. In my talk, I will use multipolar analysis to show that such materials exhibit ferroic ordering of hidden magnetic multipoles [1, 2]. Specifically, the presence of a magnetic octupole is dictated by both the arrangement of surrounding nonmagnetic atoms and the underlying magnetic dipolar order. These factors, in turn, control the non-relativistic splitting of spin-polarized bands. This insight offers a novel approach to tuning non-relativistic spin splitting without altering the magnetic order itself. Instead, by adjusting the geometry of nonmagnetic atoms surrounding the magnetic ion—governed by specific phonon modes—we can systematically modulate spin splitting. By varying the amplitude of these phonon distortion modes, the positions of nonmagnetic ions can be precisely controlled, providing a powerful tool for engineering spin splitting across different material systems. Using first-principles calculations, I will illustrate this concept in two key materials: $LaMnO_3$ [3], a perovskite oxide, and MnF_2 [4], a rutile fluoride. These findings highlight the intricate coupling between charge, spin, and lattice degrees of freedom in spin-split antiferromagnets, opening new avenues for phonon-mediated control of non-relativistic spin splitting in a wide range of materials.

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Van der Waals Magnets: Exploring Near-Half-Metallicity and Spin-Polarized Tunneling for Future Spintronic Applications

Anita Halder [1,2], Declan Nell[2], Akash Bajaj[2], Antik Sihi[2], Stefano Sanvito[2] and Andrea Droghetti[2, 3]

[1]Department of Physics and Centre for Computational and Integrative Sciences, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India.
[2]School of Physics and CRANN Institute, Trinity College Dublin, The University of Dublin, Dublin 2, Ireland.
[3]Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Italy.

In recent years, the discovery of long-range magnetic ordering in two-dimensional (2D) van der Waals (vdW) materials—despite the Mermin-Wagner theorem—has opened up new possibilities for using 2D materials in future spintronic applications. The use of 2D materials is particularly advantageous due to their van der Waals gap, which leads to ease of exfoliation, making them ideal for device integration. Among these materials, Fe_nGeTe_2 (FGT) [1] (n = 3–5) has attracted significant attention for potential spintronic applications, primarily due to its high Curie temperature.

In my talk, I will present the spin-dependent transport properties of Fe_4GeTe_2 (F4GeT), investigated using density functional theory (DFT) and the non-equilibrium Green's function (NEGF) method. Our findings [2] reveal that the conductance exhibits remarkably high spin polarization (SP), attributed to the unique half-metallic nature of the band structure along the direction perpendicular to the 2D vdW layers. Notably, this high SP remains robust when transitioning from the bulk material to a monolayer interfaced with model electrodes. Furthermore, we observe a substantial spin-polarized current when the system is driven out of equilibrium under significant bias. Importantly, this spin-dependent transport remains largely unaffected by spin-orbit coupling and electron-electron correlation effects.

The exceptional spin-filtering capability of monolayer F4GeT presents a promising opportunity for designing magnetic tunnel junctions (MTJs) based on 2D vdW materials, offering high tunnel magnetoresistance (TMR). Our study demonstrates that an MTJ device using model electrodes, with the vdW gap acting as an insulating barrier between two F4GeT layers, can achieve a TMR of nearly 500%.

Additionally, I will discuss the dual nature of electron correlation in this material, which exhibits both itinerant and localized behavior, making it intriguing for fundamental physics. To better understand this aspect, we employ a theoretical framework that combines DFT and dynamical mean-field theory (DMFT) to explain photoemission spectroscopy results [3].

We extend our analysis [4] to other materials in this family, including Fe_3GaTe_2, and find that all compounds exhibit strong spin-filtering properties due to their unique electronic structures along the transport direction. We anticipate that these findings will inspire further theoretical and experimental efforts to develop more practical spintronic devices, potentially replacing conventional ferromagnets with 2D vdW materials.

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Magnetic Property Calculations with DFT: When GGA Functionals Outperform Hybrid Functionals

Suranjan Shil

Manipal Center for Natural Sciences, Manipal Academy of Higher Education

Manipal 576104, Karnataka, India, Email: suranjan.shil@manipal.edu

The calculation of magnetic property is critical to design new magnetic molecules. Generally, the hybrid functionals are used to calculate and said to be accurate when compared to experimental results. While Hybrid functionals typically offer improved accuracy by incorporating a fraction of exact exchange, they can also be computationally expensive and, in some cases, less effective for certain magnetic systems. This study explores the conditions under which GGA functionals outperform Hybrid functionals in predicting magnetic properties of critical molecules like polyacene based magnetic molecules, non-alternant hydrocarbon based diradicals. We have found that the Hartree-Fock exchange significantly influences a functional's ability to predict magnetic nature of a system. By analyzing a range of magnetic systems, this work highlights the strengths and limitations of each functional type.

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Spin-Orbit Coupling and Emergent Topological Phases in Two Dimensional Ferromagnets

Indra Dasgupta

School of Physical Sciences
Indian Association for the Cultivation of Science
Jadavpur, Kolkata 700 032
(E-mail: sspid@iacs.res.in)

The theoretically predicted Chern insulators have highlighted the potential of easy-axis 2D ferromagnets to host the quantum anomalous Hall effect. This phenomenon can also emerge from in-plane ferromagnetism in such systems via the breaking of both out-of-plane and in-plane mirror symmetries. In this talk, we shall demonstrate that the interplay between magnetism and mirror symmetries makes ferromagnetic 2D systems a versatile platform for realizing nontrivial topological phases, with the orientation of magnetic moments at lattice sites serving as a key tuning parameter. We show that the Rashba spin-orbit coupling (SOC) induced by broken out-of-plane mirror symmetry together with the intrinsic SOC incorporated in a tight-binding model captures the rich topological phase diagram of these systems as a function of in-plane magnetization. In particular, the restoration of in-plane mirror symmetry upon orientation of the moments promotes topological phase transition. Our model calculations will be corroborated with first principles electronic structure calculations for the ferromagnetic kagome monolayer Co_3Pb_3S [1] and 2D honeycomb system $OsCl_3$[2]. Next we shall consider honeycomb 2d ferromagnet, namely CrI_3 and analyse its magnetic properties by calculating various exchange interactions and show that it has the possibility to be a Chern magnon insulator [3]. Finally various applications of these emergent phases in 2D ferromagnets will be highlighted.

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DAY 2 : 20 May 2025

Session 4

Computational Design of High-Performance Electrode Materials for Next-Generation Li-ion and Na-Ion Batteries

Priya Johari*

[1]*Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence,*

Dadri, Gautam Buddha Nagar, U.P. – 201314.

**Email: priya.johari@snu.edu.in*

Abstract

Computational methods have emerged as powerful tools for accurately predicting promising electrode materials for rechargeable batteries in a cost-effective and time-efficient manner. These approaches provide valuable insights that guide experimental research in improving battery performance, particularly in terms of capacity and energy density, thereby advancing next-generation energy storage solutions for grid applications and electric vehicles. In this study, we employ a combination of first-principles density functional theory (DFT) and evolutionary algorithms to investigate a diverse range of materials at the atomic level. By analyzing their structural, electronic, and electrochemical properties while charging/discharging, we aim to identify efficient electrode materials for Li-ion and Na-ion batteries, paving the way for enhanced energy storage technologies.

Designing Cathode Materials for Li-Ion and Na-Ion Batteries Using Advanced Computational Methods

Mudit Dixit

CSIR-Central Leather Research Institute (CSIR-CLRI), Sardar Patel Road, Adyar, Chennai 600020, India

The rapid discovery of advanced materials with superior performance through large-scale computational screening is crucial for the development of future technologies in energy conversion and storage. Inverse materials discovery, which leverages electronic structure to design materials with specific properties, offers a powerful and cost-effective approach to expediting this process. This methodology not only guides experimental efforts toward the most promising material candidates but also optimizes the use of human resources and efforts. In this presentation, I will discuss the progress of some of our work on sodium-ion batteries, lithium-ion batteries, and Li-sulfur batteries. I will present plausible redox models, including cationic and ionic redox in Ni-rich cathodes, and discuss the hypothesis of primary anionic redox in LNO and NMCs. Next, I will demonstrate how electronic structure tuning methods can be utilized to discover improved positive electrode materials for high-capacity sodium-ion batteries. Then, I will present our work on designing moisture- and air-stable O3-cathodes for sodium-ion batteries. Finally, I will discuss our recent work on dual-atom catalysts for Li-sulfur batteries. Furthermore, I will demonstrate the capability of machine learning interatomic potentials to accurately pre-screen a wide range of crystal structures for applications in electrochemical energy storage.

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Revolutionizing Energy Storage: The Role of DFT in Battery Material Innovation

W.Wasanthi P De Silva

Department of Physics, University of Sri Jayewardenepura, Sri Lanka

Batteries are essential for powering modern technology, from smartphones to electric vehicles, enabling portable energy storage and renewable energy integration. Lithium-ion batteries are the most popular commercial type of battery, which is one of the most popular energy storage devices. However, in order to achieve greater capacity, longer life cycles, lower costs, and improved safety, battery materials must undergo significant improvements due to the rapid advancements in modern society. Researchers are actively creating and investigating novel battery systems and energy storage materials to address these issues, but before they can be used in industry, a basic understanding of how they operate is necessary. In the field of energy storage, Density Functional Theory (DFT) has become a potent computational tool that allows for the virtual screening of promising battery materials and provides crucial insights into electrochemical reaction mechanisms. Cohesive energy, formation energy, Gibbs free energy, and phonon dispersion analysis are used to investigate structural stability. Gibbs free energy calculations are used to evaluate electrochemical performance, forecasting theoretical capacity and open-circuit voltage [1, 2]. Additionally, the study investigates electronic characteristics such as charge distribution, density of states (DOS), band structures, and molecular orbitals. It also studies adsorption and ion transport kinetics, offering information on interfacial interactions and ion diffusion that are essential for battery efficiency. Among various ion-based materials, Al-ion batteries are currently gaining significant attention. Organic electrode materials for rechargeable aluminum-ion batteries (AIBs) have drawn interest lately because of their intrinsic safety, affordability, and environmental sustainability. With an emphasis on ion interactions and charge storage mechanisms at active sites, in here examines the basic characteristics of organic compounds and how they affect AIB performance. Additionally, it explores the role of cutting-edge analytical tools in improving comprehension of AIB electrochemical processes and creative design approaches to overcome the limitations of different organic materials [3].

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DFT perspectives on piezoelectricity and spin-orbitronics in selected functional 2D materials

Abir De Sarkar

Institute of Nano Science and Technology, Knowledge City, Sector 81, Manauli, Mohali, Punjab – 140306, India

Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the materials. HfN_2 monolayers [1] exhibit valleytronic properties complementary to that in single-layer MoS_2, while the merger of spin (valley) Hall effect with the Rashba effect is observed in h-NbN, h-TaN and monolayers screened via high throughput studies [2, 3]. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS_2/BP and MoSSe/BP vdWHs. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated [4] together with strain tunability in ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb) [5]. 2D monolayers showing the simultaneous occurrence of ferroelectricity, ferroelasticity and large in-plane piezoelectricity will also be presented [6].

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Atomistic Insight to Non-Volatile Restive Switching in 2D Materials

Santanu Mahapatra

Department of Electronic Systems Engineering
Indian Institute of Science Bangalore
Bangalore 560012

Non-volatile resistive switching devices, referred to as memristors, are becoming increasingly significant for in-memory computing, which enables the data-intensive computations necessary for deep neural networks. Memristors are simple structures that consist of a metal-insulator-metal (MIM) matrix, with the insulator serving as the active layer. Upon the application of electrical field, these devices can shift from a high resistive state (HRS) to a low resistive state (LRS), emulating the function of biological synapses. Following Hewlett-Packard's (HP) announcement of the development of a memristor in 2008, transition metal oxides, such as titanium oxide, have been employed as active layers. Notwithstanding the significant advancements made in recent years, oxide-based memristors have not satisfied the critical performance metrics. Consequently, new active layer materials are being explored globally to enhance memristive device performance.

In this talk we focus on the recent advancement of memristor technology utilizing 2D semiconductor as active layer. We discuss the remarkable resistive switching exhibited at the mono-atomic-layer limit, and at the system level, how deep learning algorithms have been directly implemented on wafer-scale two-dimensional memristor arrays. Despite such fascinating advancements, the fundamental mechanism of resistive switching (RS) in these 2D material-based MIM devices has remained elusive, which may impede the optimisation of such disruptive technology. We finally discuss some recent results from our laboratory towards understanding this obscure phenomena adopting state-of-the-art computational techniques such as reactive-molecular-dynamics-simulations, first-principle-based electronic structure calculation and quantum transport modelling.

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Role of Interlayer coupling on electronic and optical properties of MX_2 (M= Mo / W, X= S / Se) Heterobilayers

Appalakondaiah Samudrala

Department of Physics, School of Physical, Chemical and Applied Sciences, R V. Nagar,
Kalapet, Pondicherry - 605 014, India

In this talk, we present the electronic and optical properties for MX_2 (M= Mo / W, X= S / Se) transition metal dichalcogenide (TMD) heterobilayers for different system compositions based on first principles density functional theory calculations. The obtained band gaps for these stacking configurations typically range between 1.4-2.0 eV (1.2 to 1.31 eV) and are direct/indirect for different/same chalcogen atom systems G_0W_0 (G_0W_0 + SOC) calculations and can often be induced through expansive/compressive biaxial strains of a few percent. Our studies strongly indicate the influence of interlayer interactions on electronic properties, and a direct-to-indirect gap transition is verified for heterobilayers upon the application of a minimal strain that weakens interlayer coupling. The large interlayer exciton binding energies in the order of ~ (240 to 250) meV are estimated by solving the Bethe-Salpeter equation without spin-orbit corrections. These values are enriched as ~ (270 to 290) with SOC corrections to optical absorption due to band gap reduction, suggesting these are amenable to be studied through infrared and Raman spectroscopy. We also used the a scissors-correction method to calculate the second-harmonic generation (SHG) susceptibilities and results show that the calculated SHG spectra of different stacking heterobilayers are large, being in the order of 10^3 pm V^{-1} for AA and AB stacking's, in comparison with monolayer and few-layer TMDs. In addition, the calculated linear electro-optical coefficients remains superior, being $r_{xyz} \sim 3.5$ pm V^{-1}, in the low photon energy. These enhanced properties suggest the potential of these MX_2 heterobilayers stacking's for nonlinear applications and demonstrate the amenability towards spectroscopic investigation. These results have potential implications for the design of optoelectronic devices leveraging the distinctive interlayer coupling and recent moiré pattern effects in TMD heterobilayers.

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Plasmon Induced Energy and Charge Transfer Dynamics in Metallic Nanoparticle-$MoSe_2$ Nanoflake Heterostructures

Varadharajan Srinivasan

Department of Chemistry, IISER Bhopal

Plasmon-induced hot carrier dynamics are crucial in various practical applications such as water splitting and photovoltaics. We propose a hybrid system formed by interfacing plasmonic Au or Ag metal nanoparticles with triangular $MoSe_2$ nanoflakes, which also possess edge-localized plasmons. [1] Using time-dependent density functional theory-based simulations, this bi-plasmonic system is shown to exhibit interfacial charge transfer induced by plasmonic excitations of either component. Tracking the fate of photoinduced plasmons in the system reveals that a significant pathway to their decay involves directly transferring hot-carriers across the interface. Our study [2] finds that while the likelihoods of both the direct hot-electron and hot-hole transfers are comparable, in most cases considered, the latter dominates. The extent and net direction of direct charge transfer depended on various tunable interface features, including the plasmon mode (nanoparticle or nanoflake) excited and the polarization of the light used. This platform could prove extremely useful for widening the substrate scope in photocatalysis and photodetection applications.

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DAY 3 : 21 May 2025

Session 1

Machine Learning aided efficient screening and inverse design of materials using generative models

Prasenjit Sen

Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj, UP 211019, India
&
Homi Bhabha National Center, Anushakti Nagar, Mumbai 400094, India.

The traditional trial-and-error experimental approach to materials design is time consuming, expensive and uncertain. Over the past couple of decades, rapid progress in computational hardware and software have helped accelerate materials design and discovery. High throughput computing strategy has been particularly helpful in these efforts. Yet, a comprehensive search of the chemical space to identify materials with a desired set of properties is highly computation-intensive, and is time consuming.

In recent years, Machine Learning methods have emerged as an alternative to expensive first principles calculations. We have adopted two strategies to use ML for search and design of useful materials. In the first strategy, available materials data is used to train a series of ML models to predict material properties. These models are used to hierarchically screen a set of new materials to identify the ones that satisfy all the desired properties. The small set of materials identified via this screening procedure is tested in DFT. Materials passing the DFT test are proposed as new candidate materials with specific functionalities. Success in designing new rare earth free permanent magnets will be presented.

The second strategy is to ‘inverse’ design materials with a set of target properties using generative artificial intelligence (AI). We have used two different generative AI models: constrained variational auto-encoder (cVAE), and a diffusion-based model, to design novel magnetic materials. Success of the property-embedded cVAE over previous models, and that of the diffusion-based model over the cVAE in generating novel magnetic materials will be highlighted.

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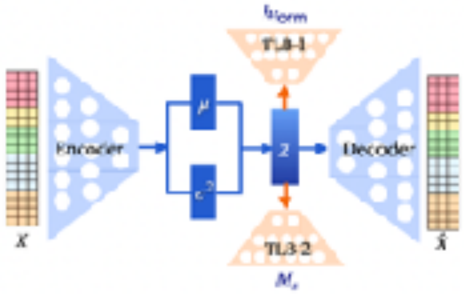

cVAE with property-embedded latent space.

Machine Learnable Representations of Materials, Molecules, and Reactions for Accelerating Materials and Mechanism Discovery

Ananth Govind Rajan
Department of Chemical Engineering, Indian Institute of Science, Bengaluru

Developing machine-learning models for expensive electronic-structure calculations has prompted the design of manually defined and learnable descriptors over the years. In this talk, we will outline the development of machine learnable representations for nanoporous two-dimensional (2D) materials, molecules, and elementary chemical reactions. We will discuss a framework called STring Representation Of Nanopore Geometry (STRONG) for 2D materials to discover nanoporous graphene structures that can be used to sieve CO_2 from air. We will explain the development of machine learning models to predict activation (free) energies of elementary chemical reactions on a catalyst using various physical features of adsorbate species and chemical transformations. Coupled with automated reaction enumeration and elementary reaction identification strategies, the use of such predictive machine learning models allows the exploration of complex reaction pathways involving thousands of elementary steps. Finally, we will present work on a physically inspired, error-free and easy-to-compute representation of electronic structure in atoms, which employs graph attention networks to accurately predict atomization of molecules and formation/adsorption energies on catalyst surfaces. Overall, the work presented in this talk will advance the use of machine learning to develop structure-property relationships for various application areas pertaining to materials for clean energy and air.

Artificial Intelligence-Enabled Molecular Simulations: Making Computers Learn Chemistry at Aqueous Oxide Interfaces

Abhinav S. Raman

Department of Chemical Engineering, IIT Madras

Chemistry at aqueous oxide interfaces plays a prominent role in several contemporary applications such as (electro/photo)catalysis and environmental geochemistry. These complex systems are challenging to probe experimentally, with computer simulations often being used to obtain atomistic insights. While first-principles-based methods have been at the forefront of making significant advances, they are severely constrained by their high computational cost, limiting the exploration of configuration space to short length and time scales. In this talk, I will discuss the application of deep learning accelerated molecular simulations coupled with enhanced sampling methods to probe the chemistry at these interfaces well beyond the reach of *ab initio* methods. I will briefly present results on proton transfer [1] and ion-exchange processes [2], as well as a more detailed picture of a long-standing puzzle in surface and interface science: the hydrophobicity of TiO_2 in the dark [3, 4].

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Computing properties of charged molecules and surfaces using efficient periodic density functional theory implementation of Coulomb kernel truncation and machine learning interatomic potentials

Sudarshan Vijay

Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, Maharashtra, India

Density functional theory (DFT) calculations of charged molecules and surfaces are critical to applications in electro-catalysis, energy materials and related fields of materials science. Periodic DFT implementations such as the *Vienna ab-initio Simulation Package* (VASP) compute the electrostatic potential under 3D periodic boundary conditions, which necessitates charge neutrality. In this work, I will discuss our recent implementation of 0D and 2D periodic boundary conditions using the Coulomb kernel truncation method [1]. Unlike 3D boundary conditions, our implementation allows for calculations of charged molecules and surfaces.

I will discuss three applications of this method to charged and polarized systems. First, to illustrate the computational efficiency of our method, we perform large supercell calculations of the formation energy of a charged chlorine defect on an NaCl(001) surface. Second, we determine the electrochemical capacitance of an Au — water electrode-electrolyte interface by training kernel-based machine learning interatomic potentials on a database of first principles calculations with 2D boundary conditions. Finally, we rationalise trends in multipole moments of small molecule adsorbates on the surface of doped transition metal surfaces.

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Distributed QPU+GPU implementation of Tensor Factorized Hamiltonian Downfolding for electronic structure modelling

Anirban Mukherjee

TCS Research

Distributed QPU-GPU algorithms for simulating chemical complexes and reactions may lead to practical quantum advantage. However its a hard problem to quantify the optimal classical-quantum resources needed for modelling chemical reactions of real world practical use. In this work we report a novel quantum chemistry

algorithm-tensor factorized Hamiltonian downfolding of coupled cluster level accuracy that can be implemented as a family of tensor products and contractions on GPU-only and on distributed GPU-QPU setup by block-encoding the tensor operations via distributed independent quantum circuits. On only GPU we show a nearly quadratic speedup and on distributed GPU-QPU we show a superquadratic speedup over CCSD. We provide accuracy benchmarks for GPU-only setup. Finally we present a real use-case of drug synthesis reaction, computing energetic and runtime on distributed GPU-only setup and detailing the QPU-GPU resources needed for performance crossover over the classical approach.

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DAY 3 : 21 May 2025

Session 2

Engineering 2D Monolayers for Optimized Hydrogen Evolution: A Computational Perspective

Prafulla K Jha

Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda,
Vadodara, Gujarat, 390002, India.

Hydrogen-based energy technologies are pivotal for achieving a sustainable, carbon-neutral future. Hydrogen's high energy density and zero-emission characteristics make it an ideal clean fuel for transportation, energy storage, and industrial applications [1-3]. One of the most promising methods for hydrogen production is electrochemical water splitting, which involves the hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode. This process efficiently converts water into hydrogen and oxygen, offering a sustainable pathway for large-scale hydrogen production. HER involves the reduction of protons to molecular hydrogen, often facilitated by catalysts that reduce activation energy and improve reaction kinetics. While platinum-based catalysts exhibit excellent HER activity, their scarcity and cost drive the search for alternative, earth-abundant catalysts. Two-dimensional (2D) materials, with their large surface area, unique electronic properties, and tuneable catalytic activity, have gained significant attention as promising candidates for efficient hydrogen production. Literature reveals that the pristine form of most of the 2D materials is not well-suited for HER activity, making modifications necessary for improvement. Strategies such as defect creation, substitutional doping, and transition metal decoration have been reported as important for enhancing performance. In our study, we have selected different monolayers, such as holey graphyne (HGY), orthorhombic diboron dinitride (o-B_2N_2), and α-SiX (X = N, P, As, Sb, Bi), as HER catalysts. We have employed dispersion-corrected density functional theory (DFT) to investigate defect creation, substitutional doping, and transition metal decoration as single-atom catalyst (SAC) strategies for enhancing HER performance. Our DFT findings predict that Ni@α-SiX and Cr@HGY SACs emerge as highly efficient catalysts for HER, exhibiting remarkably low Gibbs free energy change (ΔG_H) values of -0.04 eV and -0.05 eV, respectively [1,2]. The strong bonding between Ni metal and 2D α-SiX monolayers, as well as between transition metals and the HGY monolayer, facilitated by p-d hybridization, enhances both reactivity and conductivity. This effect is further attributed to the reduction in the band gap of the semiconducting α-SiX and HGY monolayers. Furthermore, for o-B_2N_2 monolayer, introducing BN vacancy defects and substituting C atoms at N sites enhances HER activity by 86.71% and 83.59%, respectively, compared to the pristine monolayer [3]. This improvement is attributed to charge redistribution induced by the defects and dopants. Notably, C doping renders o-B_2N_2 metallic, making it a promising electrocatalyst, while the BN-vacancy-defected o-B_2N_2 remains semiconducting with a band gap of approximately 1 eV, highlighting its potential as a photocatalyst for HER. Overall, our findings suggest that C-doped o-B_2N_2, Ni@α-SiX, and Cr@HGY SACs are highly promising catalysts for efficient hydrogen production.

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CO_2 Reduction to Methanol: DFT Microkinetic Insights into Catalytic Structure-Activity Relations

Jithin John Varghese

Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India 600036

Carbon capture and chemical utilization is attracitve as a means of mitigating the impact of CO_2 emissions and in enabling circular chemical process. Utilizing the captured CO_2 to make methanol is highly desirable for a methanol economy but has limited commercial success. Understanding the active sites on industrial catalysts, structure-activity relations and operando reaction mechanisms are crucial for enhancing performance of catalysts and for reactor optimization and design. We carried out multiscale analysis of CO_2 reduction to methanol on $Cu/ZnO_x/ZrO_x/Al_2O_3$[1] and $Cu/ZnO_x/Al_2O_3$[2] catalysts using the microkinetic modelling approach to predict reactor scale performance using the kinetic parameters derived from atomistic scale simulations within the Density Functional Theory framework. The active site features on the operando catalyst were identified using computational infrared spectroscopic analysis of key reaction intermediates and validation against *operando* IR spectroscopic data from the literature. The validated microkinetic models predicted lab-scale reactor performance on these catalysts at a wide range of operational conditions of temperature, pressure, inlet gas composition and gas hourly space velocity. With insights from the DFT analysis, the microkinetic modelling enabled us to connect the catalyst microstructure to reactor performance.

Although CO_2 adsorption is stronger on the Cu/ZrO_x interfacial sites on the $Cu/ZnO_x/ZrO_x/Al_2O_3$ catalyst, the Cu/ZnO_x interfacial sites form the primary active sites for CO_2 reduction [1]. The simulations indicated an indirect promotional role of ZrO_x in proximity via electronic interactions, lowering activation barriers for the key steps on the Cu/ZnO_x interfacial sites. Both formate and carboxyl pathways lead to the formation of methanol at different axial positions of a fixed bed reactor. A combination of Wulff construction and computational IR spectrocopic analysis indicated that the Cu(111) and Cu(100) facets on copper nanoparticles are key contributors to CO_2 reduction on $Cu/ZnO_x/Al_2O_3$ catalysts [2]. The ZnO_x/Cu(111) interfacial sites are active for methanol synthesis from CO_2 via the formate route while ZnO_x/Cu(100) interfacial sites are active but less selective on $Cu/ZnO_x/Al_2O_3$. Cu nanoparticles of 10 nm size have an optimum mix of Cu(111) and Cu(100) surfaces to enable high activity in CO_2 hydrogenation. ZnO_x/Cu(100) interfacial sites are active for CO hydrogenation making small Cu nanoparticles with larger fraction of Cu(100) surface useful for CO rich syngas conversion to methanol.

Our analayses clearly establish the active sites distributed across the metallic and metal oxide components of the catalyst. We also identify structural features of metal oxide and metal interfaces on the inverse catalysts and the desired Cu facets for high activity and selectivity during methanol synthesis from different industrially relevant CO/CO_2 gases.

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Biphenylene: A Promising Candidate for Renewable Energy Applications

Aftab Alam
Materials Modeling Group, Department of Physics, Indian Institute of Technology Bombay, India

Designing efficient, metal-free, and inexpensive catalyst for the electrochemical hydrogen evolution reaction (HER) and CO_2 reduction is crucial for large-scale clean and green energy production. In this talk, I will present a first principles calculation of the electronic structure, electrocatalytic activity and CO_2 reduction of a recently synthesized low dimensional system, namely Biphenylene. The structure of this compound acquire a unique co-existence of 4, 6 and 8-coordinated carbon rings. Nanoribbon counter part of Biphenylene with a specific width is found to be most promising candidate for electrocatalytic activity, with extremely small overpotential (~0.005 V) and a high exchange current density, much better than the state of the art Pt(111). A close inspection of the elementary reactions of the HER (Volmer, Heyrovsky, and Tafel reactions) shows that the Volmer-Tafel mechanism is most dominant for this nanoribbon, with the Tafel mechanism as the rate-determining step, with a barrier of 0.56 eV. I will also show some preliminary results on the electrocatalytic CO_2 reduction of pristine, defective and Cu-decorated 2D-Biphenylene sheet (BPH). CO_2 molecule is found to bind weakly on the pristine BPH, indicating its chemical inertness, while the same binds strongly (with binding energy -3.23 eV) when absorbed at a Carbon single-vacancy defects. I will further show the potential of of Cu-decorated BPH as a single-atom-catalyst (SAC) for the CO_2 catalytic activity, eventually producing CH_3OH.

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Computational Design of Functional Materials: From Super Capacitor to Green Hydrogen

Saroj Nayak

IIT Bhubaneswar

One of the sustainable development goals (SDG-7) by the United Nations General Assembly is to ‘Ensure access to affordable, reliable, sustainable and modern energy for all”. Energy from the sun (solar energy) is clean energy, and due to its abundance, it is highly scalable. Energy storage is a big part of the total energy solution. Emerging materials such as graphene and other 2-dimensional materials provide advanced storage options through batteries, supercapacitors, etc. This talk will present our recent computational study of developing such materials in collaboration with experiments. For example, a novel approach was applied to develop aluminum graphene (AlGra) composite materials for the fabrication of energy storage devices such as supercapacitors and batteries that are affordable and environmentally friendly. As the world goes through an energy transition from a carbon-rich fuel to renewable energy solutions, demand for various metals such as lithium and copper increases. We have recently shown that composite materials could provide highly attractive functional materials to meet this emerging demand. In collaboration with MIT, USA, and through our startup, we introduced the world’s first lightweight and rollable solar panel for mobile irrigation that could provide clean energy solutions for livelihoods worldwide. Our green hydrogen work could help hard-to-abate industries such as steel. This talk will provide an overview of our energy research and its translations for societal impact.

Engineering 2D Electron and Hole Gases at Semiconductor Heterostructure Interfaces

Shobhana Narasimhan

Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India

Two-dimensional electron or hole gases can, in some cases, arise at the interface of two semiconductors. This fact has been known for decades, and has been exploited to study exotic phenomena in fundamental physics (such as the quantum Hall effect and the fractional quantum Hall effect). It has also been utilized in applications such as MOSFETs, and is now being used to engineer semiconducting spin qubits for use in quantum computers. However, there is a lack of first-principles calculations determining the conditions under which the two-dimensional electron gas (2DEG) or hole gas (2DHG) arises, and the electronic properties of the 2DEG or 2DHG.

In our group, we have performed density functional theory calculations to study this problem, focusing on strained-Si/SiGe interfaces. While some of our results serve to confirm longstanding empirical knowledge, other findings are rather unexpected. We will present these results, and discuss them. This work has been performed in collaboration with the group of Anil Shaji at IISER Thiruvananthapuram. The DFT calculations I will present have been carried out by my student Garima Ahuja.

A Computational Insights into the Messy World of Quantum Dot Surfaces

Dibyajyoti Ghosh

Department of Materials Science and Engineering and Department of Chemistry
Indian Institute of Technology, Delhi, India
**Email: dibyajyoti@iitd.ac.in*

Semiconductor quantum dots (QDs) exhibit exciting photophysical properties for various applications, including energy conversion, lighting, and, more recently, quantum communication. The photophysics underpinning these applications at ambient conditions strongly depends on their stoichiometry and dynamic surface, making the materials design challenging. In this talk, I will illustrate our attempt to explore complex structure-property-performance relationships by performing cutting-edge computational modeling of these nanomaterials. Our detailed study depicts that the surface passivating ligands substantially impact the surface phonon modes of QDs and consequently impact their emission properties.[1-2] Investigating less studied non-stochiometric QDs employing time-dependent density functional theory, we reveal that ligand passivation can substantially impact the emission properties.[2] Strategic ligand passivation appears to eliminate the transient trap-states, improving the optical properties. The phonon-mediated charge carrier relaxation dynamics with non-adiabatic molecular dynamics further reveal that the size of the surface ligands controls the crystal vibrations and electron–phonon coupling, impacting the optoelectronics of semiconductor QDs.[3-5] These overall insights emphasize the importance of ligand engineering in non-stoichiometric QDs for photoinduced dynamics and guide future work for the implementation of improved materials for optoelectronic devices.

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Epitaxial growth of thin film of germanium on 2×1 reconstructed silicon (001) surface: A kinetic Monte Carlo study

Paramita Ghosh,
Centre for Development of Advanced Computing, Panchavati, Pashan, 411 008, Pune, Maharashtra

Heteroepitaxial semiconductor thin films have attracted scientific interest for several years due to many reasons. These are technologically relevant for fabrication of various electronic and optoelectronic devices. There is also a fundamental scientific interest in these systems since they show the spontaneous formation of different dislocation-free nanostructures. Germanium grown on silicon (001) substrate (Ge/Si(001)) is one of the most widely studied heteroepitaxial systems. Thin film growth of Ge/Si(001) in a molecular beam epitaxy (MBE) chamber shows spontaneous formation of quantum dots. Due to their quantum behavior, quantum dots receive significant attention from both experimental and theoretical perspectives. Their properties are highly dependent on the size and shape of the dots. These shapes and organization of quantum dot can be controlled by varying growth conditions. The ultra-clean conditions of the MBE growth have made this system a fertile testing ground for theoretical studies of crystal growth and morphological evolution. The observed behavior of these systems is conveniently rationalized in a few physical concepts. There are energetic terms involved – wetting, anisotropic surface energy, elastic energy, surface reconstruction energy – each of which contributes differently to the observed behavior. Then, there are kinetic processes involved – deposition, surface and bulk diffusion, defect formation and migration – whose interplay with the energetic and thermal effects leads to a great variety of structures. Various theoretical models and computer simulations of heteroepitaxial growth have incorporated these features. However, their effectiveness has been limited due to the inherent multi-scale nature of the problem, caused by the long range of the elastic interaction. In this regard, lattice kinetic Monte Carlo methods (kMC) that explicitly incorporate elastic effects have been proved to be the most successful tool to study the detailed morphological evolution in these systems.

A refined kMC model is developed and applied to investigate the growth of Ge on Si (001). Using this model, growth is simulated over a range of coverage from submonolayer to approximately ten monolayers (ML), and the results are compared with experimental observations in each regime. The model is also used to analyze behavior under different experimental conditions, such as varying growth fluxes and temperatures. Several prominent experimental features are successfully captured [1, 2, 3, 4], including Stranski–Krastanov growth, the transition from bimodal to unimodal size distribution [5] of quantum dots.

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DAY 3 : 21 May 2025

Session 3

In search of rare earth free permanent magnets

Amrita Bhattacharya

AbCMS lab, Department of Metallugical Engineering and Materials Science,
Indian Institute of Technology, Bombay, Mumbai-400076, Maharashtra,

Considering the vast compositional space of Heusler alloys, first-principles-based calculations are ideally suitable for predicting the ground state structure and tailoring the magnetic properties of these alloys. We perform density-functional-theory-based calculations for step-by-step identification of the most stable phase, taking into account all the different structural phases exhibited for this alloy (viz., cubic, cubic XA, tetragonal L21, tetragonal XA, and hexagonal D019), followed by the calculations of magnetic properties. We identify the magnetic ground state of each phase and then the most stable structural phase by taking into account electronic and geometric relaxation, spin polarization, and vibrational free energy contributions. The ferromagnetic configuration of all the phases is found to be energetically the most favorable magnetic state, while the ferromagnetic hexagonal phase is identified to be the stable structural phase of Fe2MnSn, with a sizable magnetization. Furthermore, the exchange interactions in the hexagonal phase are calculated using the Liechtenstein approach, and this phase shows a high Curie temperature attributed to the strong Fe-Fe exchange coupling. The stable hexagonal phase reveals an in-plane magnetic anisotropy [1]. However, in order to explore the possibility of using this alloy as a gap magnet, via achieving uniaxial anisotropy, interstitial doping is employed for various light elements viz. B, C, H, O, N and F with different doping concentration ranging from 1.56 % to 12.5 %. These interstitial atoms prefer octahedral sites in the stable hexagonal phase of Fe2MnSn, altering the local atomic arrangement and enhancing the magnetic properties. At 12.5 at% doping, B, C, N, and O dopants induce a significant shift in magnetic anisotropy from in-plane to out-of-plane, with N-doped Fe2MnSn showing the largest uniaxial anisotropy, followed by B-doped alloy. Enhanced Curie temperature, uniaxial anisotropy and high magnetization make these candidates promising for permanent magnet applications [2]. Finally, we demonstrate one high throughput data driven technique to identify permanent magnet materials [3].

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The Complex Topological Order In Functional Materials.

Dr. Kartick Tarafder

Department of Physics , NITK-Surathkal, Mangaore, Karnataka

In this presentation, I will examine the electronic, magnetic, and dynamic properties of functional materials, with a particular emphasis on the Kagome lattice, MXenes, and a series of 4D transition metal compounds based on our theoretical findings. I will introduce our first predictions of non-trivial topological properties in two recently synthesized Kagome compounds and an MXene system.

Additionally, I will highlight the fascinating non-trivial topological order found in Yttrium Iodide (YI), which reveals a unique electronic structure encompassing both spin-polarized Dirac and Weyl nodes within the same phase. Our analysis uncovers pairs of nodal points within both spin-up and spin-down channels. The presence of Weyl nodes is corroborated by the source and sink characteristics observed in the Berry curvature, along with the identification of Fermi arcs in the surface band structure. The system also exhibits a high Fermi velocity for Dirac fermions, estimated at 3.4×10^5 m/s, as well as a significant anisotropic intrinsic anomalous Hall conductivity reaching up to 933 S/cm.

Furthermore, I will discuss the non-trivial topological behaviour of two Kagome lattice systems, specifically $InCu_3(OH)_6Cl_2$ and $TlCu_3(OH)_6Cl_2$, which we have recently predicted to display Dirac nodal line semimetallic characteristics. Noteworthy features such as the presence of Weyl and Dirac points in these materials and high intrinsic quantum anomalous/spin Hall conductivity underscore their promising potential for spintronic applications.

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Fermionic and Bosonic Topologies in Pyrite-Structured SiX_2 (X = P, As)

G Vaitheeswaran

School of Physics, University of Hyderabad, Gachibowli, Telangana, India, 500046

The discovery and classification of novel topological phases have emerged as central themes in condensed matter physics over the past two decades. While Dirac and Weyl fermions have garnered considerable attention, recent efforts have shifted towards identifying unconventional quasiparticles that have no direct analogues in high-energy physics. In this work, we investigate the emergence of multi-fold degenerate fermions in pyrite-structured SiX_2 compounds (X = P, As), expanding the landscape of topological excitations beyond the Dirac and Weyl paradigm. By employing symmetry analysis and first-principles calculations, we reveal the presence of four-fold and six-fold degenerate fermions at the high-symmetry Γ and R points of the Brillouin zone. These topological nodes are protected by crystalline symmetries, offering a robust framework for exploring the exotic physical phenomena associated with multi-fold fermions. Beyond their electronic structure, SiX_2 compounds exhibit remarkable topological features in their phonon spectra. Notably, we identify a coexistence of three topological nodal surfaces and a Dirac nodal-line (DNL) network in momentum space. This DNL network comprises three mutually orthogonal nodal lines located in the k_x, k_γ, and k_z planes, intersecting at a single nodal point - a highly uncommon configuration in phononic systems. The unique topology of these nodal features suggests the existence of surface phonon states, potentially observable in spectroscopic experiments. Collectively, our findings position the SiX_2 family as a versatile platform for probing topological fermionic and bosonic excitations. The identified multi-fold fermions and intricate phononic topologies provide new avenues for advancing the understanding of topological matter and may inspire future experimental and theoretical investigations in solid-state systems.

Magnetostrictronics: A bi-directional exchange of magnetic anisotropy and elastic energies

Tilak Das

Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur - 721302, India
Email: tilak.das@phy.iitkgp.ac.in

Harvesting and utilizing the internal *energy* of a magnetic solid is sustainable approach by exploring its microscopic origin of spins alignment bound to the crystal orbitals [1]. Novelty arises due to its phenomenological implementation and possible future applications would be guided by the bi-directional energy exchange between the elastic and magnetic anisotropy energies. Thus, energy generation without external electric and or magnetic field has become pioneering domain of research, which is essentially unfolding the deeper understanding of the elastic and magnetic ground states of hard magnetic solids [2]. Thus, modelling and quantification of the magnetocrystalline anisotropic energy (MCAE) and the associated magneto-elastic stress-strains and strain-energies are key to the next generation magnetostrictive applications –pioneering to *magnetostrictronics*. The outcome of strain while magnetized, was earlier observed by Joule, 1842, and now-a-days it is exploited via computational first-principles modelling and numerical tools [3,4]. An accurate first-principles calculations in the scarcity of the computational issues and numerical instability, this microscopic origin of the MCAE is still elusive even for mono- or double sub-latticed metals [5,6]. Recently, we have re-investigated these magnetostrictive properties in the available limit of the numerical stability and accuracy of the density functional theory (DFT) calculations of the $L1_0$-*A*Pt order (*A*= Fe, Mn) with some future note to the reliability of the DFT tools [7,8]. Thus, in the seminar, I will derive and discuss the well-known textbook phenomena on the rationalization of volume magnetostrictive parameters and its corelation with the anisotropic linear magnetostrictive measures of the given magnetic solids, including the $L1_0$-FePt and extended to its anisotropic polycrystal models. Thus, using the basic condensed matter physics, we explored MCAE to decouple the spin- and orbital parts in the easy-axis vs. easy-plane anisotropy of $L1_0$-*A*Pt hard magnets. We believe, future development in this domain may help us to get novel technological devices *i.e.*, sonography and internal energy perturbed spin-currents in the bulk to quantum-size solids [9,10].

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Competing Interactions, Spiral Order, and Emergent Spin Liquid Behaviour in Trigonal $CaMn_2P_2$

Swarup Kumar Panda
Department of Physics, Bennett University, India
Email : swarup.panda@bennett.edu.in

In this talk, I will present a comprehensive theoretical investigation of the magnetism in $CaMn_2P_2$, a trigonal 122-type compound. Our *first-principles* calculations reveal that $CaMn_2P_2$ is an indirect-gap semiconductor hosting a highly localized Mn^{2+} ($3d^5$, $S = 5/2$) moment, with negligible spin-orbit coupling, placing it squarely in the regime of classical spin physics. By employing a Green's function-based approach, we extract the full set of interatomic exchange interactions and demonstrate that its magnetism is well captured by an isotropic Heisenberg spin model. Spin dynamics simulations, based on the Landau-Lifshitz-Gilbert (LLG) formalism, uncover a noncollinear spin-spiral ground state characterized by a propagation vector $q = (1/6, 1/6, 0)$, consistent with neutron diffraction measurements. We identify two key competing interactions driving the complex magnetic behaviour: the nearest-neighbour interlayer coupling (J_1) and a frustrated next-nearest-neighbour in-plane coupling (J_2), which forms a geometrically frustrated network within the hexagonal layers. Tuning the J_2/J_1 ratio unveils a rich magnetic phase diagram, encompassing collinear Néel order, spin-spirals, and a disordered phase with signatures of spin-liquid-like behaviour at high frustration. The resulting phase diagram provides a unifying theoretical framework for understanding and predicting magnetic phases in a broader class of trigonal Mn-based compounds, opening new avenues in the exploration of classical spin liquids and complex magnetism in frustrated 3D systems.

Quantum Geometry and Dynamical Axion in antiferromagnetic topological insulator $MnBi_2Te_4$

Dr. Barun Ghosh

Department of Condensed Matter and Materials Physics, S.N. Bose National Center for Basic Sciences, Kolkata, India

In this talk, I will present our recent discoveries in the antiferromagnetic topological insulator $MnBi_2Te_4$, highlighting quantum geometry related effects, and the realization of dynamical axion quasiparticles. I'll discuss about the quantum metric, which refers to the real part of the complex quantum geometric tensor. Although the imaginary part (Berry curvature) of the this tensor has been the basis of new discoveries in the field of topological materials for many years, the importance of the quantum metric in driving new phenomena has emerged very recently. In this connection, I'll discuss our recent efforts on probing the quantum metric through transport and optical responses[1-4]. Finally, I'll discuss our recent work on the experimental observation of the dynamical Axion quasiparticle in $MnBi_2Te_4$ [5]. These discoveries not only extend our fundamental understanding of quantum geometry and axion electrodynamics but also provide exciting new avenues for technological innovations leveraging topological quantum materials.

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Nonsymorphic symmtery enforced band topology

Sudipta Kanungo

School of Physical Sciences, Indian Institute of Technology Goa, Goa 403401, India

In the Landau-Ginzburg paradigm, different phases of matter are distinguished by their symmetry. The discoveries of the topological insulator clearly distinguish this fact that the insulators with the same symmetries and particle numbers can be topologically distinct phases of matter. In spite of that the symmetries play important roles in the classification of topological phases, for ex. noninteracting TIs and topological superconductors characterized by time-reversal symmetry, particle-hole symmetry, and chiral symmetry, Dirac semimetal characteristized by four fold rotational symmetry and Weyl semimetal by combined parity-time reversal symmetry. This scenario is substantially modified for a broad class of crystals having nonsymmorphic symmetries, namely, the spatial symmetries that unavoidably translate the spatial origin by a fractional lattice vector. Nonsymmorphic symmetries guarantee that at certain integer fillings the phase of matter must always be gapless. This robust and unavoidable metallicity originates from the nontrivial connectivity of elementary energy bands which can bring many more fancy degeneracies in the band structures, say, unconventional new fermions beyond Dirac and Weyl fermions.

Recently we have investigated the nonsymmorphic symmetry enforced band degeneracy that leads to fascinating phenomena such a nodal line semimetal, where two bands can touch each other through a line due to some special symmetry protection and can form a one-dimensional line in the momentum space. If such one dimensional band degeneracy is protected by nonsymmorphic crystal symmetry then such band degeneracy remains protected against the strong spin orbit coupling and shows gapless quasiparticles. We also found such a nodal line can be intact in the absence of the time reversal symmetry and spectropically evidenced by the drumhead-like surface state close to Fermi energy. We also found the moderate Berry curvature driven intrinsic anomalous Hall conductivity which can be tuned by the geometry confinement in the thin film form.

We also have extended our investigation to other nonsymmorphic systems among some of them show non-collinear spin structures and some of them are nonmagnetic altogether. The presentation will discuss how the special symmetry enforced band degeneracies lead to other fascinating effects such as flat band physics, chemical control of topology and Rashba effect as well.

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DAY 3 : 21 May 2025

Session 4

Solving the band gap and optical absorption problems of density functional theory

Leeor Kronik

Weizmann Institute of Science, Rehovoth, Israel

Density functional theory (DFT) has struggled, often even qualitatively, in the description of electron and optical spectroscopy. Specifically, the band gap of semiconductors and insulators has been thought to be outside the reach of DFT even in principle, and the associated optical absorption spectrum outside the reach of time-dependent DFT with standard approximate functionals. Charge transfer excitations have also presented significant difficulties in both molecular and solid-state systems.

Here, a novel approach to overcoming these difficulties, involving Wannier-localization based optimal tuning of a screened range-separated hybrid functional, is presented. It is shown that quantitative accuracy for a wide range of systems, from molecules to 3d and 2d materials, is achieved without any empiricism. This opens the door to many DFT-based true predictions of electronic and optical properties, to high-throughput calculations, and to a systematic choice of the starting point for many-body perturbation theory calculations.

Semi-universal solution of Thomas-Fermi equation for jellium spheres

Manoj K. Harbola and Subas Rana

Department of Physics, IIT Kanpur

Density-functional theory has been most widely applied in its Kohn-Sham (KS) version, which is orbital based. However, orbital-free density functional theory (OFDFT) is also being applied over the past couple of decades to study large systems. The original OFDFT is the Thomas-Fermi (TF) theory that has a universal solution for neutral atoms. We have investigated TF theory in this connection and have looked for other systems that may also have such solutions. We find that Thomas-Fermi equation has semi-universal solutions for neutral jellium spheres in that a single parameter determines the density for a wide number of jellium spheres with different density parameter r_s and number of electrons N. In this talk we will discuss how we obtain this results and present some results.

Towards Accurate Material Properties: New Computational Methodologies for Quantum Materials

Prasanjit Samal

School of Physical Sciences, National Institute of Science Education and Research, An OCC
of Homi Bhabha National Institute, Bhubaneswar 752050, India

Accurate prediction of material properties is crucial for the development of next-generation quantum materials. In this talk, we explore new computational methodologies within the density functional theory (DFT) formalism to improve the precision of electronic structure calculations [1, 2]. Traditional DFT approaches, while widely successful, often struggle with accurately capturing many-body interactions, excitonic effects, and electronic correlations in low-dimensional and strongly correlated systems. To address these challenges, we integrate advanced exchange-correlation functionals, self-consistent GW corrections, and hybrid functionals tailored for quantum materials. Additionally, we employ beyond-DFT methods, such as many-body perturbation theory and machine-learning-assisted simulations, to refine bandgap predictions and optical response properties. Our results demonstrate significant improvements in agreement with experimental data for transition metal dichalcogenides (TMDs), van der Waals heterostructures, and topological materials. This study establishes a robust computational framework for accurate material property predictions, paving the way for rational material design in quantum technologies.

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Levy-Perdew-Sahni equation and its application to perform atomic calculations

Rabeet Singh,[1, *] Ashish Kumar,[2, †] and Manoj K. Harbola[3, ‡]
[1] *Department of Physics, Institute of Science, Banaras Hindu University, Varanasi 221 005, India*
[2] *School of Physical Sciences, National Institute of Science Education and Research, HBNI, Bhubaneswar 752050, India*
[3] *Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208 016, India*

(Dated: March 25, 2025)

Levy-Perdew-Sahni (LPS) derived[1] the connection between the asymptotic decay of density and the ionization potential of a many-electron system using the equation for the square root of density. For this, they employed an expression for the corresponding effective potential in terms of the wavefunction of the system. In this paper, we explore the possibility of solving the LPS equation in conjunction with approximate wavefunction. For this, we first do the variational derivation of the equation and use this to set up a self-consistent cycle to get the ground state properties of two-electron systems using the modified form of Le Sech wavefunction[2]. Furthermore, using the observation that even the approximate wavefunctions give the accurate effective potential[3] for the LPS equation, we show that accurate densities are obtained through using the LPS equation with these wavefunctions. We demonstrate our method by performing calculations for closed-shell atoms.

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[*] E-mail: rabeet@bhu.ac.in

[†] E-mail: ash.phy7@gmail.com

[‡] E-mail: mkh@iitk.ac.in