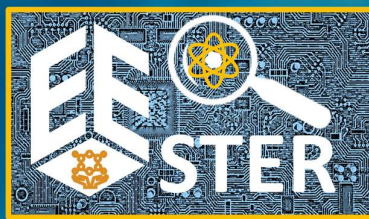


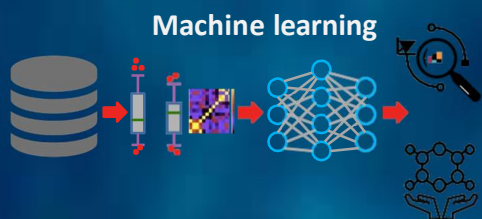


International school and conference on Evolution of Electronic Structure Theory and Experimental Realization (EESTER 2025, 4th Edition)



Abstract Book

January 3 - 11, 2025, Chennai, India
(3-7 @ SRMIST KTR, 8-11 @ IITM)



Molecular Dynamics

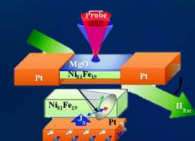
$$\dot{x} = v \quad \dot{v} = \frac{F(x)}{m} \quad MX = -\nabla U(X) - \gamma MX + \sqrt{2M\gamma} k_B T R(T)$$

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(r) + \int \frac{\rho(r')}{|r-r'|} dr' + V_{xc}(r) \right] \Psi_i^\sigma(r) = \epsilon_i^\sigma \Psi_i^\sigma(r)$$

Density Functional Theory



Experimental



Web address: <http://cammd.iitm.ac.in/eester-2025/>

Email: eester2025@cammd.iitm.ac.in

Dear Colleagues and Young friends,

Wishing you a very happy, healthy, prosperous and productive 2025!

It is a great pleasure to welcome you all to the fourth edition of the international school and conference on the Evolution of Electronic Structure Theory and Experimental Realization (EESTER).

The journey of EESTER started in 2018 on an experimental basis to see if the unique idea of having a school and a conference together, where both of them are equally prioritized, will be successful. The thought that went behind is to let our students and postdocs pursuing research in condensed matter physics, to know the various fundamental concepts, broadly in the domain of electronic structure and their utilization in predicting the materials' properties, designing new materials and exploring non-trivial quantum states of matter. It is equally important for all of us, students and scientists alike, to learn about the recent advances in the frontier areas of research in condensed matter physics and materials science. Therefore, an international conference of highest academic rigour and quality, complimenting the school, is a must.

Your enthusiastic participation in 2018, 2020 and 2023, has convinced us that the unique idea is indeed successful. It is wonderful to notice that in the last couple of years, many of our colleagues in India, have implemented this idea of organizing a joint academic event of school and conference.

In every subsequent edition, the EESTER has grown. The seed that we planted in 2018, has become to a fully grown tree, and is eager to spread knowledge and curiosity. In this edition, we have 22 lectures for the school, 74 invited talks, 24 oral presentations and more than 100 poster presentations for the conference. Keeping the national mission in mind and to stay in tune with the progress occurring in the international arena, in this fourth edition, our focussed areas are on quantum materials, energy materials, and AI/ML.

We sincerely hope that each one of you will get an enthralling experience of learning about new progresses made in the last few years, the new inventions and discoveries in these domains. With more than 300 inquisitive brains, EESTER 2025 is certainly going to be a platform of discussion, deliberation and collaboration. It is not an understatement to say that EESTER 2025 is going to provoke us to germinate new research ideas and out of box solutions.

The city of Chennai has a lot to offer as far as the history, culture, arts, and music are concerned. We believe that you will have a great time in exploring and to make your stay pleasant and memorable.

Best regards,

Conveners, and Co-conveners of EESTER 2025



Dr. Ranjit Nanda
Convener
IITM, India



Dr. Saurabh Ghosh
Convener
SRMIST KTR, India



Dr. Sudhakar Chandran
Co-convener
IITM, India



Dr. Biplab Sanyal
Co-convener
Uppsala, Sweden



Dr. Jaivardhan Sinha
Co-convener
SRMIST KTR, India

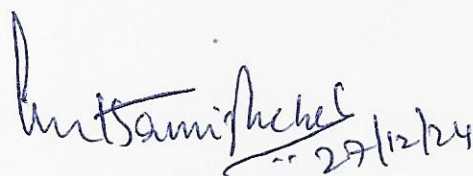


MESSAGE

I am extremely happy to know that the 4th Edition of the International Workshop and Conference on “Evolution of Electronic Structure Theory and Experimental Realization” (EESTER 2025) is organized jointly by the Dept. of Physics and Nanotechnology SRMIST, Kattankulathur campus, the Dept. of Physics, IIT Madras, CLRI, Anna University, India and Uppsala University Sweden, scheduled to be held from January 3rd – 11th, 2025.

The evolution of electronic structure theory and its experimental realization highlights the critical interplay between theoretical predictions and practical validation in understanding material properties. Theoretical methods offer powerful tools to model electronic behaviours, but their accuracy often depends on approximations. Experimental techniques provide tangible insights and serve as benchmarks to refine and validate these models. Together, they drive innovation across chemistry, materials science, and nanotechnology, while also revealing challenges in bridging theoretical assumptions with experimental complexities. This synergy underscores the importance of advancing both domains for scientific and technological progress. I am sure EESTER 2025 will provide a unique platform for researchers, scientists, and industry experts to converge and share pioneering advancements in electronic structure theory and its experimental applications. As this field forms the backbone of modern scientific and technological progress, the knowledge exchanged during this conference will play a significant role in shaping future innovations, promoting knowledge sharing, fostering new collaborations, and exploring emerging trends.

I wish the Conference a grand success.



Prof. C. Muthamizhchelvan
VICE CHANCELLOR
SRM Institute of Science and Technology
SRM Nagar, Kattankulathur - 603203
Chengalpattu Dist. Tamilnadu, India.

Invited Speakers



Richard M Martin
University of Illinois
Urbana - Champaign



Jagadeesh S. Moodera
MIT, USA



Sokrates Pantelides
Vanderbilt University,
USA



Sashi Satpathy
University of Missouri,
USA



Rampi Ramprasad
School of Materials
Science and
Engineering at Georgia
Tec



Rajeev Ahuja
IIT Ropar



D. D. Sarma
Indian Institute of
Science Bangalore



G. P. Das
TCG Crest



Indra Dasgupta
Indian Association for
the Cultivation of
Science Jadavpur



Carsten Ullrich
University of Missouri,
USA



Bartomeu Monserrat
University of
Cambridge, United
Kingdom



Udo Schwingschlögl
King Abdullah
University of Science
and Technology
(KAUST), Thuwal



Suchi Guha
University of Missouri,
USA



Jainendra K. Jain
Penn State, Eberly
College of Science



Bhaskaran Ganapathy
IMSc or IIT Madras



Suchitra Sebastien
University of
Cambridge



Shiram Ramanathan
Rutgers University



HE Qian
National University of
Singapore



Swapan Pati
JNCASR



Awadhesh Narayan
IISc Bangalore



Ashok Kumar Nanjundan
University of Southern
Queensland



Naga Phani B Aetukuri
IISc Bangalore



Pavan Nukala
IISc Bangalore



Manoj Harbola
IIT Kanpur



Abhishek Singh
IISc Bangalore



Anoop Krishnan
IIT Delhi



Biswarup Pathak
IIT Indore



Kartik Tarafdar
NIT-Suratkal



Pranaba Muduli
IIT Delhi



Narendra Kurra
IIT Hyderabad



K G Suresh
IIT Bombay



Mukul Kabir
IISER Pune



Mukesh Kumar
IIT Ropar



Manoj A G Namboothiry
IISER TVM



M B Sahana
ARCI



Dhanvir Singh Rana
IISER Bhopal



Ravi Kashikar
IITRAM



Prasanjit Samal
NISER Bhubaneswar



Ganapathy Vaitheeswaran
University of
Hyderabad



Kanchana V
IIT Hyderabad



Swastika Banerjee
IIT Roorkee



Sudhir Sahoo
IIT Dharward



Amrita Bhattacharya
IIT Bombay



Bahadur Singh
TIFR Mumbai



Aftab Alam
IIT Bombay



Satya Sahoo
IOP Bhubaneswar



Ranjit Thapa
SRM-AP



Sudip Chakraborty
HRI, Allahabad



Abir De Sarkar
INST



Ajaya Nayak
NISER Bhubaneswar



Ananth Govindrajn
IISc Bangalore



Dibyajyoti Ghosh
IIT Delhi



Tanmoy Das
IISc Bangalore



Priya Johri
Shiv Nadar University



Alok Shukla
IIT Bombay



Sudeshna Sen
IIT(ISM) Dhanbad



Sudip Kumar Batabyal
Amrita University,
Coimbatore



Arghya Taraphder
IIT Kharagpur



Anjali Kshirsagar
Savitribai Phule Pune
University



Ranjith Pai
DST, India



Yasir Iqbal
IIT Madras



Abhishek Misra
IIT Madras



E. Senthil Kumar
SRMIST



Satyesh K. Yadav
IIT Madras



Chiranjib Majumdar
BARC



P. Ravindran
Central University of
Tamil Nadu



Sougata Mallick
SRMIST



Dhavala Suri
IISc Bangalore



Pramoda Kumar Nayak
Jain University



Manas Dalai
IMMT, Odisha



Jyoti Mohanty
IIT Hyderabad



Raghavan Ranganathan
IIT Gandhinagar



Thangavelu Paliniselvam
IIT Madras



Surendra B Ananthraman
IIT Madras



Prakash Parida
IIT Patna



Prafulla K Jha
MSU Baroda



S N Pandey
MNNIT Allahabad



Debakanta Samal
IOP Bhubaneswar



Sudhir Sahoo
IIT Dharward



Dibakar Roy Chowdhury
Anurag University



Rajamani Raghunathan
RRCAT



Prakash Muthuramalingam
SRMIST



Subramaniam Chandramouli
IIT Bombay

Program Schedule (Workshop)

Evolution of Electronic Structure Theory & Experimental Realization (EESTER-2025)

Organized by SRMIST KTR and IIT Madras

3 - 7 January 2025, SRM Institute of Science and Technology, Chennai, India

8 - 11 January 2025, Indian Institute of Technology Madras, Chennai, India

Day 1: January 3, 2025, Friday Workshop at SRMIST

Electronic Structure Theory

Venue: Mini Hall 2, T. P. Ganesan Auditorium SRMIST KTR

8:00 am to – 9:00 am : Registration

9:00 am – 9:30 am	Inaugural Session		
Day 1: Morning Session	Chair: Prof. G. P. Das TCG Crest, Kolkata		
Time	Lecture	Speaker	Title of The Talk
9:40 am – 10:30 am 40 minutes talk +10 minutes Q&A	Plenary Lecture (PL1)	Prof. D. D. Sarma IISc Bangalore	The synergy between experiment and electronic structure theory in condensed matter physics
10:30 am – 11:20 am 40 minutes talk +10 minutes Q&A	Plenary Lecture (PL2)	Prof. Rajeev Ahuja IIT Ropar	Computational materials science and its applications in the area of materials for sustainable development
11:20 am – 12:00 pm (40 minutes)	High Tea / Coffee Break / Registration Contd.		
12:00 pm – 1:00 pm Interactive 60 minutes	Workshop WL 1	Prof. Manoj Harbola IIT Kanpur	Introduction to density-functional theory
1:00 pm – 2:00 pm	Lunch Break		
Day 1: Afternoon Session	Chair: Prof. Venkatesan Subramanian SRMIST KTR		

2:00 pm – 3:00 pm Interactive 60 minutes	Workshop WL 2	Prof. Manoj Harbola IIT Kanpur	Introduction to exchange- correlation functionals
3:00 pm - 4:00 pm Interactive 60 minutes	Workshop WL 3	Prof. G. P. Das , TCG Crest, Kolkata	Plane Wave versus Atom-Centered Basis in DFT
4:00 pm – 4:30 pm (30 minutes)	Tea /Coffee Break		
4:30 pm – 5:30 pm Interactive 60 minutes	Workshop WL 4	Prof. Indra Dasgupta IACS, Kolkata	Modeling Emergent Phases of Quantum Matter-Lecture-1
5:30 pm - 6:30 pm Interactive 60 minutes	Workshop WL 5	Prof. Sashi Satpathy University of Missouri USA	Berry Phase in Condensed Matter Physics: Concepts and Applications - Lecture-1
6:30 pm - 7:30 pm (60 minutes)	Own Discussion Session / Time	Interactive Discussions on the topics covered with available faculty members /Discussions in small groups /Campus tour	
7:30 pm - 8:30 pm	Dinner at conference		
8:15 pm - 8.45 pm	Buses to accommodation places		

Day 2: January 4, 2025 Saturday

Electronic Structure Theory and Experimental Realization

Venue: Mini Hall 2, T. P. Ganesan Auditorium SRMIST KTR

<u>Day 2: Morning Session</u>		Chair: Prof. Manoj Harbola IIT Kanpur	
Time	Lecture	Speaker	Topic to be covered
9:30 am - 10:20 am 40 minutes talk +10 minutes Q&A	Plenary Lecture (PL3) (online)	Prof. Richard M. Martin Illinos Urbana-Champaign University of Chicago, USA	Electronic Structure: A grand challenge of theoretical physics that is useful for many fields of science and technology
10:30 am - 11:30 am Interactive 60 minutes	Workshop WL 6	Prof. Indra Dasgupta IACS, Kolkata	Modeling Emergent Phases of Quantum Matter-Lecture 2
11:30 am – 12:00 pm (30 minutes)	Tea /Coffee Break		
12:00 pm – 1:00 pm Interactive 60 minutes	Workshop WL 7	Prof. Sashi Satpathy University of Missouri USA	Berry Phase in Condensed Matter Physics: Concepts and Applications – Lecture 2
1:00 pm – 2:00 pm	Lunch Break		
<u>Day 2: Afternoon Session</u>		Chair: Prof. Tumpa Sadhukan SRMIST	
2:00 pm – 3:00 pm Interactive 60 minutes	Workshop WL 8 (online)	Prof. Biplab Sanyal Uppsala Univ. Sweden	Magnetism and spin transport in advanced functional magnets
3:00 pm - 4:00 pm Interactive 60 minutes	Workshop WL 9	Prof. Jaivardhan Sinha SRMIST KTR	Current Induced Dynamics of Topological Spin Textures
4:00 pm – 4:30 pm (30 minutes)	Tea /Coffee Break		
4:30 pm – 5:30 pm Interactive 60 minutes	Workshop WL 10	Prof. Pavan Nukala IISc Bangalore	Physics of correlated materials and

			engineering of various devices
5:30 pm – 6:30 pm Interactive 60 minutes	Workshop WL 11 (online)	Prof. Naga Phani IISc Bangalore	Diagnostics for Better Batteries
Day 2: Evening Session	Chair: : Introduction of Prof. Sokrates Pantelides by Dr. Saurabh Ghosh		
6:30 pm – 7:20 pm 40 minutes talk + 10 minutes Q&A	Plenary Lecture (PL4) (Online)	Prof. Sokrates Pantelides Vanderbilt University, Nashville USA	Theory plus spatially resolved vibrational spectroscopy – a new frontier
7:30 pm – 9:30 pm	Banquet Dinner @ SRM HOTEL, 7:30 pm onwards		
9:30 pm	Buses to respective accommodation places		

Day 3: January 5, 2025 Sunday

Day 3: Morning Session	
9:30 am – 7:30 pm	Excursion for Registered Participants

Day 4: January 6, 2025 Monday

Machine Learning for Materials

Venue: Mini Hall 2, T. P. Ganesan Auditorium SRMISTKTR

<u>Day 4: Morning Session</u>		Chair: Prof. Rudra Banerjee SRMIST KTR	
Time	Lecture	Speaker	Topic to be covered
9:30 am – 10:30 am Interactive 60 minutes	Workshop WL 12	Prof. Saurabh Ghosh SRMIST KTR	An Overview of Machine Learning for Multiferroic and Nuclear Materials
10:30 am – 11:30 am Interactive 60 minutes	Workshop WL 13 (online)	Prof. Anoop Krishnan IIT Delhi	Machine learning for materials modelling - Lecture 1
11:30 am – 12:00 pm (30minutes)	Tea /Coffee Break		
12:00 pm – 1:00 pm Interactive 60 minutes	Workshop WL 14 (online)	Prof. Anoop Krishnan IIT Delhi	Machine learning for materials modelling - Lecture-2
1:00 pm – 2:00 pm	Lunch Break		
<u>Day 4: Afternoon Session</u> 2:00 pm – 6:00 pm Hands On		Hands on Machine Learning: Materials Database and Model Building Venue: iMac Lab1 and iMac Lab2, 14th Floor Tech Park Dept. of Computing Technologies, School of Computing, SRMIST KTR	
<u>Day 4: Evening Session</u> <u>Sponsor presentation</u> <u>6:00 pm – 7:30 pm</u>		Wiley journal workshop Overview of various Willy Journals and paper writing approach	
7:30 pm – 8:30 pm	Dinner		
8:15 pm – 8.45 pm	Bus to accommodation places		

Day 5: January 7, 2025 Tuesday

Electronic Structure Theory, ML and Experimental Realization

Venue: Mini Hall 2, T. P. Ganesan Auditorium SRM IST

<u>Day 5 Morning Session</u>		Chair: Prof. Madhuparna Karmakar SRMIST KTR	
Time	Lecture	Speaker	Topic to be covered
9:30 am – 10:30 am Interactive 60 minutes	Workshop WL 15	Prof. Biswarup Pathak IIT Indore	An Introduction to Machine Learning Approaches in Materials Science
10:30 am – 11:30 am Interactive 60 minutes	Workshop WL 16	Prof. Rohit Batra IIT Madras	Efficient and Accelerated Materials Discovery with Active Learning
11:30 am – 12:00 pm (30 minutes)	Tea /Coffee Break		
12:00 pm – 1:00 pm Interactive 60 minutes	Workshop WL 17	Prof. Carsten A. Ullrich University of Missouri USA	TDDFT: Concepts and Applications- Lecture-1
1:00 pm – 2:00 pm	Lunch Break		
<u>Day 5 Afternoon Session</u>		Chair: Prof. Jaivardhan Sinha SRMIST KTR	
2:00 pm – 3:00 pm Interactive 60 minutes	Workshop WL 18	Prof. Carsten A. Ullrich University of Missouri USA	TDDFT: Concepts and Applications- Lecture-2
3:00 pm – 4:00 pm Interactive 60 minutes	Workshop WL 19	Prof. Ramesh Babu Pondicherry Univ.	Spin transport across polar- Polyvinylidene fluoride thin films
4:00 pm – 4:30 pm	Workshop Concluding Session		
@ 4:30 pm	High Tea /Coffee		
@5:00 pm	Buses to IIT Madras from SRMIST		
@7.30 pm	Dinner at IIT Madras		

Day 1: January 8, 2025, EESTER-2025

Morning Session-1

Registration and Inauguration: 8:15 – 9:00 AM
Plenary Talks, Chair: TBA
PT-1: 1: 9:00 – 9:40 AM Title: Seeking Majorana Bound States and Diode Phenomenon in Superconductor-Ferromagnet Proximity Coupled Systems Jagadeesh Moodera, MIT, USA
PT-2: 9:40 – 10:20 AM Title: Fermi-volume-changing quantum phase transitions and the cuprate phase diagram Subir Sachdev, Harvard University, USA
Tea Break: 10:20 – 10:35 AM

Morning Session -2

Bose Gharana (BG)	Raman Gharana (RG)
BG-A: Correlated Electron Physics - I Chair: TBA	RG-A: Exciton Physics - I Chair: TBA
BG-KT-1: 10:35 – 11:05 AM Title: Wannier Orbitals and Wannier Cooper Pair in Phase Space Tanmoy Das, IISc Bangalore	RG-KT-1: 10:35 – 11:05 AM Title: Exciton dynamics and nonlinear optical properties of quantum confined halide perovskites Suchi Guha, University of Missouri, USA
BG-KT-2: 11:05– 11:35 AM Title: Charge Order Induced Altermagnetism in bipartite lattice Rajamani Raghunathan, UGC-DAE CSR, Indore	RG-KT-2: 11:05– 11:35 AM Title: Computational Roadmap of Emerging Materials: Implications of Rashba and Excitonic Physics Sudip Chakraborty, HRI, Allahabad
BG-KT-3: 11:35 AM - 12:05 PM	RG-KT-3: 11:35 AM - 12:05 PM

<p>Title: Ligand Tunability of Emergent Non-collinear Magnetism in Cu-based Layered Hybrid Perovskites</p> <p>Debakanta Samal, IOP Bhubaneswar</p>	<p>Title: Electronic Structure of Noncentrosymmetric AgCd₂GaS₄ Using High-Resolution Photoemission Spectroscopy</p> <p>Manas Kumar Dalai, CSIR - IMMT</p>
<p>BG-IT-1: 12:05 - 12:30 PM</p> <p>Title: Many-Body Quantum Interference Route to the Two-Channel Kondo Effect: Inverse Design for Molecular Junctions and Quantum Dot Devices</p> <p>Sudeshna Sen, IIT-ISM Dhanbad</p>	<p>RG-IT-1: 12:05 - 12:30 PM</p> <p>Title: Strong Light-Matter Interactions in Two-dimensional Materials for Optoelectronic Devices</p> <p>Surendra B. Anantharaman, IIT Madras</p>
<p>ORAL Presentations</p>	<p>ORAL Presentations</p>

1:15 – 2:00 PM
Lunch break + Networking

<p>BG: Quantum Transport & Topology - I Chair:</p>	<p>RG: Electrochemistry - I Chair:</p>
<p>BG-KT-4: 2:00 – 2:30 PM</p> <p>Title: Topological quantum phase transition in magnetic topological insulator bilayer</p> <p>Mukul Kabir, IISER Pune</p>	<p>RG-KT-4: 2:00 - 2:30 PM</p> <p>Title: Hydrogen Storage in Functionalised Carbon Systems – A DFT study</p> <p>Prafulla K Jha, MSU Baroda</p>
<p>BG-KT-5: 2:30 – 3:00 PM</p> <p>Title: Non-Linear Hall Effect in Flatlands and Chiral Crystals</p> <p>Awadhesh Narayan, IISc Bangalore</p>	<p>RG-KT-5: 2:30 - 3:00 PM</p> <p>Title: C₂ over C₁ during CO₂ER: Can we tune the activity of 111 Plane of Cu based catalysts</p> <p>Ranjit Thapa, SRMAP, Amaravati</p>
<p>BG-KT-6: 3:00 - 3:30 PM</p> <p>Title: Topological heterostructure based spintronic devices for optoelectronic application</p> <p>Pramod Kumar, IIT Allahabad</p>	<p>RG-KT-6: 3:00 - 3:30 PM</p> <p>Title: DFT Studies on CO₂ Reduction at Functionalized IL@Au(111) Surface</p> <p>Prakash Muthuramalingam, SRMIST</p>
<p>BG-IT-2: 3:30 - 3:55 PM</p>	<p>RG-IT-2: 3:30 - 3: 55PM</p>

<p>Title: Proximity Coupling in Topological Materials</p> <p>Dhavala Suri, IISc Bangalore</p>	<p>Title: Advancement in Next Generation Energy Materials and Neuromorphic Paradigm: A Guide Through DFT</p> <p>Tisita Das, HRI</p>
<p>ORAL Presentations</p>	<p>ORAL Presentations</p>
<p>4:15 – 4:45 PM</p> <p>High Tea</p>	
<p>Evening Session: 4:45 – 7:00 PM</p>	
<p>Quantum Transport & Topology-II Chair:</p>	<p>Electrochemistry-II Chair:</p>
<p>BG-KT-7: 4:45 – 5:15 PM</p> <p>Title: Computational Pathways in Topological Quantum Materials: Insights from DFT</p> <p>V. Kanchana, IIT Hyderabad</p>	<p>RG-KT-7: 4:45 – 5:15 PM</p> <p>Title: Designing 2D photocatalysts for Green Hydrogen Production</p> <p>P. Ravindran, CU, Tamil Nadu</p>
<p>BG-KT-8: 5:15 – 5:45 PM</p> <p>Title: Exploring Novel Topological States: Multi-Fold Fermions and Dirac Nodal-Line Net Bosons in SiX₂ (X = P, As)</p> <p>Ganapathy Vaitheeswaran, University of Hyderabad</p>	<p>RG-KT-8: 5:15 – 5:45 PM</p> <p>Title: TBA</p> <p>Anjali Kshirsagar, Savitribai Phule Pune University</p>
<p>BG-IT-3: 5:45 – 6:10 PM</p> <p>Title: The Complex Topological Landscape of 4D Transition Metal Systems</p> <p>Kartick Tarafder, NIT Surathkal</p>	<p>RG-IT-3: 5:45 – 6:10 PM</p> <p>Title: Energy storage materials for supercapacitor application</p> <p>S. N. Pandey, MNNIT Allahabad</p>
<p>PT-3: 6:20 – 7:00 PM: Evening Talk</p> <p>Title: A Century of Quantum Physics is only a Warm up Exercise</p> <p>G. Baskaran, IIT Madras</p>	

7:00 – 9:00 PM Conference Dinner - I , Alumni Club, IIT Madras

DAY-2: 9th January, 2025

Morning Session-1

Plenary Talks, Chair: TBA
PT-4: 8:45 – 9:25 AM Title: Topological Hall effect in skyrmion crystals via spin-orbit coupling Sashi Satpathy, University of Missouri, USA
PT-5: 9:25 – 10:05 AM Title: Fermi Surfaces in Unconventional Insulators Suchitra Sebastian, University of Cambridge, UK
Tech-Talk-1 10:05 – 10:30 AM (TBA)
Tea Break: 10:30 – 10:45 AM

Morning Session -2

Bose Gharana (BG)	Raman Gharana (RG)
BG-B: Correlated Electron Physics -II Chair:	RG-B: Solar Cell – I Chair:
BG-KT-9: 10:45 – 11:15 AM Title: Emergent moments and metal-insulator transition in charge density wave heterostructures 1T-NbSe₂/1T-TaX₂ Arghya Taraphder, IIT Kharagpur	RG-KT-9: 10:45 – 11:15 AM Title: Solution Processed Solar Cells - A Glimpse of Organic and Perovskite Solar Cells Manoj A. G. Namboothiry, IISER TVM
BG-KT-10: 11:15 AM – 11:45 PM Title: K₂Ni₂(SO₄)₃: A quantum spin liquid under thin ice Yasir Iqbal, IIT Madras	RG-KT-10: 11:15 AM – 11:45 PM Title: Designing Layered Halide Perovskites for Optoelectronics: Insights from ab-initio modeling Dibyajyoti Ghosh, IIT Delhi
BG-KT-11: 11:45 – 12:15 PM	RG-KT-11: 11:45 – 12:15 PM

<p>Title: DFT perspectives on piezoelectricity and spin-orbitronics in selected functional 2D materials</p> <p>Abir De Sarkar, INST Mohali</p>	<p>Title: Gallium Oxide Thin Film based Solar-Blind Photodetectors: Heterojunctions and interface</p> <p>Mukesh Kumar, IIT Ropar</p>
<p>BG-IT-4: 12:15– 12:40 PM</p> <p>Title: Antiferromagnetic Skyrmions for spintronic applications</p> <p>Sougata Mallick, SRMIST</p>	<p>RG-IT-4: 12:15– 12:40 PM</p> <p>Title: Density functional theory-based study of interaction of oxygen, hydrogen and water with CuInSe₂ thin-film solar-cell material</p> <p>Sudhir K. Sahoo, IIT Dharwad</p>
ORAL Presentations	ORAL Presentations
<p>1:15 – 3:30 PM LUNCH BREAK + POSTER</p>	
Exciton Physics-II Chair:	Electrochemistry-III Chair:
<p>BG-KT-12: 3:30 – 4:00 PM</p> <p>Title: Excitations in semiconductors: phonon-driven phenomena</p> <p>Bartomeu Monserrat, University of Cambridge, UK</p>	<p>RG-KT-12: 3:30- 4:00 PM</p> <p>Title: CAMMD Database on Electrochemical Energy Storage Materials</p> <p>Satyesh Kumar Yadav, IIT Madras</p>
<p>BG-KT-13: 4:00 – 4:30 PM</p> <p>Title: Generalized Dielectric-Dependent Hybrids: A New Computational Window for Bulk to Nano-structured Quantum Materials</p> <p>Prasanjit Samal, NISER Bhubaneswar</p>	<p>RG-KT-13: 4:00 – 4:30 PM</p> <p>Title: Influence of Slurry Rheology on Electrode Laminate Properties for Enhanced Lithium-Ion Battery Performance</p> <p>M. B. Sahana, ARCI</p>
<p>BG-KT-14: 4:30 – 5:00 PM</p> <p>Title: THz magnon spintronics with non-collinear antiferromagnets</p> <p>Dhanvir Singh Rana, IISER Bhopal</p>	<p>RG-KT-14: 4:30 – 5:00 PM</p> <p>Title: Developing an in-depth understanding of promising electrode materials for the Li and Na-ion batteries</p>

	Priya Johri, Shiv Nadar University
BG-KT-15: 5:00 – 5:30 PM Title: In search of bulk Rashba ferroelectric semiconductor for spintronics applications Amrita Bhattacharya, IIT Bombay	RG-KT-15: 5:00 – 5:30 PM Title: Non-Local Interactions Governing the Local Structure and Properties of Battery Materials Swastika Banerjee, IIT Roorkee
5:30– 6:00 PM High Tea and parallel Session ends	
PT-6: 6:00 – 6:40 PM: Evening Talk Title: TBA Jainendra Jain, Pennsylvania State University	

7:00 PM - : Dinner

DAY-3: 10th January, 2025

Morning Session-1

Plenary Talks, Chair:
PT-7: 8:45 – 9:25 AM
Title: Design of Functional and Sustainable Polymers Assisted by Computations and Artificial Intelligence
Rampi Ramaprasad, Georgia Institute of Technology, USA
PT-8: 9:25 – 10:05 AM
Title: The Quantum Materials-Neuroscience-Artificial Intelligence Interface
Shriram Ramanathan, Rutgers University, USA
PT-9: 10:05 – 10:45 AM
Title: Computational Modeling of Semiconducting Materials for their Applications in Thermoelectric and Magnetic Properties
Swapan K Pati, JNCASR
Tea Break: 10:45 – 11:00 AM

Morning Session -2

Bose Gharana (BG)	Raman Gharana (RG)
BG: Quantum Transport & Topology - III Chair:	RG: Materials Design-I Chair:
BG-KT-16: 11:00 – 11:30 AM	RG-KT-16: 11:00 – 11:30 AM
Title: Exciton Dissociation by Topological Edge States	Title: Harnessing Molecular Simulations for Advanced Materials Design
Udo Schwingenschlögl, KAUST, Saudi Arabia	Sriram Krishnamurthy, Schrödinger, Inc., Chennai
BG-KT-17: 11:30 AM – 12:00 PM	RG-KT-17: 11:30 AM – 12:00 PM
Title: Recent studies on spintronic and topological aspects of certain Heusler alloys	Title: Machine Learnable Representations for Materials, Molecules, and Reactions

K. G. Suresh, IIT Bombay	Ananth Govind Rajan, IISc
BG-KT-18: 12:00 – 12:30 PM Title: Strategies for realizing double quantum spin Hall effect Bahadur Singh, TIFR	RG-KT-18: 12:00 – 12:30 PM Title: Discovery of Unconventional and Non-intuitive Self-assembling Peptide Materials using Experiment Driven Machine Learning Rohit Batra, IIT Madras
BG-IT-5: 12:30 – 12:55 PM Title: Floquet quasi energy spectrum of graphene and kagome lattices Prakash Parida, IIT Patna	RG-KT-19: 12:30 – 1:00 PM Title: Visualizing long-range solid state amorphization in ferroic In₂Se₃ Pavan Nukala, IISc
1:10 – 3:30 PM LUNCH BREAK + POSTER	
Quantum Transport and Ferroelectrics Chair:	Materials Design -II Chair:
BG-KT-19: 3:30 – 4:00 PM Title: Coupling between magnetic and ferroelectric orders through lattice deformations Daniel Cabra, UNLP, Argentina	RG-KT-20: 3:30 - 4:00 PM Title: Designing materials for photon-phonon conversion : From science to translation Chandramouli Subramaniam, IIT Bombay
BG-KT-20: 4:00 – 4:30 PM Title: Second-principles Method for Statics and Dynamics of Ferroelectric Halide Perovskites Ravi Kashikar, IITRAM, Ahmedabad	RG-KT-21: 4:00 – 4:30 PM Title: Surface Charges of Nanostructured Materials: A New Frontier in Hydrovoltaic Power Generation Sudip Kumar Batabyal, Amrita Vishwa Vidyapeetham
BG-KT-21: 4:30 – 5:00 PM	RG-KT-22: 4:30 – 5:00 PM

Title: TBA Dibakar Roy Chowdhury, Anurag University	Title: First Principles Modelling of Liquid Water: Structure, Reactivity and Optics Ali Hassanali, ICTP
ORAL Presentations	ORAL Presentations
5:15 – 5:35 PM High Tea	

Conference Dinner-II at Coral Beach Resort, Mahabalipuram

DAY-4: 11th January, 2025

Morning Session-1

Plenary Talks, Chair:
PT-10: 9:00 – 9:30 AM
Title: Energy density and stress fields in quantum systems
Richard M Martin, University of Illinois, USA
PT-11: 9:30 – 10:10 AM
Title: Anomalous magnetism induced by 4f hybridization – An overview
E. V. Sampathkumaran, TIFR, IIT Roorkee
10:10 – 10:40 AM
Tech-Talk-2 TBA
Tea Break: 10:40 – 11:00 AM

Morning Session -2

Bose Gharana (BG)	Raman Gharana (RG)
BG: Chair:	RG: Electrochemistry - IV : Energy Storage Chair:
BG-KT-21: 11:00 – 11:30 AM Title: Thermoelectric Properties of Topological Semimetal Cu₂ZnGeTe₄: A New Paradigm to Renewable Energy Aftab Alam, IIT Bombay	RG-KT-23: 11:00 – 11:30 AM Title: Local Electronic and Structural Influence on the Li-ion Conduction in Grain Boundary-Tailored Li_{1.3}Al_{0.3}Ti_{1.7}(PO₄)₃ Solid-State Electrolyte Sudakar Chandran, IIT Madras
BG-KT-22: 11:30 AM – 12:00 PM Title: Tuning magnetic anisotropy in thin film for possible application	RG-KT-24: 11:30 AM – 12:00 PM

Jyoti Ranjan Mohanty, IIT Hyderabad	Title: MXene-Organic Hybrids for Electrochemical Storage of Divalent Metal-ions Narendra Kurra, IIT Hyderabad
BG-KT-23: 12:00 – 12:30 PM Title: Spin-Orbit Torques in Topological Quantum Materials Pranaba Kishor Muduli, IIT Delhi	RG-KT-25: 12:00 – 12:30 PM Title: TBA Sooraj K., IIT Madras
BG-KT-24: 12:30 – 1:00 PM Title: Room Temperature Dipolar Excitons in van der Waals Heterostructures Abhishek Misra, IIT Madras	RG-KT-26: 12:30 – 1:00 PM Title: Mechanisms of Thermal Rectification in Semi-Stochastic Graded Graphene Microstructures Raghavan Ranganathan, IIT Gandhinagar
BG-KT-25: 1:00 – 1:30 PM Title: Stacking and layer dependent thermal conductivity in van der Waals materials Pramoda Kumar Nayak. Jain University	RG-KT-27: 1:00 – 1:30 PM Title: Wafer-scale production of 2D TMDs via Metalorganic Chemical Vapor Deposition E. Senthil Kumar, SRMIST
1:30 – 2:30 PM LUNCH BREAK ORAL SESSION STARTS	
ORAL PRESENTATION	ORAL PRESENTATIONS
High Tea: 4:00 – 4:30 PM	
4:30 PM – 5:00 PM PANEL DISCUSSION and FEEDBACK SESSION	
5:00 – 6:00 PM Conclusion and Award Ceremony	

ORAL Presentations - EESTER - 2025

Registration Number	Name and Affiliation	Title	Category	Oral No/Paper ID	Schedule
25014	JIJILA B (Queen Marys College)	Employing Machine-Learned Functionals to Generate Potential Energy Surface for Small Molecule	ML	OP-1 eester072	
25036	Subhojit Roy (IIT Madras)	Unconventional pairing in Ising superconductors	DFT	OP-2 eester050	
25037	Sourin Chatterjee (IIT Madras)	Symmetric spin liquids on the trellis lattice	DFT	OP-3 eester049	
25038	Soumyasree Jena (IIT Madras)	Cr-benzene Complex as a new candidate for molecular spin qubit	DFT	OP-4 eester047	
25069	Sanchi Monga (IIT Delhi)	Theoretical Insights into Inorganic Antiperovskite Nitrides (X ₃ NA; X = Mg, Ca, Sr, Ba; A = As, Sb): An Emerging Class of Materials for Photovoltaics	DFT	OP-5 eester039	
25076	BUBUNU BISWAL (IIT Madras)	Substrate Dependent Energy Dissipation and High Field Breakdown in PtSe ₂	EXP	OP-6 eester069	
25084	Sarga P K (Bits Pilani Goa)	Designing MXene/blueP heterostructures for device application	DFT	OP-7 eester058	
25092	Sachin Kumar (BARC Mumbai)	Phenomena of quantum magnetization plateau(s) in a class of spin s = 1/2 Heisenberg J ₁ -J ₁ -J ₂ trimerized quantum spin chains	DFT	OP-8 eester018	
25101	Subhajit Sau (IIT Hyderabad)	Ferroelectric Polymorphism and Epitaxial Strain Effect on Polarization and Electronic Structure of Cu(OH) ₂	DFT	OP-9 eester048	
25103	Lokesh Yadav (IIT Indore)	Platinum-adsorbed defective 2D monolayer boron nitride: a promising electrocatalyst for O ₂ reduction reaction	DFT	OP-10 eester010	
25104	Joyeta Saha (NISER)	Distribution of Charge Centers in Matter from Geometric Phases of Electrons	DFT	OP-11 eester070	
25110	Manpreet Kaur (IIT Ropar)	Irida-Graphene: A New Two-Dimensional Electrode Material for Sodium-ion Batteries	DFT	OP-12 eester013	

25135	Pratik Kumar Sahu (IIT Madras)	Chiral orbital texture and Edelstein effect in monolayer Janus TMDs	DFT	OP-13	
25150	Shanu Bandyopadhyay (IoP, Bhubaneswar)	Study of sputter-grown Nitride-based memristive devices for bio-synaptic and non-volatile memory application	EXP	OP-14 eester102	
25151	Priyadharshini S (SRMIST, KTR)	Band convergence and defect engineering synergistically revamping the carrier-phonon dynamics in Mg _{3-x} ZnxSb ₂ solid solutions: An experimental and theoretical insights	EXP-DFT	OP-15 eester084	
25178	Arunava (Int.Phy. Center.Spain)	Frustrated charge density wave and quasi-long-range bond orientational order in the magnetic Kagome FeGe	EXP-DFT	OP-16 eester009	
25191	Buveneswaran (SRMIST, KTR)	Design of Ferroelectric Double Perovskite Oxides as Photovoltaic Materials	DFT	OP-17	
25183	Gayathri P (SRMIST, KTR)	Machine learning insights into Polarization and Magnetization switching dynamics in Hybrid Improper Ferroelectric Double Perovskites Oxides	DFT-ML	OP-18	
25192	Priyanka S (SRMIST, KTR)	The Stabilization Effect of Agmatine-Salicylate Ionic Liquids on PARP-1 for Parkinson's Disease: A Perspective from DFT and MD Simulations	DFT	OP-19	
25183	Shivendra Kumar Gupta (VNIT Nagpur)	Unveiling the Coexistence of Giant Rashba Splitting and Topological properties in hexagonal crystal structure	DFT	OP-20	
25214	Poonam Sharma	Defect engineering in two dimensional PdTe ₂ pentagonal: Tuning electronic, optical, and magnetic properties	DFT	OP-21	
25082	Dipanwita Banerjee (IIT Bombay)	Identification of disorder and its influence on transport properties of half-Heusler compound	EXP-DFT	OP-22	
25215	Sayan Ghosh (IIT Madras)	TBA		OP-23	
25	Gowsalya R (SRMIST, KTR)	First principles studies on functional mode couplings in oxide superlattices DFT	DFT	OP-24	

POSTER Presentations - EESTER – 2025

Registration Number	Name and Affiliation	Title	Category	Poster No/Paper ID	Schedule
25001	Abinaya.V (SRMIST, KTR)	DFT Study on the Functionalization of Aluminum Nitride Nanotubes with Organic Acids for Targeted Delivery of Carmustine	DFT	PP-1 eester104	
25002	Sneha.J (SRMIST, KTR)	Dft Study on Functionalization of Boron Nitride Nanotube With Non-Essential Amino Acids For Targeted Delivery of Allicin In Cancer Treatment	DFT	PP-2 eester105	
25003	S.Susannal Ezhilarasi (Queen Marys College)	Exploring Hydrogen Bonding Interactions Using Neural Density Functional	ML	PP-3 eester073	
25005	S.M. Esther Rubavathy (SRMIST, KTR)	Molecular Mechanism behind Cholinium-Taurate Ionic Liquid in Stabilisation of HDAC2 for Alcohol Use Disorders: Insights from DFT and MD Simulations	DFT	PP-4 eester076	
25007	Viveka N (SRMIST, KTR)	A DFT Study of Doped MoSe2 Monolayer for Improved Sensing of H2S and HCN Gas Molecules	DFT	PP-5 eester078	
25008	Nivethitha Ganesan (SRMIST, KTR)	A DFT study on the drug delivery nature of Zinc Oxide nanocluster for anti-inflammatory drugs.	DFT	PP-6 eester113	
25009	A Sakthi Balaji (SRMIST, KTR)	DFT+NEGF Insights on Thermoelectric Transport Properties of GeTe/arsenene vdW Heterostructure: Interface Engineering	DFT	PP-7 eester092	
25013	Lakshmi Naga Sai Laya Pagadala (SRMIST, AP)	The Role of Backbone Rigidification in Thermally Activated Delayed Fluorescence: A Structure-Property Analysis	DFT	PP-8 eester065	
25019	S. Saral Sessal (SRMIST, KTR)	Superior Anchoring behaviour of Calcium Polysulfides through the Integration of ZIF-8 MOF as a substantial cathode in Ca-S Battery: A DFT study	DFT	PP-9 eester077	
25021	Rama Chandra Moharana (IIT Tirupati)	Electronic Structure and Magnetic Properties of S = 1/2 Alternating Spin Chain System KCuGa(PO4)2.	DFT	PP-10 eester112	
25025	Gowthami S (Jain, Bangalore)	Facile synthesis of large area single crystal MoS2 for photodetector	EXP	PP-11 eester060	

25026	Thameemul Ansari A (SRMIST, KTR)	Theoretical Investigation of Ba ₃ XO (X = Si, Ge, Sn): Exploring Structural, Electronic, and Elastic Properties in Inverse Perovskites	DFT	PP-12 eester099	
25027	Dr. Pooja Vyas (IIT Bombay)	Role of structural disorder on the electronic and magnetic properties of Cr ₃ Al	DFT	PP-13 eester057	
25028	Hariharan Ramesh (SRMIST, KTR)	First Principles Calculations of Argyrodite Compounds Ag ₉ XSe ₆ (where X = Al, Ga and In) for Thermoelectric Applications	DFT	PP-14 eester095	
25029	Hema G (SRMIST, KTR)	Selective Targeting of KRAS Mutations via Machine Learning-Assisted Molecular Docking and Dynamics Simulations	DFT	PP-15 eester115	
25030	Gopalakrishnan C (SRMIST, KTR)	Screening of Anion in Ionic Liquid - Graphene Interface for the Energy Storage Applications: First Principles Approach	DFT	PP-16 eester054	
25031	Giri Lakshman N (SRMIST, KTR)	Identification of Dual Inhibitors Targeting VEGFR2 and HDAC: A Computational Study	DFT	P-17 eester071	
25033	Arka Bhowmick (IIT Hyderabad)	Unveiling Topological Phenomena and Spin Hall Conductivity in NaCdBi	DFT	PP-18 eester059	
25034	Namrata Das (IIT Hyderabad)	Thermoelectric Properties of layered Bi ₂ YO ₄ Cl : a cageless rattler host structure	DFT	P-19 eester052	
25035	Sonali Srotaswini Pradhan (IIT Hyderabad)	Exploring Spin Hall Conductivity and Magnetotransport in the Rare-Earth Topological Antiferromagnetic Dirac Semimetal: GdCuSn	DFT	P-20 eester051	
25041	Thillaiarasi S (SRMIST, AP)	Azole-Based Diarylethene Photoswitches for Molecular Solar Thermal Energy Storage: A Computational Study	DFT	P-21 eester066	
25042	Zayid Ahmed (Birla Goa Campus)	Strain Tuning of TiN for Thermoelectric Applications	DFT	PP-22 eester096	
25043	Rishab Sahoo (IIT Kharagpur)	Ab-initio calculation of Lattice Thermal Conductivity of Janus Graphene	DFT	PP-23 eester067	
25048	Deepak Upadhyay (MSU Baroda)	Polymorph exploration of niobium oxynitride using first-principles calculations	DFT	PP-24 eester042	

25049	Kusum Kumari (IIT Hyderabad)	Computational Modelling of Single-Molecule Magnet (SMM) behavior in 1D nanotubes and 3D Metal-Organic Framework by embedding Dyprocenium-based SMM in their voids	DFT	PP-25 eester081	
25050	Priyanka Ghosh (IIT Indore)	Unveiling the Role of Surface Redistribution of High-Index Cu ₂ O on CO ₂ RR	DFT	PP-26 eester053	
25053	Heli Jatin Mistry (MSU Baroda)	Interaction Study of Toxic gases with Nickel decorated alpha-CN: A First-principles Study	DFT	P-27 eester056	
25055	Heera T Nair (MSU Baroda)	V-decorated Graphdiyne for Efficient Hydrogen Storage- Insights from DFT	DFT	PP-28 eester030	
25057	Dhori Bhautik Rameshbhai (MSU Baroda)	Topological signatures of Triply Degenerate nodal point Fermions in TbPtBi Heusler Alloy	DFT	P-29 eester025	
25060	Zarna D. Ponkiya (MSU Baroda)	Machine Learning Force Field-Accelerated Prediction of Lattice Thermal Conductivity in Strained WS ₂ Monolayer	ML	P-30 eester026	
25062	Maricherla Hemalatha (SRMIST, AP)	Rational Design of D- π -A- π -A(C60) and D- π -D- π -A(C60) Architectures: Electric Field-Mediated Charge Transfer Dynamics for Single-Component Organic Solar Cells	DFT	PP-31 eester063	
25063	Monikana Gope (IIT Roorkee)	Prediction of SJTM Observables in Putative PDW State in Cuprates	EXP-DFT	PP-32 eester055	
25065	Arkamitra Sen (IACS)	Topological phases of Honeycomb system with broken in-plane mirror symmetry	DFT	PP-33 eester088	
25066	Anupam Mondal (IACS)	Effect of spin-orbit coupling in non-centrosymmetric Heusler family(half-Heusler, inverse-Heusler and quaternary-Heusler)	DFT	PP-34 eester080	
25067	Ayan Chakravorty (Shiv Nadar Insti.)	Unlocking the Optoelectronic Potential of AGeX ₃ (A = Ca, Sr, Ba; X = S, Se): A Sustainable Alternative in Chalcogenide Perovskites	DFT	PP-35 eester027	

25068	Sanjay Kumar (SRMIST, KTR)	Effect of Metal-based Anion in Ionic Liquid@UiO-66 MOF for Selective CO ₂ Capture and Separation: A Computational study	DFT	PP-36 eester061	
25070	Shantanu Pathak (IIT Delhi)	Exploring Spin Textures and Modulating Spin-Splitting in Layered Perovskites: A First-Principles Computational Approach	DFT	PP-37 eester040	
25071	Mani Bharathi M (SRMIST, KTR)	Back-to-Back Successful Transformation of Domain Wall Pair and Skyrmion in a Specially Designed Racetrack for Memory Storage Application	DFT	PP-38 eester068	
25073	Ankita Narwal (IIT Madras)	AB-stacked bilayer β 12–borophene as a promising anode material for alkali metal-ion batteries	DFT	PP-39 eester074	
25074	K. Saikumar (SRMIST, KTR)	Interplay of coherence dynamics and particle Current in Quantum double dot system coupled to fermion reservoirs: Insights for predicting transport in molecular devices	DFT	PP-40 eester123	
25075	Mohd Rashid (IIT Indore)	Effect of Graphene Electrode Functionalization on Machine Learning aided Single Nucleotide Classification	ML	PP-41 eester045	
25078	Bommareddy Poojitha (IIT Tirupati)	Electronic and phonon studies of B-site ordered double perovskites Nd ₂ BTiO ₆ (B = Zn, Ni)	DFT	PP-42 eester028	
25079	Pritish Ranjan Joshi (CREST, Kolkata)	Inverse design of cathode materials for metal-ion batteries using Variational Auto-Encoder neural network architecture	ML	PP-43 eester111	
25080	Sk.Soyeb Ali (Bennett Univ)	Strain induced electronic and magnetic transition in S=3/2 ferromagnetic spin chain compound SbCrSe ₃	DFT	PP-44 eester046	
25081	Shovan Gayen (Bennett Univ)	Pressure Induced electronic and magnetic transition in antiferromagnetic NiS: A combined DFT+U and Monte-Carlo study	DFT	PP-45 eester021	
25083	Ibtesham Tarannum (IIT Hyderabad)	Unravelling Electronic Structure, Bonding and Magnetic Properties of Dysprosocene Single Molecule Magnets	DFT	PP-46 eester089	

25086	Kahkasha Parveen (IIT Indore)	Unveiling the Electrocatalytic Activity of Metallophthalocyanine based Covalent Organic Frameworks towards CO ₂ Reduction Reactions	DFT	PP-47 eester020	
25088	Basantia Saswat Abhilash (IIT Hyderabad)	Computational Modelling of Electron Transport through the Spin Cross-Over (SCO) complex [Co(3,4lutidine) ₄ X] ⁺ (X=F, Cl, Br)	DFT	PP-48 eester023	
25093	Karthik HJ (Bits, Goa Campus)	Janus van der Waals Heterostructures: Unlocking Ultra-High Thermoelectric Efficiency in SnS ₂ and its Janus monolayer based Systems	DFT	PP-49 eester017	
25094	Abhishek Hota (IoP, Bhubaneswar)	Exploring Frustration in the Hollandite Lattice and Its Connection to the 3D Triangular Lattice	DFT	PP-50 eester062	
25100	Singdha Sagarika Behera (KIIT, Bhubaneswar)	Deciphering the Insulating Behavior of pentavalent Ir-based perovskite oxide: Interplay of Spin-Orbit Coupling and Hubbard U	DFT	PP-51 eester107	
25106	Dr. Nila Pal (shiv Nadar Univ)	Cost-effective ZnO/GeOx/Ge Heterostructure for Broadband Photodetection Applications	EXP	PP-52 eester006	
25108	Vineeta Yadav (IIT Tirupati)	Pressure studies on Os-based double perovskite oxides	DFT	PP-53 eester029	
25109	Divya (IIT Ropar)	Reversible Hydrogen Storage in NLi ₄ -Decorated Boron Phosphide Biphenylene	DFT	PP-54 eester015	
25111	Shikha (IIT Ropar)	Designing high-performance doped Ni(OH) ₂ electrocatalyst for Oxygen Evolution Reaction(OER) through water splitting	DFT	PP-55 eester-12	
25112	Manorama Pandey (IIT Bhubaneswar)	Enhancing the Electrochemical Properties of LiFePO ₄ by Fe-Site Doping: An ab initio Study	DFT	PP-56 eester007	
25113	Abhishek (IIT Jodhpur)	Tuning the Selective Sensing Properties of Molybdenum Carbide MXenes, (Mo ₂ CT ₂ : T ₂ = -O, -S and -F) Towards Volatile Organic Compounds (VOCs): An Ab-initio Approach	DFT	PP-57 eester114	
25116	Varinder Pal (IIT Kharagpur)	Thermoelectric behaviour of directionally solidified Bi ₂ Te ₃ -Ga ₂ Te ₃ eutectic	EXP	PP-58 eester004	

25117	Subham Chattopadhy (Visvesvara, Nagpur)	Water Assisted Photoinduced Tautomerization in a Potential Bioactive Semicarbazone Schiff Base	EXP-DFT	PP-59 eester003	
25119	Shrestha Banerjee (Visvesvara, Nagpur)	Unveiling the Dynamics of Triplet Exciton in Chalcone-based Donor-Acceptor System	EXP-DFT	PP-60 eester002	
25120	Anupama S (IISER Pune)	High-temperature magnetism and strong spin-phonon coupling in two-dimensional CrTe ₂	DFT	PP-61 eester008	
25123	Rose Jose (MAR, Pazhanji)	First-Principle Study on Structural and Charge Conduction Parameters of CsPbX ₃ (X= Cl, Br, I) for Memristor Applications	DFT	PP-62 eester041	
25124	Purushothaman M (IIITDM Kanchi)	A Density Functional Theory Based Study of the Optical properties of Oxygen-deficient SrVO ₃	DFT	PP-63 eester064	
25127	Rashi Jain (IIT Dharwad)	Molecular Insights into Alkali Metal Interaction with Redox Active Covalent Organic Framework as Cathode in Batteries	DFT	PP-64 eester024	
25129	Surya S (SRMIST, KTR)	Tailored Surface Functionalization of Ti ₃ C ₂ T _x MXenes through Transition Metal Doping : A DFT Study	DFT	PP-65 eester093	
25141	Arijit Mandal (IIT Madras)	The role of orbital interplay in the formation of alter magnetism	DFT	PP-66 eester124	
25145	Santanu Kumar Nayak (CUTM, Odisha)	Exploring Elastic Properties of ZnO Single-Walled Nanotubes: Insights from Zigzag, Chiral, and Armchair Configurations Using the Universal Force Field	DFT	PP-67 eester075	
25146	Kavyasree N (Central Univ, Kerala)	Effects of Surface functionalization on electronic properties of Ti ₂ C MXene.	DFT	PP-68 eester079	
25149	Subarna Ray (IISER Berhampur)	Lead-Free, Vacancy-Ordered Double Halide Perovskite based material for Thermoelectric Energy Utilization	DFT	PP-69 eester103	
25154	Dipan Kumar Das (CUTM, Odisha)	Assessing Ai's Potential In Gallium Nitride Material Design For Spintronic Applications	ML	PP-70 eester082	
25156	Shweta Choudhary (IIT Roorkee)	Lithium and Sodium Superionic Conduction in Metal Borohydride Framework	DFT	PP-71 eester087	

25158	Selvamani E (SRMIST, KTR)	A first principle characterization on structural & electronic properties of 2D HfS ₂ monolayer	DFT	PP-72 eester110	
25160	Deepak (NIT KKR)	A DFT Investigation of Tungsten(W) Doped and Decorated Pristine Graphene and Graphene with Stone-Thrower-Wales (55-77) Defects for hydrogen adsorption	DFT	PP-73 eester125	
25161	Yammala Eliya (IIT Madras)	Defect engineering and its impact on electrocaloric properties in non-stoichiometric BaTiO ₃ -based system	EXP	PP-74 eester094	
25162	Utkarsh Jain (IIT Madras)	Study of glassy transitions in modified barium titanate system.	EXP	PP-75 eester090	
25163	Bhargab Kakati (IASST, Guwahati)	Berry curvature induced anomalous Hall effect in Pt ₂ MnGa	DFT	PP-76 eester091	
25164	Ankita K (IIT Madras)	Flexible Triboelectric Nanogenerator based on PVDF-BCZT Nanocomposite Films for piezo-tribo Hybrid Energy Harvesting	EXP	PP-77 eester097	
25165	Aravind V Raj (IIT Mandi)	Transport Properties of AM ₄ X ₈ type Tetrahedral Cluster Compounds	EXP	PP-78 eester108	
25166	Vivek Gusain (IIT Delhi)	First-principles study of the electronic structure, Z ₂ invariant and Quantum oscillation in the kagome material CsV ₃ Sb ₅	DFT	PP-79 eester100	
25167	M. Julie Therese (IIITDM, Kanchi)	Role of Defect Migration in Wide-Bandgap Semiconductor for Memristor Application: An Ab-initio Analysis	DFT	PP-80 eester101	
25171	Namitha Dsouza (IIT Madras)	Modulating the sub-gap defects in titanium oxide using atomic layer deposition for the application in carrier selective Si solar cell	EXP	PP-81 eester106	
25172	Saurabh Kumar Sen (VNIT, Nagpur)	Exploring Three-Dimensional Topological Weyl Semimetals Featuring Robust Fermi Arcs and Lifshitz Transition	DFT	PP-82 eester109	
25174	Manuj Ahuja (Shiv Nadar Univ)	Unraveling K-ion storage in MXenes films for flexible supercapacitor applications	DFT	PP-83 eester086	
25185	Ashish Kumar Panigrahi (IoP, Bhubaneswar)	Resonance Raman and Temperature-Dependent Photoluminescence in MoS ₂ -WS ₂ Vertical Heterostructures	DFT	PP-84 eester126	

25186	Alok Kumar (IoP, Bhubaneswar)	Unveiling structural phases and correlated thermal conductivities in bilayer WS ₂	DFT	PP-85 eester127	
25195	Perarasan (SRMIST, KTR)	Field-free Perpendicular Magnetization Switching by Spin-Orbit Torque in Exchange Bias System: A Micromagnetic Study	DFT	PP-86 eester122	

LIST OF ABSTRACTS IN WORKSHOP MODE

Plenary Lecture 1

Synergy between experiment and electronic structure theory in condensed matter physics: A couple of examples

D. D. Sarma

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru 560012,
India

Email: sarma@iisc.ac.in

The intrinsic link between electronic structure theories and experimental practices in condensed matter physics is well-established and requires no further justification. The dynamic interplay between these two research methodologies has significantly advanced the field, sometimes through mutual challenges and at other times through cooperative efforts. This synergy will be illustrated with two examples from our work.

First, I will discuss an unusual phase transition in VO₂ and present a unified quantum-entanglement description of its polymorphs.[1] Second, I will address the paradoxical achievement of thermal conductivity lower than the expected minimum in a specific system.[2]

References

1. Banabir Pal, Amar Srivastava, Abhinav Kumar, Sumanta Mukherjee, Indranil Sarkar, Suman Mandal, Mihaela Gorgoi, Paola Di Pietro, Stefano Lupi, W. Drube, E. Arenholz, J. Chakhalian, A. Perucchi, T. Venkatesan, S. Biermann, Jan M. Tomczak, and D. D. Sarma, Unpublished.
2. Debasmita Pariari, Paribesh Acharyya, Arijit Sinha, Ashutosh Mohanty, Shaili Sett, Navkiranjot Kaur Gill, Arindam Ghosh, Umesh V Waghmare, Kanishka Biswas, and D. D. Sarma, ACS Energy Letters 9, 2128 (2024).

Bio of the Speaker:

DD Sarma is J.N. Tata Chair Professor at the Solid State and Structural Chemistry Unit of the Indian Institute of Science. Besides heading the Solid State and Structural Chemistry Unit, he served as a guest professor at the Uppsala University, Sweden, a Distinguished Scientist at the CSIR-Network Institutes of Solar Energy, an honorary professor at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru and a distinguished visiting professor at the Indian Association for the Cultivation of Science, Kolkata



Computational materials science and its applications in the area of materials for sustainable development

Rajeev Ahuja

Indian Institute of Technology (IIT) Ropar, Rupnagar 140001 Punjab, India

&

Department of Physics & Astronomy, Uppsala University, 751 20 Uppsala, Sweden

Email: rajeev.ahuja@iitrpr.ac.in

Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modelled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."

The purpose of this talk is to provide an overview of the most recent studies in the field of computational materials science and how computational material science can play an important role in search, design, improve and understand of materials? How computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

Bio of the Speaker:

Prof. Rajeev Ahuja has joined Indian Institute of Technology (IIT) Ropar director from April 1st, 2021. He is also professor of computational Materials science at Uppsala University, Sweden. He is one of the most highly cited researchers in Sweden & India. He is in top 5 materials scientists in India & Sweden. He has done his Ph.D. from I.I.T. Roorkee in India in 1992. Same year he has joined Uppsala University, Sweden as postdoctoral fellow. He became Assistant Professor in 1996, Associate Professor in 2002 and become Professor in 2007 at Uppsala University, Sweden.



Introduction to density-functional theory and exchange-correlation functionals

Manoj Harbola

Department of Physics, Indian Institute of Technology, Kanpur, 208 016, India

Email: mkh.iitk.ac.in

Lecture 1: Introduction to density-functional theory and exchange-correlation functionals
In this lecture, we will give a general introduction to density-functional theory (DFT) covering both orbital-free DFT and Kohn-Sham DFT. We will then turn our attention to exchange-correlation functional and discuss it in terms of the Fermi-Coulomb hole. Some exact properties of these functionals will be presented and it will be shown how these are employed to obtain accurate functionals.

Lecture 2: Exchange-correlation potential This lecture will discuss exchange-correlation potential and how to generate exact potentials for a given density. Ionization potential theorem and derivative discontinuity of exchange-correlation potential will be discussed. Finally, we will present optimized potential method and how it can be used to get exchange-correlation potential in terms of Kohn-Sham orbitals.

Bio of the Speaker:

Dr. Manoj Kumar Harbola joined the Department in 2000. He obtained his doctoral degree at the City University of New York, USA, working under the supervision of Prof. Viraht Sahni. Subsequently he carried out postdoctoral research at the University of North Carolina, Chapel Hill, USA before joining the Centre for Advanced Technology, Indore as a Scientist.

He is a theoretical physicist, whose chief interest lies in Electronic Structure of Atoms, Molecules and Solids using Density Functional Methods.



Plane Wave versus Atom Centered Basis in DFT

G.P. Das

Research Institute for Sustainable Energy (RISE),
TCG Centres for Research and Education in Science and Technology,
Sector V, Salt Lake, Kolkata-700091, India
Email: gour.das@tcgcrest.org

The two broad categories of Kohn-Sham DFT implementations viz. pseudo-potential methods based on plane waves and atom-centered localized basis functions, have their respective strengths and weaknesses. The precision with which one can estimate various properties from these codes, as well as their accuracy to validate with the corresponding experimental results, have been studied extensively. While plane-wave based methods are being widely used for tackling a large variety of problems, atom-centered (spatially localized) basis functions are quite handy in extracting the chemical information of molecular as well as condensed systems in a transparent way. I shall try to give a ‘guided tour’ of these practical aspects of DFT calculations for real materials.

Bio of the Speaker:

Prof. G.P. Das is a Condensed Matter Physicist cum Materials Scientist, whose research interests include electronic structure and properties of materials from bulk to nano, with specific applications in materials science and nano-devices. He did his Masters in Physics from Calcutta University, PhD from Bombay University, followed by post-doctoral research in Max Planck Institute for Solid State Research in Stuttgart. He served as Senior Scientist in BARC Mumbai, Senior Professor in IACS Kolkata, Visiting Professor in IIT Kharagpur and more recently as a Distinguished Visiting Faculty in St. Xavier's College Kolkata. He made important contributions in the field of first principles investigation of alloys and intermetallics, energy materials, two-dimensional materials as well as semiconductor spintronics. He has authored and co-authored more than 150 research publications in peer reviewed journals, book chapters etc.



Modeling Emergent Phases of Quantum Matter

Indra Dasgupta

School of Physical Sciences

Indian Association for the Cultivation of Science

Jadavpur, Kolkata 700 032, India

Email: sspid@iacs.res.in

In this talk, we shall describe in detail the key ingredients that are necessary to model quantum materials. In particular, we shall illustrate the important role of structure and chemistry in deriving low energy tight-binding Hamiltonian that serve as the single electron part of the many body Hamiltonian like Hubbard and Kanamori models employed to describe emergent properties of quantum materials. We shall show in the strong coupling limit, one can derive spin models, Heisenberg model and in the presence of strong spin-orbit coupling the Kitaev model from Hubbard and Kanamori models respectively. Finally we shall illustrate such models with built in chemical realism help us to understand emergent phases of quantum materials from Kitaev Spin Liquids to Magnon Chern Insulators. This talk will be divided into two parts, in the first part we shall discuss strongly correlated systems without spin orbit coupling and in the second part we shall illustrate the important role of spin orbit coupling in modeling such systems.

Bio of the Speaker:

Dr. Indra Dasgupta is a leading expert in Theoretical and Computational Condensed Matter Physics, focusing on electronic structure calculations, strongly correlated systems, quantum spin systems, and nanoscale magnetic materials. Since 2013, he has served as a Senior Professor at the School of Physical Sciences. Previously, he was a Professor at IIT Bombay. His research combines numerical and analytical techniques, often collaborating with experimentalists to address key challenges in condensed matter physics.



Berry Phase in Condensed Matter Physics: Concepts and Applications

S. Satpathy

Department of Physics & Astronomy
University of Missouri, Columbia, MO 65211, USA
Email: satpathys@missouri.edu

Berry phase is a seminal concept in quantum mechanics with wide ranging applications in a variety of fields in physics. In these lectures, I will introduce the concepts and give some examples of applications in condensed matter physics. Notable applications will include electric polarization in solids, quantum and anomalous Hall effects, and topological insulators.

Bio of the Speaker:

Prof. Satpathy's research is focused on a theoretical description of the physical phenomena in solids resulting from the fundamental behavior of the interacting electrons. A variety of computational techniques are employed, principally the Density-Functional Methods, but also Exact Diagonalization, mean-field methods, as well as the Quantum Monte Carlo Methods. Current research problems span a wide variety of research areas including Correlated Oxide interfaces, Spin Ice Materials, Charge Orbital Ordering in solids, Jahn-Teller effects, Graphene Physics including the RKKY interaction, and method development including the Gutzwiller Density Functional theory and the Muffin-Tin Orbitals methods.



Electronic Structure: A grand challenge of theoretical physics that is useful for many fields of science and technology

Richard M. Martin

University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

Stanford University, Stanford, CA 94305, USA

Email: rmartin@illinois.edu

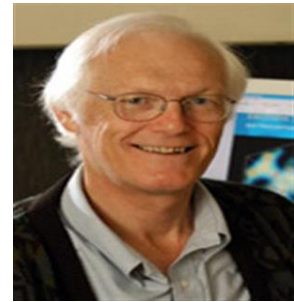
The many-body problem of interacting electrons is the grand challenge in physics, for which the solutions are truly useful. Starting with Schrodinger's equation and Dirac's relativistic quantum mechanics in the 1920's, there was great progress in 1930's using independent particle approximations, including the basic ideas of almost all methods used today. Despite the elegant many-body theory of the 1940's - 1960's, no method came close to quantitative calculations for materials. It was an entirely new approach, Density functional theory in 1964, that made possible quantitative methods to calculate some (but not all!) properties of the full interacting system using independent-particle methods and approximate (but very good!) functionals. The first part of this talk is on the ideas behind DFT, what the Kohn-Sham formulation can and cannot do, and some of the stunning advances that revolutionized the roles of experiment and theory. The second theme returns to the grand challenge: How and when is it possible to use independent-particle methods with approximate functionals to confidently draw conclusions about the full interacting system? What about "strongly interacting" systems and questions like "Can DFT describe a Mott insulator?" In addressing such issues, the guiding principle is continuity as expressed in the work of Landau and Luttinger in the 1950's and 1960's. Perhaps surprisingly, temperature plays a key role in understanding the issues. Such topics are difficult to cover even in an entire course, but I hope to bring out the importance of basic guiding principles alongside the capabilities of DFT.

References

1. Richard M. Martin, "Electronic Structure: Basic theory and practical methods," Cambridge University Press, 2004, Second Edition, 2020.
2. Richard M. Martin, Lucia Reining and David M. Ceperley, " Interacting Electrons: Theory and Computational Approaches ," Cambridge University Press, 2016.

Bio of the Speaker:

Professor Richard Martin obtained his Ph.D. in physics from the University of Chicago in 1969, after earning a S.B. in engineering physics from the University of Tennessee, Knoxville, in 1964. He worked as a member of the technical staff at Bell Labs (1969-71) and then as a principal scientist at the Xerox Palo Alto Research Center and a consulting professor at Stanford University. He joined the physics faculty at the University of Illinois in 1988. In 2007 he retired from the University of Illinois. He now lives in Palo Alto, CA and is a consulting professor in the Department of Applied Physics at Stanford.



Magnetism and spin transport in advanced functional magnets

Biplab Sanyal

Uppsala University, Sweden, Ångströmlaboratoriet, Lägerhyddsvägen 1, 751 20 UPPSALA

Email: biplab.sanyal@physics.uu.se

For centuries, magnetism has brought new surprising phenomena, which have contributed extraordinarily to new technological innovations. Fundamental understanding of the experimental observations is always demanded for further development. In this lecture, I will demonstrate how density functional theory coupled with several sophisticated theoretical methods has been instrumental in the microscopic understanding of several aspects of magnetism, viz., magnetic exchange interactions, magnetic anisotropy, electron correlation, x-ray spectroscopy and spin transport.

Bio of the Speaker:

Dr. Biplab Sanyal is a prominent researcher in Materials Theory, specializing in graphene and 2D materials, multiferroics, random alloys, organometallics, clusters, time-dependent electron dynamics, and spin-phonon coupling. Based at the Ångström Laboratory in Uppsala, he works on theoretical and computational approaches to study material properties at the atomic and molecular levels. With a focus on advancing fundamental understanding and applications of materials, Dr. Sanyal contributes to cutting-edge developments in condensed matter and materials science.



Current Induced Dynamics of Topological Spin Textures

Jaivardhan Sinha^{1*}

¹Department of Physics and Nanotechnology, SRM Institute of Science and Technology,
Kattankulathur 603203, Tamil Nadu, India

Email: *jaivardr@srmist.edu.in

Understanding the mechanism of stabilization and dynamic control of topological spin textures, such as, magnetic domain walls, vortex, skyrmions, fractional skyrmions and bimerons is crucial for fundamental physics as well as memory applications. In order to efficiently control the dynamics of these spin textures it is crucial to utilize spin torque efficiently. Role of spin-transfer torque (STT) and spin orbit torque (SOT) in governing the spin dynamics requires thorough analysis. While STT results from exchange interactions in ferromagnet, the SOT arises from the spin-orbit interaction in an adjacent non-magnet. Two important mechanisms of spin current generation, viz., using spin Hall effect and spin pumping have significant application potential in magnetic memory devices. We will first discuss the factors governing the transfer of spin current across the interface and experimental analysis of transparency of interface. Subsequently we will develop the understanding to STT induced domain wall motion and vortex dynamics in magnetic nanostructures. In particular, using micromagnetic simulation we study the effect of STT in transforming magnetic domain wall to skyrmion or bimeron. Interestingly, we observe that the domain wall with zero topological charge gains a non-zero topological charge in the simultaneous presence of STT and exchange, Dzyaloshinskii-Moriya, and Zeeman interactions. Furthermore, SOT driven dynamics of topological spin textures will be discussed. We study the SOT induced propagation of bimeron in ferromagnetic (FM) racetrack as a function of current density (j) and Gilbert damping (α) values. Also, we investigate the dynamics of bimeron by introducing semi-circular notch along one edge of the FM racetrack. Depending on the notch size and critical current density, bimeron dynamics gets substantially affected. We further propose bimeron based racetrack model can perform logic operations by effectively tailoring the strength of current density for a fixed notch diameter. We believe, all the discussed results provide useful insight into the understanding of current induced dynamics of topological spin textures which are key to applications in low power consumption magnetic memory as well as logic devices.

Bio of the Speaker:

Dr. Jaivardhan Sinha is working as Research Associate Professor at SRM Institute of Science and Technology and is leading the Spintronics and Nanomagnetism for nearly six years. He has experience of performing experiments along similar lines for more than seven years in National Institute of Materials Science (NIMS), Tsukuba, Japan and S. N. Bose National Centre for Basic Sciences (SNBNCBS), Kolkata India. He mainly investigated various interfacial effects e.g., perpendicular magnetic anisotropy (PMA), spin Hall effect, and IDMI in ferromagnetic thin film heterostructures at NIMS.



Physics of correlated materials and engineering various devices

Pavan Nukala

Center for Nanoscience and Engineering, Indian Institute of Science, Bengaluru, 560012,
India

Email: pnukala@iisc.ac.in

In this talk, I will first discuss the physics of Mott Insulators with particular emphasis on metal-insulator transitions. I will review the various experiments in the field that show tuning of the MIT through strain, doping, field engineering, and how decoupling individual effects is in general difficult. I will discuss some very nice recent experiments from IISc (NagaPhani's group[1]) based on modulation doping, which help us decouple these effects and answer questions such as electron densities required to change the ground state of these materials as a metallic phase (spoiler: very difficult to happen). We will take a moment to reflect on the smart experimental design and transport measurements that allows one to make claims only about the effect of doping on Mott insulators without worrying about changing stoichiometry, strain etc..In the later part, I will talk about how such beautiful physics of phase transitions can be used to create several functional devices by coupling them with other materials and with each other. In particular, I'll discuss how large pyroelectric/electrocaloric coolers, sub-Boltzmann limit switching transistors, and electromechanical neuronal oscillators [2,3,4] that arise from the metal-insulator phase transition and it's field/carrier induced tunability. Again, I'll spend considerable time on experimental design aspects of these works

References

1. D. Mondal et al., Modulation doping a correlated electron insulator, Nature Comm, 6210, 2023
2. U. Khandelwal et al., Dynamics of voltage driven self-oscillations in NdNiO₃ neuristors, ACS AELM, 5, pp:3859, 2023
3. U. Khandelwal et al., Large electro-opto-mechanical coupling in VO₂ neuristors, Applied Physics Reviews, 11, 02140, 20242023
4. Jalaja NM, Sooraj S, et al., Emerging devices out of proximity coupled Mott insulator and ferroelectric layers. (arXiv)

Bio of the Speaker:

Dr. Pavan Nukala is an Assistant professor at CeNSE from Aug 2020. He is a materials scientist/engineer by training and works in the broad fields of oxides (correlated oxides, ferroelectric and piezoelectric oxides), phase-change memories (chalcogenides) for electronic applications (neuromorphic computation, in particular) and topological insulators. He has expertise in in situ electron microscopy, spectroscopy (EELS) and x-ray diffraction techniques, especially on real working devices. He also has expertise in ferroelectric and piezoelectric materials, measurements.



Diagnostics for Better Batteries

Naga Phani B Aetukuri

Associate Professor

Solid State and Structural Chemistry Unit

Indian Institute of Science, Bangalore, 560012, India

Email: phani@iisc.ac.in

Making better batteries requires an in-depth understanding of the microscopic mechanisms that lead to their failure. Such an understanding needs to be developed at time and length scales that span nearly 10-orders of magnitude. For example, it is necessary to optimize material compositions at an atomic scale and optimize cell and battery pack designs at scales that are about 10 orders of magnitude larger than the atomic scale. Similarly, it is necessary to minimize charge transfer time scales that occur over microsecond time scales while also maximizing degradation time scales, of the order of years, for better battery life. In this talk, we will discuss some of our work on Solid State Li-ion and Li-O₂ batteries, wherein we employ electrochemical mass spectrometry and impedance analysis to understand rate limiting process in these systems. We will discuss the implications of our work for building batteries that could afford better rate capabilities.

Bio of the Speaker:

Dr. Naga Phani B. Aetukur is an Associate Professor, at Solid State and Structural Chemistry Unit, IISc Bangalore and a leading materials scientist specializing in energy-efficient electronics and energy storage. With a Ph.D. from Stanford University and postdoctoral research experience at IBM Research, Almaden, his work focuses on designing novel materials and devices, particularly high-energy-density batteries. His research employs advanced thin-film synthesis techniques to develop transition metal compound thin films and heterostructures for applications in energy-efficient electronics, energy storage, and electrocatalysis. Dr. Aetukur's work bridges fundamental science and application-driven innovation in materials chemistry.



Theory plus spatially resolved vibrational spectroscopy – a new frontier

Sokrates T. Pantelides

Department of Physics and Astronomy and Department of Electrical and Computer
Engineering

Vanderbilt University, Nashville, Tennessee 37235, USA

Email: pantelides@vanderbillt.edu

Phonons in solids have, for the most part, been studied in perfect bulk and 2D crystals by both theory and experiments because there has been a lack of experimental techniques with spatial resolution. All that changed recently with the advent of new monochromators that achieve electron-energy-loss spectroscopy (EELS) with high energy resolution in scanning transmission electron microscopes (STEM), which already feature atomic-scale spatial resolution. It is now possible to use vibrational EELS (vEELS) to investigate vibrational modes that are localized at point defects, dislocations, grain boundaries, stacking faults, interfaces in heterostructures and superlattices and to distinguish isotopes in isotope alloys. Density-functional-theory (DFT)-based calculations have been an indispensable companion of such experiments to enable identification of the observed modes through their frequencies and go beyond experiments' reach to determine the corresponding vibrational patterns. Knowledge of both phonons and localized vibrational modes are essential for understanding and engineering the thermal properties of materials and nanostructures. In this talk we will describe several examples of probing localized vibrational properties in diverse systems – the evolution of phonons in $(\text{SrTiO}_3)_n/(\text{CaTiO}_3)_n$ superlattices from large n to $n=1$ [1] and of their impact on the thermal conductivity [2], and atom-by atom vEELS of Si impurities in graphene, demonstrating chemical-bond sensitivity [3], which led to the theoretical discovery of vibrational vortices at heavy substitutional impurities [4]. We will then describe the first case of using vEELS/DFT to resolve a long-standing problem that is at the heart of nanofluidics, namely the structure of water confined in carbon nanotubes (CNTs). Prior research had led to the conclusion that the CNT vibrations have a negligible effect. We now demonstrate that the combination of confinement and the CNT vibrations in medium-diameter CNTs lead to effectively total disruption of the H-bond network, with O-H stretch frequency the same as that of vapor – the water molecules are in close proximity, but random rotations disrupt the intermolecular bonding. Cryo-STEM vEELS and DFT provide support. This work was supported by the U.S. Department of Energy. Key vEELS collaborators are Jordan Hachtel [1,5] at Oak Ridge National Laboratory in the U.S.A. and Wu Zhou [3,4] at the University of the Chinese Academy of Sciences in Beijing, China. Theory by D.-L. Bao [1-5]], X. Zhang [2], X. Jin [5], H. A. Walker [5].

1. E. R. Hoglund et al., *Nature* **601**, 556 (2022)
2. M. Lu et al., Senior Honors Thesis, Vanderbilt University (Dec. 2024).
3. M. Xu et al., *Nature Mater.* **22**, 612 (2023).
4. D.-L. Bao et al. *Nanoscale Horiz.* **9**, 248 (2024) 5. X. Xu et al., *Nature*, to be published

Bio of the Speaker:

Dr. Sokrates Pantelides, University Distinguished Professor of Physics and Engineering, William A. & Nancy F. McMinn Professor of Physics, and Professor of Materials Science and Electrical Engineering at Vanderbilt University, is a leading expert in theoretical and computational studies of nanoscience and nanotechnology. His research encompasses semiconductors and semiconductor devices at the atomic scale, focusing on defects, defect-mediated device degradation, and radiation effects, as well as quantum theory, complex oxides, heterostructures, ferroelectrics, and two-dimensional materials, driving advancements in both fundamental science and practical applications.



An Overview of Machine Learning for Multiferroic and Nuclear Materials

Saurabh Ghosh

Dept. of Physics and Nanotechnology

SRM Institute of Science and Technology, Kattankulathur, Chennai 603203 India

Email: saurabhs@srmist.edu.in

Integrating predictive machine learning (ML) with hypothesis-driven active learning and causal inference offers a powerful framework for advancing materials discovery and design in multiferroics and nuclear materials. Predictive ML techniques enable the analysis of complex, high-dimensional datasets to uncover hidden patterns, guiding the exploration of material compositions and structures with exceptional precision. Hypothesis-driven active learning complements this by strategically prioritizing experiments and simulations, iteratively refining the search for optimal material candidates. Incorporating causal ML provides a deeper understanding of the underlying mechanisms, distinguishing mere correlations from true causal relationships, and enabling the design of materials with targeted, multifunctional properties.

For multiferroics, this approach can uncover new materials with coupled magnetic and ferroelectric behaviors, addressing challenges in energy-efficient data storage and spintronic applications. In the nuclear domain, the methodology accelerates the discovery of advanced fuels, cladding, and structural materials, enhancing radiation tolerance, thermal stability, and safety. By unifying these cutting-edge techniques, this framework not only fosters breakthroughs in multiferroic and nuclear materials but also establishes a generalizable paradigm for hypothesis-driven, efficient, and scalable materials innovation.

References [1] [Insights into cation ordering of double perovskite oxides from machine learning and causal relations](#), A Ghosh, G Palanichamy, DP Trujillo, M Shaikh, S Ghosh, Chemistry of Materials 34 (16), 7563-7578 (2022), [2] [Predictive Design of Hybrid Improper Ferroelectric Double Perovskite Oxides](#), P Gayathri, S Ghosh, A Ghosh, Chemistry of Materials 36 (2), 682-693 (2024), [3] [Structural mode coupling in perovskite oxides using hypothesis-driven active learning](#), A Ghosh, P Gayathri, M Shaikh, S Ghosh Journal of Physics: Materials 7 (2), 025014 (2024), [4] [Insights into Prismatic Loop Formation in Irradiated Fe–Cr Alloys from Hypothesis-Driven Active Learning and Causal Analysis](#), S Ghosh, A Tom, D Dasgupta, A Ghosh, BD Wirth, ACS Applied Energy Materials 7 (15), 6123-6134 (2024), [5] [Mapping causal pathways with structural modes fingerprint for perovskite oxides](#), A Ghosh, S Ghosh Machine Learning: Science and Technology 5, (4), 045014 (2024)

*All the work referred here is done in collaboration with Dr Ayana Ghosh, Staff Scientist, Oak Ridge National Laboratory, TN USA.

Bio of the Speaker:

Dr. Saurabh Ghosh joined the Department of Physics and Nanotechnology at SRM Institute of Science and Technology, Tamil Nadu, India, as an Assistant Professor in June 2017. He earned his PhD from Jadavpur University, Kolkata, in 2011, after completing his doctoral research at the Indian Association for the Cultivation of Science. Prior to SRM, Dr. Ghosh held postdoctoral positions in the USA from 2011 to 2017, first at Cornell University in Ithaca, NY, then at Vanderbilt University in Nashville, TN, and Oak Ridge National Laboratory in Oak Ridge, TN. At SRM, Dr. Ghosh leads the 'Functional Materials by Design' (FMD) group, which focuses on applying first-principles calculations and machine learning techniques to design materials with tailored structure-property relationships, particularly in oxide electronics, spintronics, and nuclear and quantum materials. In 2023-2024, he completed a sabbatical as a visiting scientist in the Department of Nuclear Engineering at the University of Tennessee Knoxville, where he worked on machine learning for nuclear materials.



Machine learning for materials modeling

N. M. Anoop Krishnan

Department of Civil Engineering
School of Artificial Intelligence (Joint Appt.)
Indian Institute of Technology Delhi, 110016, India
Email: krishnan@iitd.ac.in

Machine learning for materials modeling - 1

In this session, we will discuss about the basics of machine learning techniques. We will discuss processing including outlier, removals, and data imputations. Following this., we will focus on linear regression and neural networks. We will briefly discuss about the idea of regularization and back propagation.

Machine learning for materials modeling - 2

In this session, we will discuss about several applications of machine learning in the materials domain. To this end, we will discuss how physics based inductive biases can be incorporated in machine learning through physics informed machine learning. Further, we will also discuss about graph neural networks and how those can be used for modelling atomic systems.

Bio of the Speaker:

Dr. N. M. Anoop Krishnan, Associate Professor in the Department of Civil Engineering at IIT Delhi, leads the Multiphysics & Multiscale Mechanics Research Group (M3RG). After earning his Ph.D. in Civil Engineering from IISc Bangalore in 2015, he worked as a postdoctoral researcher at the University of California, Los Angeles, from 2015 to 2017. Dr. Krishnan's research focuses on the response of materials across different length and time scales, with emphasis on multiphysics problems such as radiation damage, corrosion, and dissolution, as well as multiscale issues like fracture, indentation, and creep. His group's philosophy integrates a two-way informed analysis-design methodology to optimize material selection and design for applications in nuclear, armament, naval, automotive, and construction industries.



An Introduction to Machine Learning Approaches in Materials Science

Biswarup Pathak

Department of Chemistry, Indian Institute of Technology (IIT) Indore, Indore, Madhya Pradesh, 453552, India

E-mail: biswarup@iiti.ac.in

Machine learning (ML) has become a transformative tool in materials science, enabling the discovery, design, and optimization of materials with unprecedented speed and precision. By leveraging data-driven models, ML approaches can predict material properties, identify new compounds, and optimize processes, all while reducing the reliance on trial-and-error experimentation. Techniques such as regression, neural networks, support vector machines, and reinforcement learning are increasingly applied to tasks ranging from predicting the mechanical, thermal, and electronic properties of materials to identifying novel materials for energy storage, catalysis, and electronics. Additionally, ML helps to analyze complex datasets from experiments and simulations, offering insights that may be challenging to derive using traditional methods. Despite its promise, challenges such as data quality, model interpretability, and transferability across different systems remain. Nevertheless, ML is poised to revolutionize materials discovery, offering new pathways to advanced, high-performance materials with applications in a wide range of industries, including energy, electronics, and others.

Bio of the Speaker:

Dr. Biswarup Pathak is a distinguished Professor in the Department of Chemistry at IIT Indore, India, where he leads the Computational Materials Designing Research Group. His research integrates advanced computational modeling with machine learning and artificial intelligence to design nanomaterials for applications in catalysis, energy, and molecular sequencing. Dr. Pathak has published over 290 papers in prestigious international journals, garnering more than 7,500 citations. His contributions to the field have earned global recognition, including the Early and Mid-Career Research Award from the Indian National Science Academy (INSA) in 2017 and the IIT Indore Best Researcher Award in 2016, 2023, and 2024. He has secured numerous national and international grants supporting his research on nanomaterials for energy and catalysis.



Efficient and Accelerated Materials Discovery with Active Learning

Rohit Batra

Department of Metallurgical and Materials Engineering, IIT Madras, Chennai, TN 600036,
India

Email: rbatra@iitm.ac.in

The discovery of new materials is vital part of technological progress, yet the process often involves high-dimensional search spaces and costly experimental evaluations. Bayesian Optimization (BO) has emerged as a powerful framework for efficiently navigating these challenges by balancing exploration and exploitation in the search for optimal material properties. This talk will introduce the core principles of BO and its integration with active learning to accelerate the discovery process. The role of probabilistic surrogate models, such as Gaussian Processes, in guiding the search for new materials will be discussed, along with acquisition functions that quantify trade-offs between exploring unknown regions and exploiting promising candidates. We will also delve into the design of experiments (DOE) as the foundation for initiating BO workflows, with special emphasis on techniques such as Latin Hypercube Sampling to ensure diverse and well-distributed initial data points. Practical examples from materials science will highlight how BO can be applied to optimize different materials properties like hardness, conductivity, or thermal stability, with significant reductions in experimental and computational costs.

Bio of the Speaker:

Dr. Rohit Batra joined the Department of Metallurgical and Materials Engineering at IIT Madras as Assistant Professor in July 2022. Prior to this, he had completed two Post-doctoral appointments, one at the Center for Nanoscale Materials, Argonne National Lab, and the other at the School of Materials Science and Engineering, Georgia Institute of Technology. Rohit received his PhD in Materials Science and Engineering from the University of Connecticut and B.Tech. in Metallurgical and Materials Engineering from IIT Roorkee. Before joining IIT Madras, he also had a 4-month stint at Rivian Automotive LLC R&D lab for cell manufacturing and battery development. Rohit's research interest lies in the area of combining computational and data-driven methods to design new materials. He has expertise in first-principles electronic structure methods, molecular dynamics simulations, and many machine learning (ML) based techniques, particularly geared towards the general field of chemical and materials science.



Time-dependent density-functional theory: formal framework and applications

Carsten A. Ullrich

Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211, USA

Email: ullrichc@missouri.edu

Time-dependent density-functional theory (TDDFT) describes the quantum dynamics of interacting electronic many-body systems out of equilibrium formally exactly and in a practical and efficient manner. TDDFT has become the leading method for calculating excitation energies and spectroscopic properties of molecules and materials, with accuracies that rival traditional wave-function-based methods, but at a fraction of the computational cost.

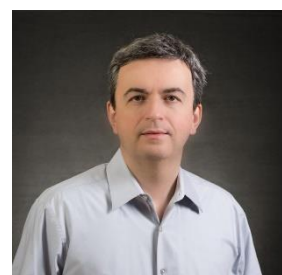
This tutorial will present two lectures on TDDFT. The first lecture will give a concise discussion of the formal framework of TDDFT, focusing on the Runge-Gross theorem, the time-dependent Kohn-Sham formalism, common approximations for the exchange-correlation functionals, and the linear-response formulation of TDDFT and the calculation of excitation energies via the Casida equation. The second lecture will then give an overview of various applications of TDDFT, with an emphasis on ultrafast and collective excitations in solids, such as plasmons, excitons, and spin waves. The tutorial will conclude with perspectives on current hot topics and future developments in TDDFT.

References:

1. Carsten A. Ullrich, *Time-dependent density-functional theory: Concepts and Applications* (Oxford University Press, 2012)
2. Neepa T. Maitra, Perspectives on TDDFT, *J. Chem. Phys.* **144**, 220901 (2016)
3. X. Li, N. Govind, C. Isborn, A.E. DePrince III, and K. Lopata, Real-time time-dependent electronic structure theory, *Chem. Rev.* **120**, 9951 (2020)

Bio of the Speaker:

Dr. Carsten Ullrich, Curators' Distinguished Professor in the Department of Physics and Astronomy at the University of Missouri, is an expert in time-dependent density-functional theory (TDDFT). Prof. Ullrich's research focuses on using TDDFT to investigate excitation processes and optical properties of materials and nanostructures. Additionally, he explores formal aspects of the theory, including non-adiabatic behavior and memory effects, contributing to advancements in theoretical and computational materials science. One of Ullrich's main areas of work is to study excitons, which are a key feature of the optical response in semiconductors and insulators. He and his group have developed new methods to calculate excitonic binding energies from first principles, and to simulate and visualize the formation and motion of excitons in real time.



Spin transport across polar-Polyvinylidene fluoride thin films

Gangineni Ramesh Babu

Functional Thin Films Laboratory

Department of Physics, SOPCAS, Pondicherry University, Kalapet -605014, Puducherry,
India

*rameshcu@pondiuni.ac.in, rameshg.phy@pondiuni.edu.in

Controlling spin injection, transport, and detection have been the prime objectives of inorganic (metal or insulator or polar) and organic (semiconductor or polar) spacer-based spintronic devices for low-power, multi-resistance states, high-memory density and -processing applications¹. The large magnetoresistance (MR) ratios in spin-valves (SVs) and magnetic tunnel junctions are commonly correlated to the long spin lifetimes (\sim few ms) and corresponding long spin diffusion lengths (λ_s)¹. Organic spacers are known to exhibit long λ_s of 100 nm – 300 nm due to their low spin-orbit and hyperfine coupling, compared to short λ_s of \sim 5 nm in metallic barrier-based SVs^{1,2}. Additionally, the quest to control the multi-resistance states of the SVs by electric and magnetic fields across ferroelectric spacers has risen recently and the changes in MR are linked to the variations in interfacial polarization and interfacial structure^{3,4}. In this presentation, the basics of these mechanisms in SVs will be described. Specifically, spin transport across organic ferroelectric (OFE) PVDF and PVDF-HFP barriers and their relation to the spin polarization of the electrodes, impedance mismatch across OFE/FM interfaces, and OFE crystal structure will be discussed in (PVDF or PVDF-HFP)/(CoFeNi or Fe₃O₄) bilayers and (Co or (Ta/Co))/(PVDF or PVDF-HFP)/(NiFe or Fe₃O₄ or Co) SVs by using electrical and ferromagnetic resonance excitation based spin injection methods^{5,6,7,8}.

References

1. Atsufumi Hirohata et al., J. Mag. Mag. Mate. 509 166711 (2020),
2. Rugang Geng et al., Journal of Science: Advanced Materials and Devices 1 256 (2016),
3. Quindeau, A et al., Sci. Rep. 5, 9749 (2015),
4. Xiaoshan Xu, J. Materiomics 4 1 (2018)
5. PR Teja et al, Journal of Magnetism and Magnetic Materials 609, 172478 2024.
6. J Roy et al., Journal of Physics: Condensed Matter 36 (50), 505803 2024.
7. J Roy et al., Physica B: Condensed Matter, 687, 416101 2024.
8. J Roy et al., Journal of Magnetism and Magnetic Materials 585, 171130, 2023

Bio of the Speaker:

Dr. Gangineni Ramesh Babu is currently working as Assistant Professor at the Department of Physics, Pondicherry University. He obtained his Master's degree in 2002 from the University of Hyderabad. He took his Ph.D. from Technical University Dresden & Leibnitz institute of solid-state physics and Materials Research, Dresden, Germany in 2008 under the guidance of Prof. Kathrin Doerr and Prof. Ludwig Schultz. During his



Ph.D., he indulged in the study of extrinsic magneto-transport and its dependence upon in-situ strain in Manganite thin films. After Ph.D., he worked as a post-doctoral fellow at SPINTEC/CEA/CNRS, Grenoble, France in the area of Magnetic Tunnel Junctions. He joined the Department of Physics in August 2010. Currently, he is working on the study of electronic transport across ferroelectric, ferromagnetic & multiferroic thin film devices for memory & sensing applications.

LIST OF ABSTRACTS IN CONFERENCE MODE

Plenary Talk 1

Seeking Majorana Bound States and Diode Phenomenon in Superconductor-Ferromagnet Proximity Coupled Systems

Jagadeesh Moodera¹

¹Physics Department, Plasma Science and Fusion Center and Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, MA 02139 USA

Exploration of superconductors (SC) has continued to exhibit new phenomena despite the extensive studies for over a century. The excitement and challenge become richer when SC are proximity coupled to ferromagnets (FM). Recently with strong interest, among various other schemes, the prediction of exotic Majorana bound states (MBS) to appear in superconducting proximity coupled (111) Au surface state, with SC/FM system. Combined with the ideal Heisenberg FM such as EuS and proximity coupled with superconductor V, the (111) Au gives us an excellent topological SC to seek MBS. This led us to observe the signature of candidate MBS pair by scanning tunnel spectroscopy. For further confirmation we are pursuing nanostructured planar junctions, aiming to show the highly challenging MBS pair entanglement, a precursor for enabling topological qubits. It is fascinating to note that the SC/FM platform utilized in the search of MBS has also led us to 'rediscover' another phenomenon - the observation of the nonreciprocal critical supercurrent flow, called SC diode effect. We demonstrate strong SC diode effect in conventional SC thin films interfaced with a ferromagnetic semiconductor EuS, reaching efficiencies $\sim 70\%$. We identify that the critical supercurrent nonreciprocity in SC thin films to be arising from asymmetrical vortex edge/surface barriers and the universal Meissner screening current. Furthermore, nonvolatile SC memory has been realized as well. The evolution of SC order parameter, and its influence on the magnetic ordering adds richness.

References:

1. Proc. Natl. Acad. Sci. 117 (16) 8775 (2020)
2. Phys. Rev. Lett. 131, No. 2, 027001 (2023)

Bio of the Speaker: Dr. Jagadeesh S. Moodera, Senior Research Scientist, Physics Department Group Leader - Superconductivity, Quantum Transport and Nanospintronics Plasma Science and Fusion Center/Francis Bitter Magnet Laboratory, MIT. He did his PhD in Condensed Matter Physics from IIT, Madras. Awards and Honors include 2009 Oliver Buckley Prize from APS, American NSF Competitiveness and Innovation Fellow (2008-2010). Fellow of APS (2000). IBM and TDK Research Awards (1995-1998). Distinguished Alumnus Award (IIT, Madras). Distinguished scientist at Fujitsu Company, Japan. Visiting professor, Applied Physics Dept, Eindhoven Tech. U. (The Netherlands). Distinguished Visiting Professor/Scientist, Institute for Quantum Computing, U. of Waterloo, Canada. Distinguished Institute Professor, Indian Inst. of Tech., Madras. Distinguished Foreign Scientist, National Physical Laboratory, New Delhi. Adjunct Professor (Mangalore Univ., National Institute of Technology



Fermi-volume-changing quantum phase transitions and the cuprate phase diagram

Subir Sachdev¹

¹Department of Physics, Harvard University, Cambridge MA 02138

A Fermi liquid with a ‘large’ Fermi surface (FL) can have a quantum phase transition to a spin density wave state (SDW) with reconstructed ‘small’ Fermi pockets. Both FL and SDW phases obey the Luttinger constraints on the volume enclosed by the Fermi surfaces. The critical spin fluctuations lead to spin-singlet d -wave pairing, as observed in the cuprates. Studies of the influence of spatial disorder on the FL-SDW quantum phase transition [1,2] predict an extended quantum-critical Griffiths-type phase on the large Fermi surface side. We compare these predictions to recent neutron scattering observations on LSCO.

However, this theory cannot explain the higher temperature pseudogap and strange metal phases of the hole-doped cuprates. Here we need to consider Fermi-volume-changing quantum phase transitions *without* symmetry breaking. Then the small Fermi surface phase does not obey the Luttinger constraint, and is instead a ‘fractionalized Fermi liquid’ (FL*). A theory of FL* in single band models describes photoemission observations in the pseudogap phase. The FL-FL* quantum phase transition, and the influence of spatial disorder, is described by an analysis inspired by the Sachdev-Ye-Kitaev model [3,4]. This theory successfully describes linear-in-temperature resistivity, optical conductivity and thermopower observations.

References:

1. A. A. Patel, P. Lunts, and S. Sachdev, Proceedings of the National Academy of Sciences **121**, e2402052121 (2024).
2. A. A. Patel, P. Lunts, and M. S. Alberg, arXiv:2410.05365.
3. A. A. Patel, Haoyu Guo, I. Esterlis, and S. Sachdev, Science **381**, 790 (2023).
4. Chenyuan Li, D. Valentinis, A. A. Patel, Haoyu Guo, J. Schmalian, S. Sachdev, and I. Esterlis, *Physical Review Letters* **133**, 186502 (2024)

Bio of the Speaker: Subir Sachdev is Herchel Smith Professor of Physics at Harvard University. He attended school in Bengaluru, IIT Delhi for his freshman year, and received his PhD in theoretical physics from Harvard. He has been elected to national academies of science in India and the United States, and the Royal Society in the U.K. Sachdev has made extensive contributions to the theory of the diverse varieties of states of quantum matter, and of their behavior near quantum phase transitions.



Wannier Orbitals and Wannier Cooper Pair in Phase Space

Tanmoy Das¹

¹Department of Physics, Indian Institute of Science, Bangalore, 560012

The construction of lattice models for excitation of a many-body theory remains a fundamental challenge in physics. Here, we propose a variational wavefunction approach in the position-momentum phase space which serve as the vacuum state of Wannier orbital-like excitations. The method allows us to systematically incorporate quantum statistics, correlations, and geometric properties as variational parameters. Next, we focus on the solutions of unconventional pairing symmetry calculations and the Bogoluybov-de-Gennes (BdG) equation in the phase space. We apply this framework to a square octagon (SO) lattice. First, we take a tight-binding model with artificial gauge fields to engineer a flat band on the 2D SO lattice. Then we construct Wannier orbitals and Wannier pairings states in the flat band and solve it analytically. Next we study SO material $\text{Lu}_2\text{Fe}_3\text{Si}_5$ within the DFT and solve the full pairing symmetry calculate to validate the method.

References:

1. R. O. Sharma, T. Das, manuscript under preparation.
2. K. B. Yogendra, G. Baskaran, Tanmoy Das, arXiv:2407.12559

Bio of the speaker: Prof. Tanmoy Das is an Associate Professor in the Department of Physics at the Indian Institute of Science, Bangalore. He received his Ph.D. from Northeastern University, Boston in 2010, followed by postdoctoral research at Los Alamos National Laboratory, USA. His research interests span several frontiers of quantum theory of condensed matter and materials science. Broadly, his focus is on understanding and predicting materials properties driven by quantum theory, with the goal of experimental verification and device implementation. Key areas of interest include superconductivity, emergent correlated properties, topological phases of matter, emergent excitations, and non-Hermitian and open quantum properties. The numerical techniques employed in his group include analytical models, density-functional theory (DFT), momentum-resolved density fluctuation (MRDF) theory (developed in-house), DMRG, Machine Learning, and other numerical methods. Prof. Das is the recipient of several accolades, including the Infosys Young Investigator Award, and is listed among the top 2% of the world's most-cited scientists.



Charge Order Induced Altermagnetism in Bipartite Lattice

Rajamani Raghunathan¹, Dayasindhu Dey¹, Shivam Choudhary¹ and S. Ramasesha²

¹UGC-DAE Consortium for Scientific Research, DAVV Campus, Khandwa Road, Indore - 452001.

²Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore - 560012.

Conventional ferromagnets show spin polarisation and break the time reversal symmetry (TRS). But, antiferromagnets (AFMs) do not have spin polarisation and preserve TRS. Recently, altermagnets (AMs) which conserve the TRS but also show momentum dependent spin splitting have been proposed. The occurrence of AM depends on a special geometry around the magnetic ion. Here, using numerical studies of quantum phases of bimetallic systems it will be shown that altermagnetism can be induced in a general lattice by leveraging the coupling between the charge and spin degrees of freedom. Using a mean field approach it will be shown that the occurrence of charge order and antiferromagnetic spin order in the two sub-lattices leads to AM. The origin of AM phase will be further shown analytically to stem from a unitary transformation of Hamiltonian matrix between up-spin at (k_x, k_y) and down-spin at $(k_x, -k_y)$ when the A-sublattice is charge-ordered. The proposed model will also be validated using band structures of the pristine and doped LaMnO_3 using density functional theory.

Bio of the speaker: Dr. Raghunathan obtained his Ph.D. from the Indian Institute of Science Bangalore. His thesis was on modeling magnetism in transition metal complexes using exact diagonalization techniques. He then moved to the University of California at Berkeley and then at the Massachusetts Institute of Technology under post-doctoral research fellowships. He later joined as a Scientist at the UGC-DAE Consortium for Scientific Research, Indore where he currently heads the computational group. His research interests are in understanding charge and spin orders in quantum systems using exact diagonalization technique, mean field theory, density matrix renormalization group approach and first principles modeling.



Ligand Tunability of Emergent Non-collinear Magnetism in Cu-based Layered Hybrid Perovskites

Debakanta Samal,^{1,2} P. Biswal,^{1,2} Sagar Sarkar,^{3,5} S. N. Sarangi,¹ Subhendra D. Mahanti,⁴ G. Tripathy,^{1,2} Ashis Kumar Nandy,⁵ Diptikanta Swain⁶

¹Institute of Physics, Bhubaneswar 751005, India

²Homi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India

³Department of Physics and Astronomy, Uppsala University, Uppsala, 751 20, Sweden

⁴Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

⁵School of Physical Sciences, National Institute Of Science Education and Research, An OCC of HBNI, Jatni, Odisha 752050, India

⁶Institute of Chemical Technology–Indian Oil Odisha Campus, Bhubaneswar 751013, India

Transition metal based layered organic-inorganic hybrid perovskites (OIHPs) exhibit compelling magnetic phenomena intertwined with their structure and dimensionality. This talk will illustrate a notable ligand tunability of magnetism in two new quasi 2D OIHPs $(C_7H_9NBr)_2CuX_4$ ($C_7H_9NBr=4$ -Bromobenzylammonium: A, X:Cl, Br) and provide a microscopic understanding through *ab initio* DFT calculations. Despite being isostructural, the Cl and Br analogs exhibit contrasting magnetic response, while A_2CuCl_4 shows an in-plane ferromagnetic and out-of-plane antiferromagnetic like response, A_2CuBr_4 follows the reverse trend. The underlying origin of the observed magnetism is argued to stem from Dzyaloshinskii-Moriya interaction (DMI) present in these layered systems. Based on the competition between DMI and magnetocrystalline anisotropy, a complex-canted and a transverse conical spiral spin structures are proposed for A_2CuCl_4 and A_2CuBr_4 respectively; which explains the observed magnetic response. Further we construct the respective H-T phase diagrams revealing the evolution to distinct magnetic phases. Essentially this study provides a framework to tailor and understand the possible occurrence of non-collinear spin textures in the above class of OIHPs.

References:

1. P. Biswal et al., (unpublished)

Bio of the Speaker: Dr. Debakanta Samal is working as Associate Professor at Institute of Physics, Bhubaneswar, India. He earned his Ph.D in Experimental Condensed Matter Physics from Department of Physics, IISc, Bangalore in the year 2010. He did his Postdoctoral work at MESA+ Institute for Nanotechnology, University of Twente, The Netherlands from 2011 to 2014. Later during the years 2014 to 2016, he worked as a Scientist at Max Planck Institute for Solid State Research, Stuttgart, Germany. His research interest mainly focuses on the microscopic understanding and engineering of the electronic and magnetic properties of quantum materials.



**Many-Body Quantum Interference Route to the Two-Channel Kondo Effect:
Inverse Design for Molecular Junctions and Quantum Dot Devices**

Sudeshna Sen¹ and Andrew K. Mitchell^{2,3}

¹Department of Physics, IIT(ISM) Dhanbad, Dhanbad-826004 Jharkhand, India

²School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

³Centre for Quantum Engineering, Science, and Technology, University College Dublin,
Dublin, Ireland

Molecular junctions—whether actual single molecules in nanowire break junctions or artificial molecules realized in coupled quantum dot devices—offer unique functionality due to their orbital complexity, strong electron interactions, gate control, and many-body effects from hybridization with the external electronic circuit. Inverse design involves finding candidate structures that perform a desired function optimally. Here we develop an inverse design strategy for generalized quantum impurity models describing molecular junctions, and as an example, use it to demonstrate that many-body quantum interference can be leveraged to realize the two-channel Kondo critical point in simple 4- or 5-site molecular moieties. We show that remarkably high Kondo temperatures can be achieved, meaning that entropy and transport signatures should be experimentally accessible.

References:

1. *PHYSICAL REVIEW LETTERS* 133, 076501 (2024)

Bio of the Speaker: Our Group at IIT(ISM) Dhanbad explore materials in the quantum domain using theoretical and computational approaches. Quantum Materials are currently the vanguard of modern condensed matter physics. I am interested in the quantum mechanics of strongly correlated electron systems and many-body theory of these systems. I did my Ph.D. from JNCASR, Bangalore, and worked as Post Doctoral Fellow at University College Dublin, Ireland, and TD Lee Institute, Shanghai. I collaborate with several groups from around the globe for my research.



Exciton dynamics and nonlinear optical properties of quantum confined halide perovskites

Suchi Guha¹, Dallar Babaian, Daniel Hill, and Ping Yu

¹Department of Physics and Astronomy, University of Missouri, Columbia, USA

The steep performance improvement in organic–inorganic halide perovskite solar cells over the past decade has resulted in exploiting their optical and electronic properties in a vast range of optoelectronic devices. Two-dimensional (2D) organic-inorganic Ruddlesden-Popper (RP) halide perovskites emphasize a strong excitonic contribution, which enhances their linear and nonlinear optical properties. Insights into carrier and relaxation dynamics are crucial for the application of such 2D perovskite films in optoelectronics. We present third harmonic generation and transient absorption (TA) studies from two prototypical 2D lead-iodide perovskite systems with butylammonium (BA) and phenylethylammonium (PEA) cations, which are synthesized using chemical vapor deposition. The TA features are characterized by a low and a high energy absorption peak with respect to the band-edge bleach at 520 nm. The low energy absorption peak decays faster in the PEA perovskite sample compared with the BA perovskite, indicating the role of the cation. Fast carrier cooling times of 150 fs, signaling the absence of a phonon bottleneck effect, are observed. The decay dynamics of the band-edge bleach reveal strong contributions from the Auger recombination process at early times, when the system is far from equilibrium.

References:

1. D. Babaian, D. Hill, P. Yu, and S. Guha, *J. Mater. Chem. C* (2024); DOI: 10.1039/d4tc03014a
2. C. J. Arendse, R. Burns, D. Beckwitt, D. Babaian, S. Klue, D. Stalla, E. Karapetrova, P. F. Miceli, and S. Guha, *ACS Appl. Mater. Interfaces* 15, 59055 (2023).

***Bio of the Speaker:** Suchi Guha is a Professor in the Department of Physics and Astronomy at the University of Missouri-Columbia, USA, where she joined as an assistant professor in 2003. She earned her doctorate degree in physics from Arizona State University, USA. Prior to that, she obtained master's and bachelor's degrees in physics from the Indian Institute of Technology, New Delhi and the University of Delhi, respectively. Her current research interests include charge transport mechanisms in polymeric and organic semiconductors, development of organic field-effect transistors and photodetectors, peptide electronics, and photophysics of conjugated polymers and perovskite materials using linear and nonlinear optical spectroscopy. She has co-authored over 140 publications and currently serves as an associate editor of the journal - ACS Applied Electronic Materials.*



Computational Roadmap of Emerging Materials: Implications of Rashba and Excitonic Physics

Sudip Chakraborty¹

¹Materials Theory for Energy Scavenging (MATES) Lab, Harish-Chandra Research Institute (HRI) Prayagraj (Allahabad), 211019, U.P. India

In this talk, I will start with the brief introduction of first principles electronic structure calculations in perovskite materials, and how it could be connected to the Computational Screening for achieving highly efficient and stable solar cell materials [1]. Next, I will delve into the fundamentals and possible implications of Rashba phenomena in both hybrid and inorganic perovskite materials [2-5]. The fundamental interplay between structural distortions and the Rashba splitting in the considered one-dimensional system under the influence of compression along with the evolution of spin texture could hold great potential for the pursuit of sustainable energy. The rest of the talk would be devoted to theoretical understanding of piezochromism, where hydrostatic pressure could be employed as an effective tool, giving rise to novel crystal structures and optical properties, while it has proven to be an alternative to chemical pressure [4,5]. I will end my talk touching upon our recent successful endeavour of pre-intercalation mechanism in Li-ion battery based on transition pathway prediction [6].

References:

1. S. Chakraborty* et al. *ACS Energy Letters*, 2, 837 (2017).
2. Manasa G., M. Nazeeruddin*, Sudip Chakraborty*, *Applied Physics Reviews*, 8, 041309 (2021)
3. J. Kaur, Sudip Chakraborty*, *Small*, Accepted (2024)
4. J. Kaur, Sudip Chakraborty*, *Physical Review Materials*, 8, 055405 (2024)
5. S. H. Mir, S. Chakraborty*, *Journal of Materials Chemistry A*, 12, 10287(2024)
6. Y. Luo, J. Handy, T. Das., Sudip Chakraborty*, S. Banerjee*, *Nature Materials*, 23, 960 (2024).

Bio of the Speaker: Prof. Sudip Chakraborty is leading Materials Theory for Energy Scavenging (MATES Lab) group in India's premier theoretical research Institute Harish-Chandra Research Institute (HRI) Allahabad (Prayagraj), Department of Atomic Energy, Govt. of India. After completing Ph.D. from Bhabha Atomic Research Centre and University of Pune, India, he moved to Max Planck Institute for Sustainable Materials, Düsseldorf, Germany in March, 2011 as a Max Planck Postdoctoral Fellow. In February, 2013, he joined Materials Theory Division, Uppsala University, Sweden as a Försökare. Since March, 2019, he started leading his group firstly in Department of Physics of IIT Indore and later on in HRI from May, 2021 onwards. He has been awarded the Rising Stars by ACS Materials Au 2021, among 300+ nominations worldwide, while he is the sole recipient from India. He is in the Editorial Board of *Journal of Physical Chemistry C (ACS)*, *Energy Advances (RSC)*, *Electronic Structure (IOP)*, *Chemistry of Inorganic Materials (Elsevier)* and *Graphene & 2D Materials (Springer)*. His works are appeared in *Nature Materials*, *PNAS*, *Materials Today*, *ACS Energy Letters*, *JACS*, *ACS Nano*, *ACS Catalysis*, *AngewChemie*, *Advanced Materials*, *Advanced Functional Materials*, *ChemMat*, *JMCA* etc. At present, he has 175 International publications with total 6800 citations and 45 h-index



Electronic Structure of Noncentrosymmetric AgCd₂GaS₄ Using High Resolution Photoemission Spectroscopy

Manas Kumar Dalai^{1,2}, Nitin Kumar Tripathy^{1,3}, Soumyojit Chatterjee³, Rahul Sharma³, Biju Raja Sekhar⁴ and N. Vijayan^{2,5}

¹CSIR - Institute of Minerals and Materials Technology, Bhubaneswar - 751013, Odisha, India

²Academy of Scientific and Innovative Research (AcSIR), Ghaziabad - 201002, India

³Department of Physical Sciences, Indian Institute of Science Education and Research, Berhampur - 760003, Odisha, India.

⁴Institute of Physics, Bhubaneswar - 751005, Odisha, India

⁵CSIR - National Physical Laboratory, Dr. K. S. Krishnan Marg, New Delhi - 110012, India and

Email: dalaimk@immt.res.in

Non-centrosymmetric crystals are a topic of recent interest because they exhibit non-reciprocal response leading to a wide array of phenomenology in the fields of non-linear optics, photovoltaics, superconductivity. AgCd₂GaS₄, a quaternary chalcogenide compound, arising from the quasi-ternary system Ag₂S–CdS–Ga₂S₃ is of particular interest as it offers potential applications in various fields. The noncentrosymmetric structure and wide transmission range make AgCd₂GaS₄ promising for infrared (IR) nonlinear optical applications. A detail study on the electronic structure of such materials is very important to realize their potential applications. In this talk, the temperature dependent electronic structure of AgCd₂GaS₄ near the Fermi level will be discussed. High resolution ultraviolet photoemission spectroscopy was used to investigate their near fermi level electronic structure with respect to temperature. The Density Functional Theory (DFT) was carried out in order to see the total and partial density of states, which are in well agreement with the experimental data. The Ag-d and S-p orbitals are the main contributors for the observed features near the Fermi-level. We observe the presence of two features near the Fermi level indicating the coherent and incoherent part of the spectral function similar to those found in Mott-Hubbard type systems.

References:

1. Nitin Kumar Tripathy, Soumyojit Chatterje, Rahul Sharma, Biju Raja Sekhar, N. Vijayan and Manas Kumar Dalai, "Temperature Dependent Electronic Structure Study of noncentrosymmetric AgCd₂GaS₄ Near the Fermi Level Using High Resolution Ultraviolet Photoemission Spectroscopy", Submitted for publication (2024).
2. Y. Tokura and N. Nagaosa, *Nature communications*, 9, 3740 (2018).
3. B. Sturman and V. Fridkin, Photovoltaic and photorefractive effects in noncentrosymmetric materials, (Routledge, 2021).
4. S. Yip, *Annu. Rev. Condens. Matter Phys.* 5, 15 (2014).
5. S. I. Chykhrij, O. V. Parasyuk, and V. O. Halka, *Journal of alloys and compounds* 312, 189 (2000).
6. I. Olekseyuk, O. Parasyuk, V. Halka, L. Piskach, V. Pankevych, and Y. E. Romanyuk, *Journal of alloys and compounds* 325, 167 (2001).
7. V. Atuchin, V. Pankevich, O. Parasyuk, N. Pervukhina, L. Pokrovsky, V. Remesnik, V. Uvarov, and V. Pekhnyo, *Journal of crystal growth* 292, 494 (2006).

8. L. Ma, W. Shi, and L. M. Woods, *Journal of Alloys and Compounds* 969, 172399 (2023).
9. G. Myronchuk, M. Piasecki, A. Krymus, I. Kityk, R. Vlokh, A. Fedorchuk, V. Kozer, and O. Parasyuk, *Materials Chemistry and Physics* 200, 250 (2017).
10. A. H. Reshak, V. Atuchin, S. Auluck, and I. Kityk, *Journal of Physics: Condensed Matter* 20, 325234 (2008).
11. Y. Azhniuk, B. Lopushanska, O. Selyshchev, Y. Havryliuk, A. Pogodin, O. Kokhan, A. Ehm, V. Lopushansky, I. Studenyak, and D. R. Zahn, *Physica Status Solidi (b)* 259, 2100349 (2022).
12. I. Olekseyuk, O. Parasyuk, O. Yurchenko, V. Pankevych, V. Zaremba, R. Valiente, and Y. E. Romanyuk, *Journal of crystal growth* 279, 140 (2005).
13. G. Myronchuk, M. Piasecki, A. Krymus, I. Kityk, R. Vlokh, A. Fedorchuk, V. Kozer, and O. Parasyuk, *Materials Chemistry and Physics* 200, 250 (2017).

Bio of the Speaker: Dr. Manas Kumar Dalai is currently working at CSIR-Institute of Minerals & Materials Technology (CSIR-IMMT), Bhubaneswar, Odisha, India as a Principal Scientist and Associate Professor in Academy of Scientific and Innovative Research (AcSIR) India. Dr. Dalai Obtained his M. Sc (Physics) degree from Department of Physics, Utkal University, Vanivihar, Bhubaneswar in 2001. He obtained his Ph. D in 2009 in the field of "Experimental Condensed Matter Physics" from Institute of Physics, Bhubaneswar (Degree affiliated to HBNI Mumbai). He was a post-doctoral scientist at University of Augsburg, Germany in 2009. From 2009 to 2017; Scientist at CSIR-National Physical Laboratory, New Delhi, India, where he was working in field of Surface and Interface study of materials. He was a visiting Scientist at Department of Physics, University of North Texas, USA during 2023 under the prestigious CSIR Raman Research fellowship, He was a visiting Scientist at Department of Physics, University of Illinois, Urbana-Champaign, USA during 2013 – 2014 under the prestigious Indo-US research fellowship program by IUSSTF, New Delhi. His field of research includes Electronic structure of transition metal oxides, Topological insulators, 2DEG materials, Superconductivity, Surface and interface study of thin films and multilayers, Photoemission spectroscopy (UPS & XPS), X-ray Absorption spectroscopy (XAS), Secondary ion mass spectroscopy (SIMS) etc. He has been awarded with CSIR Raman Research Fellowship 2023-2023, Indo-US Research fellowship award 2013 by Indo-US Science and Technology Forum (IUSSTF), New Delhi. Outstanding Performance Award 2018 for the "dissemination of Metrological Traceability Through Bharatiya Nirdeshak Dravya; BND - 4201", by CSIR-National Physical Laboratory, New Delhi. He was member of American Physical Society (APS), USA during 2014 – 2015. He is a life member of Indian Society for Mass Spectrometry (ISMAS), Vijnana Bharati (VIBHA India) and Indian Institute of Metal (IIM).



Strong Light-Matter Interactions in Two-dimensional Materials for Optoelectronic Devices

Surendra B. Anantharaman¹

¹Low-dimensional Semiconductors Lab, Department of Metallurgical and Materials Engineering, IIT Madras 600 036, Tamil Nadu, India

The exploration of semiconductor materials for applications in optoelectronic devices such as efficient solar cells, low-threshold lasers, and bright light emitting diodes are some of the continuous efforts among materials scientists, physicists, and chemical engineers. Often new materials possessing unique optical properties with feasibility for device integration falls under the emerging semiconductors domain. Recently two-dimensional (2D) semiconductors with strong exciton binding energy at room temperature have shown promise in solar energy harvesting and low-threshold lasers. Nevertheless, the intrinsic optical property of the 2D material remains unperturbed. In this talk, I will present the recent developments in 2D materials and how we can overcome intrinsic limitations in these materials by introducing strong coupling of light-matter interactions. Strong coupling without an external cavity to form exciton-polaritons quasiparticles for energy harvesting will be discussed.^{1,2} I will present a simple device structure of 2D perovskites on the gold substrate which can absorb photons below the semiconductor's bandgap. Efficient charge and energy transfer in a few-layer graphene-2D perovskite heterostructure will be discussed.³ Finally, I will conclude the talk on ultrastrong coupling in the 2D materials which can lead to low-threshold lasers with a narrow linewidth.⁴

References:

1. Anantharaman, S. B.; Jo, K.; Jariwala, D. Exciton–Photonics: From Fundamental Science to Applications. *ACS Nano* **2021**, *15* (8), 12628–12654. <https://doi.org/10.1021/acsnano.1c02204>.
2. Anantharaman, S. B.; Stevens, C. E.; Lynch, J.; Song, B.; Hou, J.; Zhang, H.; Jo, K.; Kumar, P.; Blancon, J.-C.; Mohite, A. D.; Hendrickson, J. R.; Jariwala, D. Self-Hybridized Polaritonic Emission from Layered Perovskites. *Nano Lett.* **2021**, *21* (14), 6245–6252. <https://doi.org/10.1021/acs.nanolett.1c02058>.
3. Anantharaman, S. B.; Lynch, J.; Stevens, C. E.; Munley, C.; Li, C.; Hou, J.; Zhang, H.; Torma, A.; Darlington, T.; Coen, F.; Li, K.; Majumdar, A.; Schuck, P. J.; Mohite, A.; Harutyunyan, H.; Hendrickson, J. R.; Jariwala, D. Dynamics of Self-Hybridized Exciton–Polaritons in 2D Halide Perovskites. *Light: Science & Applications* **2024**, *13* (1), 1. <https://doi.org/10.1038/s41377-023-01334-9>.
4. Anantharaman, S. B.; Lynch, J.; Aleksich, M.; Stevens, C. E.; Munley, C.; Choi, B.; Shenoy, S.; Darlington, T.; Majumdar, A.; Shuck, P. J. Ultrastrong Light-Matter Coupling in 2D Metal-Organic Chalcogenates. *arXiv preprint arXiv:2308.11108 (accepted in Nature Photonics)* **2024**.

Bio of the Speaker: Surendra B. Anantharaman is an Assistant Professor in the Department of Metallurgical and Materials Engineering at IIT Madras. He has been leading the Low-dimensional Semiconductors Lab since May 2023. Before joining IIT Madras, he was a Group Leader for Perovskite Optoelectronics at RWTH/AMO GmbH, Aachen, Germany. He was a Swiss National Foundation Postdoctoral Fellow at the University of Pennsylvania,

USA. During his Postdoctoral tenure, he investigated exciton-polariton dynamics upon strong light-matter coupling without an external cavity from two-dimensional (2D) perovskites, transition metal-dichalcogenides, and emerging 2D hybrid materials. He received his Ph.D. from the Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland, in 2019 on “Exciton Dynamics in 2D Organic Assemblies for Realization of Next-Generation Optoelectronic Devices”. He also had a stint working with Taiwan Semiconductor Manufacturing Company, Taiwan, in the Thin Films Division before joining the Ph.D. program. His research focuses broadly on light-emitting devices, energy harvesting systems, and neuromorphic computing in optoelectronic devices. Dr. Anantharaman is a recipient of the Swiss National Science Foundation Postdoctoral Fellowship (2019-2021), the Japan Society for the Promotion of Science Postdoctoral Fellowship (2016), and the Ministry for Human Resources and Development, India (2009-2012).



Topological quantum phase transition in magnetic topological insulator bilayer

Mukul Kabir¹, and Basavaraja G

¹Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India

Magnetic ordering in topological insulators disrupts time-reversal symmetry, transforming the topologically non-trivial surface state into a massive Dirac fermionic state. In the two-dimensional limit, MnBi_2Te_4 , an intrinsic magnetic topological insulator, emerges as an intriguing candidate for exploring controllable topological phase transitions from an axion insulator to a Chern insulator. While such phase transitions have been experimentally demonstrated, they are typically restricted to temperatures below 2 K and require significant magnetic fields above 9 Tesla. This talk will explore various methods for controlling topological phases without relying on high magnetic fields. The results are derived within first-principles calculations, supported by Hamiltonian modelling and Monte Carlo simulations.

Bio of the Speaker: Mukul Kabir earned his PhD in computational condensed matter physics in 2006 from the S. N. Bose National Centre for Basic Sciences, Kolkata. Following this, he conducted postdoctoral research at the Massachusetts Institute of Technology from 2006 to 2011. In 2012, he joined the Physics Department of IISER Pune after being awarded the prestigious Ramanujan Fellowship



Non-Linear Hall Effect in Flatlands and Chiral Crystals

Awadhesh Narayan¹

¹Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru, India

In recent years, it has been discovered that inversion symmetry broken systems can exhibit non-linear Hall effects even under time-reversal symmetric conditions [1]. The underlying quantum objects leading to this phenomena are the moments of the Berry curvature, termed the Berry curvature multipoles. This opens up avenues for exploring fundamental physics and possible applications [2,3]. However, despite such promise, the Berry curvature multipole induced non-linear Hall effect has been experimentally realized only in a handful of materials. It is, therefore, of vital importance to find materials with large and controllable Berry curvature multipoles. In this talk, I will give examples from our work where such a controllable Berry curvature dipole has been predicted. First, we propose a giant non-linear Hall effect in the elemental buckled honeycomb lattices -- silicene, germanene, and stanene [4]. We show that the Berry curvature dipole is tunable by a transverse electric field which breaks inversion symmetry. We demonstrate that the electric field induced topological phase transitions are associated with a giant Berry curvature dipole near the critical field. Next, I will present chiral systems as promising platforms to study the non-linear Hall effects [5]. We use state-of-the-art first-principles computations, in conjunction with symmetry analyses, to explore a variety of chiral material classes. We demonstrate that the two enantiomeric pairs exhibit an opposite sign of the Berry curvature dipole, which may enable their identification via a non-linear Hall response.

References:

1. I. Sodemann and L. Fu, *Phys. Rev. Lett.* 115, 216806 (2015).
2. J Z. Du, H.-Z. Lu, and X. Xie, *Nature Reviews Physics* 3, 744 (2021).
3. A. Bandyopadhyay, N. B. Joseph, and A. Narayan, *Materials Today Electronics* 8, 100101 (2024).
4. A. Bandyopadhyay, N. B. Joseph, and A. Narayan, *2D Materials* 9, 035013 (2022).
5. N. B. Joseph, A. Bandyopadhyay, and A. Narayan, *Chemistry of Materials* (2024).

Bio of the Speaker: Awadhesh Narayan is an Associate Professor at the Indian Institute of Science. He obtained his Ph.D. from Trinity College Dublin, Ireland, where his dissertation won the Dan Bradley prize. After postdoctoral appointments at the University of Illinois at Urbana-Champaign, USA and ETH Zurich, Switzerland, he joined the Indian Institute of Science in 2019. He was selected as an outstanding referee of the American Physical Society in 2023. His research interests are in solid state and materials theory, including topological phases, ferroic materials, and non-Hermitian systems.



Topological heterostructure based spintronic devices for optoelectronic application

Pramod Kumar¹, Roshani Singh¹

¹Spintronic and Magnetic Materials Laboratory, Department of Applied sciences, Indian Institute of Information Technology-Allahabad, Prayagraj, 211015, India

Topological heterostructures present a transformative approach to optoelectronic device innovation, seamlessly integrating spintronic and photonic functionalities. This work highlights the optoelectronic potential of Ni₈₀Fe₂₀/TlBiSe₂/p-Si heterostructures, which harness the unique properties of topological insulators such as robust surface states, high spin-momentum locking, and dissipationless conduction channels. By leveraging the magnetic proximity effect, a bandgap is induced in the topological surface states, enabling efficient control of light-induced charge and spin dynamics. Experimental results reveal that these heterostructures exhibit remarkable photodetection capabilities across a broad spectrum. Raman spectroscopy confirms symmetry-breaking mechanisms at the interface, while transient absorption spectroscopy under optical excitation demonstrates ultrafast charge carrier dynamics, enhanced by magnetic field-induced energy level splitting. Electrical measurements highlight superior photo response characteristics, with high photoresponsivity, sensitivity, and Detectivity, making these devices ideal for photodetection and optical signal processing [1]. These findings establish the Ni₈₀Fe₂₀/TlBiSe₂/p-Si heterostructure as a versatile platform for energy-efficient optoelectronic devices, including ultrafast photodetectors and optical switches. The interplay of spintronics and photonics in these heterostructures opens avenues for next-generation technologies, such as high-speed optical communication, quantum information systems, and advanced imaging. This work explores how the unique optoelectronic properties of topological heterostructures are paving the way for multifunctional devices that redefine the landscape of modern optoelectronics.

References:

1. Singh R, Maurya G K, Gautam V, Kumar R, Kumar M, Suresh K G, Panigrahi B, Murapaka C, Haldar A and Kumar P 2023 Proximity induced band gap opening in topological-magnetic heterostructure (Ni₈₀Fe₂₀/p-TlBiSe₂/p-Si) under ambient condition *Sci. Rep.* 13 22290.

Bio of the Speaker: Dr. Pramod Kumar is a distinguished professor and researcher at IIT Allahabad, specializing in the advanced study of magnetic and spintronic materials. With a Ph.D. in Physics from IIT Bombay and extensive postdoctoral work across leading institutions like IFW Dresden, Tulane University, and Georgia State University, his expertise spans magneto-thermal and transport phenomena, topological insulators, and quantum Hall effects. He has pioneered research in nanoscale device fabrication, cryogenic techniques, and photovoltaic effects, contributing significantly to the development of innovative technologies. Dr. Kumar has led several high-impact research projects funded by prestigious agencies like SERB, DST, and CSIR, focusing on spintronic devices, topological materials, and advanced instrumentation. He has authored numerous peer-reviewed publications in top journals and collaborated with global research leaders. His work on graphene, heterostructure devices, and novel magnetic materials underpins advancements in microelectronics and optoelectronics. An IEEE Senior Member and recipient of multiple awards, including best poster awards and international travel fellowships, Dr. Kumar is also a dedicated educator and mentor guiding numerous Ph.D. scholars and organizing workshops on material sciences. His contributions significantly enhance the understanding and application of cutting-edge materials science in modern engineering.



Proximity Coupling in Topological Materials

Dhavala Suri¹

¹Indian Institute of Science, Bengaluru 560 012, India

Proximity coupling in topological systems have been studied in several systems including coupling with 2D materials [1], superconductors [2] and ferromagnetic insulators [3]. These have resulted in emergent phenomena at the interface such as above room temperature ferromagnetism [3], interfacial non-trivial spin textures [4] and proximity coupled superconductivity. In this talk, I will present a review of this field of research that provides a comprehensive perspective of proximity coupling to topological materials. In this context, the concept of planar Hall effect will be discussed in detail [5-6].

References:

1. M. A. Haque et.al., *npj 2D Materials and Applications* 8, 10 (2024).
2. Qi-Guang Zhu and Tao Zhou *Phys. Rev. B* 107, 094506 (2023).
3. F. Katmis et. al., *Nature* 533, 513–516 (2016).
4. D. Suri et. al., *Phys. Rev. B* 110, 134433 (2024).
5. D. Suri et. al., *J. Phys.: Condens. Matter* 33 335301 (2021).
6. A. Bhardwaj et. al., *Appl. Phys. Lett.* 118, 241901 (2021).

Bio of the Speaker: Asst. Professor at CeNSE, IISc since 2023, with a lab that works on magnetic topological insulators, superconductors and proximity effects. Her lab specializes in MBE growth of materials, and quantum transport measurements. She did her PhD in BITS Pilani, K. K. Birla Goa Campus followed by postdoctoral stint with Dr. Moodera at MIT. She spent a brief time in TIFRH and then was a Marie Curie fellow at TU Munich in the group of Prof. Christian Back.



Hydrogen storage in functionalised carbon systems- a DFT study

Prafulla K Jha¹, Heera Nair¹ and Darshil Chodvadia²

¹Department of Physics, Faculty of Science, The M. S. university of Baroda, Vadodara-390002, India

² Department of Chemistry and Institute for Nanotechnology & Advanced Materials, Bar-Ilan University, Ramat-Gan, 5290002 Israel.

The increasing energy demands and diminishing traditional fuels necessitate alternative solutions, especially in transportation. Hydrogen fuel is a promising option due to its abundance, eco-friendliness, and high energy density. However, efficient hydrogen storage remains a critical challenge due to its low density and high diffusivity. Among various storage methods, solid-state storage offers safety, stability, and high-density potential. For efficient solid-state hydrogen storage, the U.S. Department of Energy (DOE) recommends an average binding energy of 0.2–0.7 eV/H₂ and a gravimetric weight percent of at least 4.5%. This talk presents advanced carbon-based hydrogen generation and storage systems using Density Functional Theory (DFT) and Ab initio Molecular Dynamics (AIMD) simulations, focusing on material design, metal decoration, and strain engineering to overcome current limitations. Transition metals enhance hydrogen storage through the Kubas interaction, facilitated by the presence of d-orbitals, while alkali and alkaline earth metals promote storage via polarization, transferring electrons to the host material and inducing a partial positive charge. Strain engineering enhances hydrogen storage in 2dpa under compressive strain, with the system adsorbing 10 H₂ molecules at -0.24 eV and achieving 6.9 wt.% under 4% biaxial strain, with a desorption temperature of 209.73 K at 12 bar. These results highlight the potential of optimized carbon-based and polymer systems, alongside strain engineering, as promising approaches for advancing hydrogen storage technologies in sustainable energy applications.

Bio of the Speaker: Prof. Prafulla K. Jha is a professor of physics at the Maharaja Sayajirao University of Baroda, Gujarat. Prof. Jha is currently Head of the Department of Physics and Chairman BoS in Physics at Faculty of Science, Maharaja Sayajirao University of Baroda, Gujarat. Over the years Prof. Jha has been recognized by several awards such as, Indian National Science Academy Teacher Award (2018), prestigious TWAS-UNESCO Associateship twice, regular associateship of International Centre for Theoretical Physics (ICTP), UGC Research Awardee, DST Young Scientist awardee and Fellow of the Royal Society of Chemistry. He has been awarded the Silver Medal-2022 of Society for Materials Chemistry for his contribution in the field of materials chemistry. He leads computational condensed matter physics lab which is actively involved in research on various problems such as, topological quantum materials, thermoelectric, heterogenous catalysis, magnetism, corelated materials, superconductivity, sensors/detectors, drug design and delivery mechanisms. As a result, he has actively contributed to the field of condensed matter physics by publishing more than 300 research papers in peer reviewed journals of national and international repute. He has h-index of 46 and citations of more than 8300. He is also serving as member of the editorial board for several journals. His dynamism is evident from the completion of 25 research projects (5 international) funded by major funding agencies and guiding 29 Ph. D Students. Furthermore, he is editor of the UGC care journal being published by the M S University of Baroda. He is also working as nodal officer of the western zone of UGC CARE.



C₂ over C₁ during CO₂ER: Can we tune the activity of 111 Plane of Cu based catalysts

Ranjit Thapa^{1,2}

¹Department of Physics, SRM University—AP, Amaravati, Andhra Pradesh 522 240, India

²Center for Computational and Integrative Sciences, SRM University—AP, Amaravati, Andhra Pradesh 522 240, India

Human activities release CO₂ through chemical reactions, increasing atmospheric CO₂ levels. Strategies to reduce these emissions include cleaner energy, improved industrial processes, and sustainable practices. Carbon capture and utilization (CCU) is a promising approach. Electrochemistry effectively converts CO₂ into valuable products using copper catalysts. While CO₂ER predominantly yields single carbon products (C₁ products) with high efficiency, there is a growing interest in producing double carbon products (ethanol, C₂ products) due to their higher energy density and greater industrial significance. However, the complexity of C₂ product formation, involving C-C bond formation, presents challenges as it competes with the hydrogenation of *CO to *CHO, reducing C₂ 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 C₂ product formation. We introduce an innovative graphical method and C₂ vs C₁ parity plot to facilitate this screening process. We believe that this user-friendly graphical screening technique for CO₂ electroreduction catalysts has the potential to gain widespread adoption, possibly becoming as prevalent as 'volcano plots' in other reaction analyses. Now we are working on descriptor and predictive model equation using Quantum mechanics/ Machine Learning approach which will help to identify the best catalyst for CO₂ER towards C₂ product.

References:

1. Anjana Tripathi, Ranjit Thapa Size, Shape, Facet and Support Dependent Selectivity of Cu nanoparticles in CO₂ reduction through multiparameter optimization, *Nanoscale*, Accepted, 2024, 10.1039/D4NR03567D.
2. Sayantan Chongdar, Rupak Chatterjee, Samim Reza, Snigdha Pal, Ranjit Thapa, Rajaram Bal, Asim Bhaumik, Low Potential Electrochemical CO₂ Reduction to Methanol over Nickel-Based Hollow 0D Carbon Superstructure, *Advanced Energy Materials*, <https://doi.org/10.1002/aenm.202403809>.
3. Asif Iqbal, Anjana Tripathi, Ranjit Thapa, C₂ product formation over C₁ product and HER on 111 plane of specific Cu alloy nanoparticle identified through multiparameter optimization, *Inorganic Chemistry*, 63, 2024, 1462.
4. Anjana Tripathi, Ranjit Thapa, Optimizing CO₂RR selectivity on Single Atom Catalysts using Graphical Construction and Identification of Energy Descriptor, *CARBON*, 208, 2023. 330-337.

Bio of the Speaker: Currently, Prof. Thapa is DEAN-Research of SRM University-AP, and a full professor in the Department of Physics, SRM University -AP. He conducting research on Computational Material Science technologies focused on QM/ML based approach for the past ten years. He has received the Young Associate Award in the year 2016 by the Indian Academy of Science, Bangalore for my outstanding research in Computational Materials Science and was also chosen for BRNS' Young Scientist's Research Award (YSRA) in the year 2018. He has published more than 190 research articles with an average impact factor of 8.1, in highly reputed international journals. His current h-index is 41 with a total citation of more than 5800. Currently, he is developing a "Materials database" (<http://energymaterials.org:3000/>) and pipelines named as "padarth khoj" to identify the various catalyst and battery materials under the different funded projects. He has guided nine Ph.D. students to date. The main contributions are: "electronic and structural descriptor", "Simple Graphical Construction to find the best catalyst of eNRR and CO₂RR", "Bond Exchange Spillover Mechanism", "Homonuclear B-B and B-B-B bond as catalytic center", and "inverse catalyst".



DFT Studies on CO₂ Reduction at Functionalized IL@Au(111) Surface

Muthuramalingam Prakash¹, Shanmugasundaram Kamalakannan¹, Majdi Hochlaf²

¹ *Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603 203, Tamil Nadu, India*

² *Université Gustave Eiffel, COSYS/IMSE, 5 Bd Descartes, 77454, Champs Sur Marne, France*

A heterogeneous catalytic environment (i.e., electrode/electrolyte) plays a major role to decide the catalytic activation and conversion of the CO₂ molecule at the interface. ADDIN CSL_CITATIO{"citationItems":[{"id":"ITEM1","itemData":{"DOI":"10.1039/c9ta11966c","ISSN":"20507496","abstract":"As a promising and important carbon source, utilization of carbon dioxide (CO₂) can effectively solve the energy crisis caused by fossil resource consumption and the environmental problems arising from the emission of CO₂. The electrocatalytic method is currently a promising research method for CO₂ reduction; however, it faces the problems of low product selectivity and poor faradaic efficiency (FE). Therefore, the design of effective catalysts with lower overpotential, high FE, and product selectivity is key consideration for the development of electrochemical CO₂ reduction (CO₂RR). Herein, we summarize the current research progress in the electrocatalytic reduction of CO₂ to fuels on heterogeneous catalysts. Progress in the electrocatalytic reduction of two types of products, C₁ products (CO, HCOOH, CH₃OH, CH₄) and C₂ products (CH₃CH₂OH and C₂H₄), are discussed. The catalytic activity, FE, product selectivity, electrocatalytic mechanisms, and challenges faced in terms of product selectivity and catalytic activity stability in electrochemical CO₂ reduction are discussed. This review can provide effective guidance for the design of effective catalysts with high activity, product selectivity, FE, and stability."},"author":[{"dropping-particle":"","family":"Liu","given":"Anmin","non-dropping-particle":"","parsenames":false,"suffix":""}, {"droppingparticle":"","family":"Gao","given":"Mengfan","nondroppingparticle":"","parsenames":false,"suffix":""}, {"droppingparticle":"","family":"Ren","given":"Xuefeng","non-dropping particle":"","parsenames":false,"suffix":""}, {"droppingparticle":"","family":"Meng","given":"Fanning","nondropping-particle":"",""}]}

Bio of the Speaker: Dr. Prakash Muthuramalingam completed his B.Sc., and M.Sc., Degrees in Chemistry from Madurai Kamaraj University, Madurai. He completed his Doctoral studies at the CSIR-Central Leather Research Institute (CSIR-CLRI) Adyar, Chennai. Before joining SRMIST, he worked as a postdoctoral fellow at Rice University (Houston, USA), CNRS-ICGM (Montpellier), and Université Paris-Est (UPEM and UPEC) Paris, FRANCE. He also worked on industrial collaborative projects at IIT-Madras and DST Indo-EU (HYPOMAP) sponsored project at CSIR-CLRI, Chennai. Currently, he is working as a Research Associate Professor at SRMIST, Kattankulathur, and his research interest involves investigating ILs-based composite materials (2D and 3D MOFs) for energy storage, gas storage (H₂, CO₂, CH₄,



etc.), carbon capture, separation, activation, and conversion applications. In addition, studies on the structure, stability, dynamics, and functions of biomolecules in ILs using QM, QM/MM and MD Simulations approaches. Currently, he is the head of Computational Chemistry Research Laboratory (CCRL) at SRMIST, Kattankulathur campus. Under his guidance, 5 Ph.D. scholars have successfully completed their doctoral degree and at present, 6 Ph.D. scholars are working in the field of Computational Modelling. He has published more than 106 articles with 6 book chapters and also signed 4 MoUs with French Institutes (UPEst & UM2) and Inha University, South Korea. He has also received several projects (5 projects) including recipient of DST-SERB ECRA and ANRF-CRG projects from the Government of India.

Advancement in Next Generation Energy Materials and Neuromorphic Paradigm: A Guide Through DFT

Tisita Das¹,

DST INSPIRE Faculty

¹Condensed Matter Physics, Harish-Chandra Research Institute (HRI), Prayagraj, India

I will start with an overview of vivid applications of computational modelling for energy harvesting. The first part will be dedicated to our computational modelling for the next generation energy materials, where I will explain the fundamental electronic structure perspective behind catalytic reaction mechanism for novel two-dimensional (2D) materials and strain induced catalytic enhancement. I will demonstrate the experimental realization of our theoretical prediction for efficient catalytic materials for water splitting and CO₂ reduction [1-5]. Subsequently, I will discuss about our recent findings of pre-intercalation mechanism in layered oxide materials for battery application based on ion migration pathway prediction, which has been experimental validated [6]. This will be followed by discussion about our research to understand the fundamental physics behind the unique electronic and optical properties of emerging hybrid perovskite materials for optoelectronic industry. The last part of my talk will be focused on the future roadmap of our ongoing research in neuromorphic computing [7] as another important implication of ion migration pathway prediction in hybrid perovskites.

References

1. Tisita Das *et al.*, *ACS Applied Energy Materials*, 2, 5074 (2019).
2. Tisita Das *et al.* *Catalysis Today*, 370, 189 (2021)
3. Tisita Das *et al.*, *Sustainable Energy and Fuel*, 6, 5621 (2022).
4. S. Mondal, S. Sarkar, D. Bagchi, Tisita Das *et al.*, *Advanced Materials*, 34, 2202294 (2023).
5. R. Belgamwar, R. Verma, Tisita Das *et al.*, *JACS*, 145, 8634 (2023)
6. Y. Luo[†], J. V. Handy[†], Tisita Das[†] *et al.*, *Nature Materials* (2024).
7. K. Sakhatskyi, ... Tisita Das *et al.*, *ACS Energy Letters*, 7, 3401 (2022)



Computational Pathways in Topological Quantum Materials: Insights from DFT

V. Kanchana¹

¹Department of Physics, Indian Institute of Technology Hyderabad,
Kandi, 502285, Sangareddy, Telangana, India

Advancing next-generation technology relies on quantum topological materials, crucial for energy-efficient processing, high-speed operation, and reliable quantum storage. Driven by principles such as magnetism, topology, correlations, and superconductivity, materials with topological properties in both electronic and phononic bands are central to this pursuit, offering wide-ranging applications. Topological metals and semimetals, known for their unique properties under various conditions, have been extensively studied but remain underexplored in certain aspects. MnRhP, for example, exemplifies a compound whose robust electronic topological properties persist under pressure [1]. On the other hand, phonon topology can suppress lattice thermal conductivity, as observed in the thermoelectric candidate CuTlS [2]. However, few materials display topological characteristics in both electronic and phononic bands. In this context, non-magnetic ThX₂ (X = As, Sb, Bi) compounds show high Fermi surface nesting, suggesting a potential charge density wave (CDW), validated by a peak in the Lindhard susceptibility [3]. Non-magnetic ZGeSb (Z = Hf, Ti, Zr) compounds, with a high density of states and dual topological properties, suggest potential superconductivity applications [4]. We also explore MnGaGe, a magnetic compound proposed as a two-terminal device model to investigate quantum transport properties [5], and the MnAlGe/TiO₂ (001) heterostructure, where proximity coupling induces spintronic effects. Electron transfer drives TiO₂ from a semiconductor to a metal, forming an Ohmic contact with non-trivial topological features, with a spin injection efficiency of 43% at a 0.2 V bias. These materials, exhibiting dual topological behaviour in both electronic and phononic bands, advance our understanding of quantum phenomena and offer potential breakthroughs in quantum computing, energy-efficient devices, and novel technologies.

References:

1. J. Singh, B. Anuroopa, S. Kharabadze, A. N. Kolmogorov, G. Vaitheeswaran, and V. Kanchana, *J. Phys. Chem. C* 126, 17328-17337 (2022).
2. Sushree Sarita Sahoo, & V. Kanchana, *Physica Scripta*, 97(12), 125820 (2022).
3. Rishi G, C.V Anusree, and V Kanchana, *J. Phys.: Condens. Matter* 34, 445502 (2022).
4. Sahoo, S. S., Mason, T. M., Dugdale, S. B., & Kanchana, V.. *Physical Review B*, 109(3), 035151 (2024).
5. Anusree, C. V., S. Pradhan, V. Kanchana, *Journal of Physics: Condensed Matter*, 36(15), 155501 (2024).

Bio of the Speaker: Dr. V. Kanchana is a Professor in the Department of Physics at Indian Institute of Technology Hyderabad (IITH). Before joining IITH, she held positions as a Guest Scientist at the Max-Planck Institute for Solid State Research in Germany and as a Researcher at the Royal Institute of Technology in Sweden. She completed her Ph.D. in Condensed Matter Physics at Anna University. Dr. Kanchana's research focuses on

quantum materials, thermoelectrics, topological insulators, and computational studies of materials under extreme conditions. Her contributions to the field are exemplified by 147 peer-reviewed publications and over 4,400 citations. Dr. V. Kanchana has received numerous prestigious awards, including the Bronze Medal from the Society for Material Chemistry (SMC) in 2023, the MRSI Medal in 2021, and the DAE Young Achiever Award in 2014. She was elected as a Fellow of the Institute of Physics (UK) in 2021 and honored with the Fellowship of the Royal Society of Chemistry (FRSC) in 2020. Additionally, Dr. Kanchana serves as an editorial member for the Journal of Electronic Structure (IOP) and is a life member of the Material Research Society of India (MRSI) and the Society for Material Chemistry (SMC).



Exploring Novel Topological States: Multi-Fold Fermions and Dirac Nodal-Line Net Bosons in SiX₂ (X = P, As)

G Vaitheeswaran¹

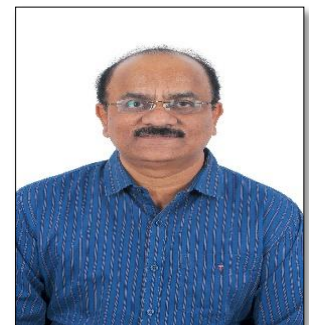
¹School of Physics, University of Hyderabad, Gachibowli, Hyderabad-500046, Telangana, India

Over the past two decades, the pursuit of novel topological phases of matter has become a major focus in condensed matter research. Beyond Dirac and Weyl particles, a variety of unique quasiparticles, distinct from those studied in high-energy physics, have attracted significant attention. This study explores multi-fold degenerate fermions beyond Dirac and Weyl types in pyrite-structured SiX₂ compounds, where X = P or As. Through symmetry analysis, we uncover the topological features of multi-fold fermions with four-fold and six-fold degeneracies located at the Γ and R points of the Brillouin zone. These nodes, protected by crystalline symmetries, present an excellent platform for investigating novel topological properties and the physical phenomena associated with them. Additionally, these compounds exhibit intriguing topological features in their phonon dispersions. Specifically, we identify the coexistence of three nodal surfaces (NSs) and a phononic Dirac nodal-line (DNL) network. This DNL network consists of three intersecting nodal lines, each residing in a distinct momentum plane (k_x , k_y , k_z) and converging at a common nodal point. Such a configuration is extraordinarily rare in phononic systems, creating opportunities for experimental validation through observable phononic surface states. These findings establish SiX₂ compounds as a promising platform for studying multi-fold fermions and their potential applications. Moreover, the discovered phononic topologies highlight these materials as exceptional candidates for investigating novel bosonic excitations, advancing the understanding of topological phenomena in solid-state systems.

References:

1. Chattopadhyay T K and Schnering H G V 1984 Zeitschrift für Kristallographie-Crystalline Materials 1671–12
2. Wu P and Huang M 2016 physica Status Solidi (b) 253862–7

Bio of the Speaker: Dr. G. S. Vaitheeswaran, Professor at the School of Physics, University of Hyderabad. His research interest is towards understanding the electronic band structures of complex materials. With a Ph.D. in Theoretical Solid-State Physics from Anna University (2004), Dr. Vaitheeswaran held post-doctoral positions at the Max-Planck Institute for Solid State Research, Stuttgart, and Royal Institute of Technology, Stockholm, Sweden. He joined as a faculty in the University of Hyderabad in 2007. His excellence in research has been recognized with numerous accolades, such as DAE-Young Achiever Award (2012), B.M. Birla Science Prize In Physics (2013), Chancellor's Award for Excellence in Teaching and Research by University of Hyderabad (2014), and the Materials Research Society of India Medal (2019).



The Complex Topological Landscape of 4D Transition Metal Systems

Kartick Tarafder¹

¹Physics Department, National Institute of Technology Karnataka, Surathakal,
Mangalore, Karnataka-575025

In this presentation, I will explore the electronic, magnetic, and dynamic properties of a few 4D transition metal compounds based on our theoretical findings. We present the non-trivial topological properties in Yttrium Iodide (YI), revealing a unique electronic structure featuring spin-polarized Dirac and Weyl nodes within the same phase. Our analysis identifies twenty-five pairs of nodal points in the spin-up channel and six pairs in the spin-down channel. The presence of Weyl nodes is confirmed by the source and sink characteristics in the Berry curvature and the observation of Fermi arcs in the surface band structure, classifying YI as a type-II magnetic Weyl semimetal. With spin-orbit coupling (SOC), eight pairs of Weyl points show robustness while a small gap opens at the spin-polarized Dirac cone. The system also demonstrates a high Fermi velocity for Dirac fermions, estimated to be 3.4×10^5 m/s, along with a significant anisotropic intrinsic anomalous Hall conductivity of up to 933 S/cm. Additionally, I shall discuss the non-trivial topological behaviour of ZrN, which we predict will exhibit Dirac nodal line semimetallic characteristics. The unique properties of these materials, including Weyl points, Dirac points, high intrinsic quantum anomalous Hall conductivity, and widely spaced Weyl points in momentum space, emphasize their promising potential for spintronic applications.

References:

1. *Nature Materials* volume 15, pages1145–1148 (2016)
2. *Annual Review of Condensed Matter Physics* Volume 8, 337 (2017)
3. *Rev. Mod. Phys.* 90, 015001 (2018)

Bio of the Speaker: Dr. Kartick Tarafder is currently serving as an Associate Professor and Head of the Physics Department at NIT Karnataka. A PhD in theoretical condensed matter physics was completed at the S.N. Bose National Centre, Kolkata. Postdoctoral research was conducted at Uppsala University, Sweden, and Lawrence Berkeley National Laboratory, USA. His current research focuses on investigating physical properties of materials through First-Principles electronic structure calculations, with particular attention to quantum materials and functional materials for spintronics, energy harvesting, and storage applications. Numerous projects in molecular spintronics and advanced solar cells have been led, and he has supervised several PhD scholars and published several articles in reputed international journals.



Designing 2D photocatalysts for Green Hydrogen Production

P. Ravindran¹

¹Department of Physics, Central University of Tamil Nadu, Thiruvarur, Tamil Nadu, 610005, India

²Simulation Center for Atomic and Nanoscale MATerials (SCANMAT), Central University of Tamil Nadu, Thiruvarur, Tamil Nadu, 610005, India

Designing functional materials with 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. 2D materials offer enormous opportunities to tune their electronic properties owing to large surface area and short diffusion length and hence can be used as an efficient photocatalyst. We have investigated the structural, electronic, and optical properties of derivative of graphene such as graphene monoxide, graphene dioxide, graphitic carbon nitride, molecule adsorbed systems and the heterostructures made with cadmium mono-chalcogenides using hybrid density functional calculations. The overall stability of these compositions were analyzed using formation energy calculation, phonon spectra, and AIMD simulations. Band gap engineering has been done by varying layer thickness, strain, electric field, isoelectronic substitution/co-substitution etc and predicted that several of these compounds has low effective mass, high carrier mobility, enhanced optical absorption, and most importantly the band edges straddle the water redox potential thus suitable to use them as photocatalyst for solar hydrogen production. C-site substitutions improve the spatial separation of e^- - h^+ pairs, which in turn suppress the recombination rate, thereby enhancing the photocatalytic activity. The CdX/C_2N heterostructures possess a type-II band alignment, where the relative and alignment of the C_2N and CdX monolayers promotes a spatial separation of the electrons (that resides in C_2N) and holes (that resides in CdX). Importantly, the band edges of the heterostructures straddle the water redox potential under different pH conditions and hence suitable to produce hydrogen from sea water.

References:

1. S.M.Thomas and P.Ravindran, Tuning the optoelectronic properties of graphene monoxide by electric field, strain and heterostructure with CdX ($X= S, Se$ or Te), *Surfaces and Interfaces* 52, 104979 (2024).



Are Vertical van der Waals Heterostructures of Transition Metal dichalcogenides useful as Efficient ultra-thin Solar Cells?

Anjali Kshirsagar¹, Laxman Tatikondewar¹ and Sudip Chakraborty²

¹Department of Physics
Savitribai Phule Pune University
Pune 411 007, India

²Materials Theory for Energy Scavenging (MATES) Lab, Department of Physics, Harish-Chandra Research Institute (HRI), Prayagraj 211019, India

Vertical bilayered heterostructures of zirconium and hafnium dichalcogenide monolayers are found to be potential materials for excitonic and Schottky barrier solar cells. The dynamic stability of these van der Waals heterostructures (vdwH) is confirmed using phonon dispersion spectra. Structural stability and hence the feasibility of experimental preparation is guaranteed from the binding energy values. Ladder calculations are performed - density functional theory for structural relaxation and electronic self-consistency, final electronic structure for better estimation of the band gap with single-shot GW calculation and solution of the Bethe–Salpeter equation to calculate the optical absorption spectra for vdwH. Using these absorption spectra, the power conversion efficiency is estimated to be ~1% for 1 nm thick device leading to considerably high power density values. ZrSe₂(1T)@ZrTe₂(1T) vdwH has not been studied to date in the literature theoretically or experimentally and it is demonstrated to have potential application as a Schottky barrier solar cell. ZrS₂(1T)@HfSe₂(1T) vdwH has type II band alignment with sufficiently high conduction and valence band offsets. These keep the photo generated electron-hole pairs as separate free carriers minimizing recombination and leading to efficient light to electricity conversion. Bader charge analysis is carried out to understand interatomic charge transfer during formation of the heterostructures.

Bio of the Speaker: Professor Anjali Kshirsagar retired as the Professor and Head of Department of Physics, Savitribai Phule Pune University (SPPU) and is currently working as an Emeritus Professor. She was the Director of Centre for Modeling and Simulation and Interdisciplinary School of Scientific Computing at SPPU. She is Co-ordinator of the Center for Science Education and Communication, SPPU. Prof. Kshirsagar was a Senior Associate of Abdus Salam International Centre for Theoretical Physics (AS-ICTP), Trieste, Italy during 2002-2014. She is Member and chartered physicist of Institute of Physics, UK since 1999 and is a Fellow of Maharashtra Academy of Science. She has received the prestigious Late Principal V. K. Joag Award of SPPU in 2011 for excellence in teaching and research. Fifteen students have obtained their doctoral degree and seven students have received M.Phil. degree under her guidance. She has set-up a world-class high-performance computing facility named SAHASRAR to carry out research in Computational Materials Science on SPPU campus worth Rs. 8 Crores through a major research project funded by DST Nanomission council. This is the largest project ever sanctioned to an individual faculty in the University and SPPU is the only University having such facility.



Energy storage materials for supercapacitor application

S. N. Pandey¹

¹Department of Physics, Motilal Nehru National Institute of Technology Allahabad,
Prayagraj-211004, India

Energy is a fundamental requirement in nearly all aspects of daily life. Developing efficient energy storage systems is an essential requirement now. Among the various energy storage options, supercapacitor has attracted significant attention due to its exceptional characteristics, such as high power density, rapid charge-discharge capabilities, and long cycle stability. Metal oxides/ hydroxides demonstrate significantly higher capacitance and energy density in comparison to carbon materials. Furthermore, the surface characteristics are crucial for supercapacitor application. Fractal analysis serves as an analytical method that extracts additional information about the surface beyond traditional analyses. This method also enhances the understanding of how surface morphology is affected by various physical and chemical properties. I shall present the electrochemical and fractal analysis of oxide and hydroxide materials.

References:

1. Kavyashree, Shrikant S. Raut, Babasaheb R. Sankapal, S. N. Pandey, Tuberoso surface architecture of Sr(OH)₂ film as supercapacitive electrode, *Electrochimica Acta*, **2017**, 258, 34-42.
2. Embedded coral reef sponge like structured Al(OH)₃/FeOOH composite for flexible solid-state symmetric supercapacitor; Shama Parveen, Kavyashree and S. N. Pandey, *Journal of Power Sources*, **2020**, 445, 227304.
3. Shama Parveen, Kavyashree., S. K. Sharma, S. N. Pandey, High performance solid state symmetric supercapacitor based on reindeer moss-like structured Al(OH)₃/MnO₂/FeOOH composite electrode for energy storage applications, *Energy*, **2021**, 224, 120137(1-12).
4. Fractal characterization of flakes covered tuberoso structured Cu: Sr(OH)₂ thin film as supercapacitive electrode; Kavyashree, R. P. Yadav, Shama Parveen, Leela Pradhan Joshi and S. N. Pandey; *Material Research Bulletin*, **2019**, 120, 110574 (1-8).

Bio of the Speaker: Dr. S. N. Pandey is working as a Professor and Head, Department of Physics, MNNIT Allahabad, Prayagraj, India. He has more than thirty years of both teaching and research experiences. He is recipient of many awards and fellowships including University Grants Commission (UGC) Research Award, Associateship of The Institute of Mathematical Sciences, SERC Visiting Fellowship, JNCASR Visiting Fellowship, etc. He is a Mentor of INSPIRE programme and Coordinator of Madhava Mathematics Competition. He is associated with many academic bodies/ societies as a life member/ member. The area of research of Prof. Pandey is both experimental and theoretical physics. A) Experimental: Nanostructured thin films, functional oxide nanomaterials, new materials for energy storage, supercapacitors and device fabrications. B) Theoretical: Dynamics of nonlinear and damped systems, symmetry and integrability, fractal analysis, quantum computing: entanglement dynamics. Prof. Pandey has published more than 60 research papers in the reputed international/ national journals like *Energy*, **Journal of Power Sources**, *Journal of Energy Storage*, *Electrochimica Acta*, *Applied Surface Science*, *Physical Review Letters*, *Chemical Physics Letters*, *Journal of Applied Physics*, etc. He has delivered keynote/ invited lectures in many international/ national conferences/ symposia/ short term courses. He is reviewer and editorial board member of many international/ national journals. Prof. Pandey has supervised seven Ph. D. scholars and two post-docs (N-PDF). Presently, four Ph. D. scholars are working with him. Prof. Pandey visited many countries like USA, Russia, Ukraine, South Africa, Singapore, Finland, etc.



A Century of Quantum Physics is only a Warmup Exercise

G. Baskaran^{1,2,3}

¹Department of Physics, IIT Madras

²Perimeter Institute for Theoretical Physics, Waterloo, ON, Canada

³Matscience, Chennai

Quantum mechanics, that began in early last century continues to engage us in science and technology. “More is Even More Different” [1] in the quantum world. The new and challenging field of quantum biology is a fascinating example. Our understanding of quantum materials in the last one century seems like a warm up exercise, to climb Mount Everest. The experimental fact that certain quantum coherence phenomena are operating at the warm and wet biological environment is a surprise. After a over view, I will briefly touch upon long distance coherent electron transfer in bio molecules and certain electron pair tunnelling processes. “Condensed matter physics – Biology Resonance” [2] is a need of the day. Further, “All Basic Phenomena in Condensed Matter Physics Mirror in Biology” [3,4].

References:

1. W. Anderson, More is Different, Science, 177, 393 (1972).
2. G. Baskaran, Condensed matter physics – Biology Resonance, Int. J. Mod. Phys. B14, 449 (2000).
3. G. Baskaran, All basic condensed matter physics phenomena & notions mirror in biology – A hypothesis, two examples and a novel prediction Pramana, 58, 427 (2002)
4. G. Baskaran, Hypotheses on Manybody Quantum Effects in Photosynthes Proceedings of QSCP 2023.

Bio of the Speaker: G. Baskaran is a theoretical physicist with a broad interest in quantum matters; also explores prospects for room temperature superconductivity, novel quantum phases and qubits at ambient conditions. Nature, Biology and Neuroscience continue to amaze him.

Baskaran completed his school education in Tamil medium at the St. Mary's High School; Pre-University, B.Sc. (Physics) at the Thiagarajar College and M.Sc. (Physics) at The American College, all at Madurai. He completed a Ph.D. in Theoretical Physics at the Indian Institute of Science, Bangalore.

He joined the Institute of Mathematical Sciences, Chennai in 1987 and is now a Professor Emeritus. He is a Distinguished Professor at IIT Madras and

Distinguished Visiting Research Chair at the Perimeter Institute for Theoretical Physics, Waterloo, Canada.

Fellow of IASc, INSA and TWAS, he has received ICTP Award, S.S. Bhatnagar Award, Distinguished Alumni Award of IISc, Thiagarajar College and G.N. Ramachandran Award of SASTRA for Theoretical Physics.

He occasionally writes on popular science in Tamil.



Topological Hall effect in skyrmion crystals via spin-orbit coupling

S. Satpathy,^{1,2,3} Arijit Mandal,^{1,2} Pratik Sahu,^{1,2} and B. R. K. Nanda^{1,2}

¹Condensed Matter Theory and Computational Lab, Department of Physics, IIT Madras, Chennai-600036, India

²Center for Atomistic Modelling and Materials Design, IIT Madras, Chennai-600036, India

³Department of Physics, University of Missouri, Columbia, MO 65211, USA

The topological Hall effect (THE) is the result of spin-asymmetric deflection of charge carriers flowing through a non-collinear spin system. Effective manipulation of the topological Hall conductivity (THC) in skyrmions is currently a vigorous area of research with an eye towards potential spintronics application. We start with a single skyrmion interacting with an electron in the presence of the spin-orbit coupling (SOC), which leads to the formation of the skyrmionic polaron. For the skyrmion crystal, electron bands are formed with topological characters. We show that the band topology can be tuned by changing the strength of the Rashba SOC, which can be accomplished via a perpendicular electric field. This results in the change of the subband Chern numbers and a transition between ordinary insulator and Chern insulator as the Rashba SOC is varied. For partially filled subbands, the Rashba SOC can tune the THC and reverse its sign, so that the direction of the Hall current is flipped. The critical Rashba strength for this depends on the skyrmion type and the carrier density. We extend our analysis to the cases of Dresselhaus and Weyl SOC as well and show that they can be directly mapped to the Rashba SOC case. Our work suggests new avenues for the control of charge transport in skyrmion crystals.

References:

1. Formation of the skyrmionic polaron by Rashba and Dresselhaus spin-orbit coupling, P. Sahu, B. R. K. Nanda, and S. Satpathy, *Phys. Rev. B* 106, 224403 (2022)
2. Tuning the band topology and topological Hall effect in skyrmion crystals via the spin-orbit coupling, A. Mandal, S. Satpathy, and B. R. K. Nanda, ArXiv: 2411.06434

Bio of the Speaker: Professor Sashi Satpathy is currently a Curators' Distinguished Professor of Physics at the University of Missouri, United States, with research area in Theoretical Condensed Matter Physics. He is an elected Fellow of the American Physical Society, the American Association for the Advancement of Science, the Institute of Physics, London, and he is a long-time Patron of the Odisha Physical Society. Currently, he is a Visiting Professor in the Department of Physics, IIT Madras, under the VAJRA advanced research award from the Government of India.



Fermi Surfaces in Unconventional Insulators

Suchitra Sebastian¹,

¹University of Cambridge, UK

In this talk I will discuss various families of unconventional insulators, in which bulk Fermi surfaces are revealed despite bulk insulating behaviour. We study complementary experiments to shed light on the potential origin of such unexpected Fermi surface observations.



Emergent moments and metal-insulator transition in charge density wave heterostructures 1T-NbSe₂/1T-TaX₂

A. Taraphder¹

¹Department of Physics, IIT Kharagpur, West Bengal 721302

The electronic properties of charge density wave (CDW) heterostructures out of monolayers of 1T-NbSe₂ and 1T-TaX₂ (where, X = S and Se) are explored using first-principles and dynamical calculations. The CDW-ordered crystal structures are simulated using $\sqrt{13} \times \sqrt{13}$ supercells of NbSe₂ and TaX₂ by stacking monolayers of NbSe₂ and TaX₂ along (001) direction. Our investigations reveal a non-zero magnetic moments in NbSe₂/TaS₂, albeit without a long-range magnetic order, raising the issue of a possible quantum spin liquid (QSL) as suggested also for monolayer 1T-TaS₂ recently. In contrast, the NbSe₂/TaSe₂ heterostructure exhibits no magnetic moment. In order to capture the dynamical effects of local correlation, we use DFT plus multi-orbital dynamical mean field theory (MO-DMFT), as implemented in TRIQS. Our findings indicate that NbSe₂/TaS₂ is influenced considerably by the dynamic corrections, whereas NbSe₂/TaSe₂ shows no significant effects. Additionally, our preliminary results suggest Mott transition (MT) in the NbSe₂/TaS₂ heterostructure at a reasonable strength of correlation.

Reference:

1. Shubham Patel and A. Taraphder, arXiv:2410.00600

Bio of the Speaker: Arghya Taraphder earned his B.Sc. Honours in Physics from Presidency College, West Bengal followed by M.Sc. from Calcutta University and Ph.D. from the Indian Institute of Science, Bangalore in 1991. He was a postdoctoral fellow at Rutgers University and the NEC Research Institute, Princeton, USA. He has also served as a visiting scientist and visiting professor at several institutions, including the Max Planck Institute for Physics of Complex Systems in Germany, Michigan State University, ICTP Trieste, CSIC, ICMM Madrid and University of Neuchatel, Switzerland. His primary research interests are in correlated and disordered quantum matter and related systems.

Currently, he is a professor in the Department of Physics at the Indian Institute of Technology (IIT) Kharagpur, where he was also affiliated to the Centre for Theoretical Studies and the Centre for Nanoscience and Nanotechnology. His work includes studies on the chiral anomaly and planar Hall effect in Weyl semimetals, investigations on the possible excitonic liquids in transition metal dichalcogenides, emergent properties in interfaces and heterostructures, CMR systems and High T_c.

In addition to his research, Dr. Taraphder serves as a referee for many esteemed journals, including those published by the American Physical Society (PRL, PRB, RMP) and the Institute of Physics (Europhysics Letters, JPCM, NJP, EPJB), among others such as Solid State Communications, Pramana, JMMM, and IJMPB.



$K_2Ni_2(SO_4)_3$: A quantum spin liquid under thin ice

Yasir Iqbal¹, Matías G. Gonzalez^{2,3}, Vincent Noculak^{2,3}, Aman Sharma⁴, Virgile Favre⁴, Jian-Rui Soh⁴, Arnaud Magrez⁵, Robert Bewley⁶, Harald O. Jeschke^{7,1}, Johannes Reuther^{2,3,1}, Henrik M. Rønnow⁴ and Ivica Živković⁴

¹Department of Physics and Quantum Centre of Excellence for Diamond and Emergent Materials (QuCenDiEM), Indian Institute of Technology Madras, Chennai, 600036, India

²Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109, Berlin, Germany

³Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195, Berlin, Germany

⁴Laboratory for Quantum Magnetism, Institute of Physics, École Polytechnique Fédérale de Lausanne, CH-1015, Lausanne, Switzerland

⁵Crystal Growth Facility, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

⁶ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0QX, UK

⁷Research Institute for Interdisciplinary Science, Okayama University, Okayama, 700-8530, Japan

Quantum spin liquids (QSLs) have become a key area of research in magnetism due to their remarkable properties, such as long-range entanglement, fractional excitations, and topologically protected phenomena. Recently, the search for QSLs has expanded into the three-dimensional world, despite the suppression of quantum fluctuations due to high dimensionality. A new candidate material, $K_2Ni_2(SO_4)_3$, belongs to the langbeinite family and consists of two interconnected trillium lattices. Although magnetically ordered, it exhibits a highly dynamical and correlated state. In this work, we combine inelastic neutron scattering measurements with density functional theory (DFT), pseudo-fermion functional renormalization group (PFFRG), and classical Monte Carlo (cMC) calculations to study the magnetic properties of $K_2Ni_2(SO_4)_3$, revealing a high level of agreement between experiment and theory. We further reveal the origin of the dynamical state in $K_2Ni_2(SO_4)_3$ to be centred around a magnetic network composed of tetrahedra on a trillium lattice.

References:

1. *Nature Communications* 15, 7191 (2024)

Bio of the Speaker: Yasir received his M.Sc from Indian Institute of Technology (IIT) Madras and Ph.D. from University of Toulouse, France. He conducted his postdoctoral research at the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste and University of Würzburg, Germany, before joining as faculty at the physics department of IIT Madras in 2017. He is a Simons associate of the ICTP and Faculty associate of the International Centre for Theoretical Sciences, Bangalore. His research spans topics in frustrated magnetism centered around spin liquids, symmetry classification schemes, and development and application of numerical quantum many-body approach.



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

Abir De Sarkar¹

¹Institute of Nano Science and Technology, Sector 81, Knowledge City, Manauli
Mohali, Punjab-140306

Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the materials. HfN₂ monolayers [1] exhibit valleytronic properties complementary to that in single-layer MoS₂, 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 MoS₂/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].

References:

1. M. K. Mohanta, A. De Sarkar, *Phys. Rev. B*, 102, 125414 (2020).
2. A. Arora, S. Sharma, A. De Sarkar, *J. Appl. Phys.*, 136, 124301 (2024).
3. R. Ahammed, A. De Sarkar, *Phys. Rev. B*, 105, 045426 (2022).
4. A. Arora, A. Rawat, A. De Sarkar, *Phys. Rev. B*, 107, 085402 (2023).
5. H. Seksaria, A. Kaur, A. De Sarkar, *Phys. Rev. B*, 108, 075426 (2023).
6. N. Tripathy, A. De Sarkar, *Phys. Rev. B*, 109, 125414 (2024).

Bio of the Speaker: Prof. Abir De Sarkar has been serving the Institute of Nano Science and Technology, Mohali as Senior Professor. In the realm of Computational Nanoscience, Prof. De Sarkar pursues research on two-dimensional materials for energy conversion and futuristic electronics. He has been recognized as the world's top 2% Scientist by Stanford-Elsevier and top 0.48% by ScholarGPS. Prof. De Sarkar has been the recipient of the President of India, medal for the year 2000 for having topped all the postgraduate disciplines in Calcutta University. The CNR Rao Award for Excellence in Nano research for the year 2018 was conferred upon him in appreciation of his work on 2D materials.

American Chemical Society has recognized him in the top 3% of highly cited authors for 2019-2020, while the Top Cited Paper Award 2023 has been conferred upon him by IOP Publishing, UK. He has also been recognized as an outstanding reviewer for 2023 by Nanoscale and JPCM. Prof. De Sarkar has published more than 120 papers in leading international journals and acquired an h-index of 36.

He has guided 6 scholars to the successful completion of their PhD. The first 5 scholars have secured h-index ~ 13 from their PhD work



Antiferromagnetic Skyrmions for Spintronic Applications

^{1,2}Mallick, S., ³Panigrahy, S., ⁴Ye, P., ¹Sassi, Y., ¹Prestes, N. F., ¹Krishnia, S., ¹Gallego, F., ¹Arche, L. M. V., ⁴Denneulin, T., ¹Collin, S., ¹Bouzehouane¹, K., ³Thiaville, A., ⁵Dunin-Borkowski, R.E., ⁴Boutu, W., ¹Bibes, M., ⁶Viret, M., ³Jeudy, V., ³Rohart, S., ¹Fert, A., ¹Reyren, N., and ¹Cros, V.

¹Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, France

²Department of Physics and Nanotechnology, CET, SRMIST, Kattankulathur, India

³Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, France

⁴Université Paris-Saclay, CY Cergy Paris Université CEA, LIDYL, France

⁵Forschungszentrum Jülich, ER-C for Microscopy & Spectroscopy with Electrons, Germany

⁶SPEC, CEA, CNRS, Université Paris-Saclay, France

Magnetic skyrmions, spin swirling particle like entities, have been in the focal point of many research in condensed matter physics due to their solitonic nature combined with chiral and topological properties. The main challenge for their practical application is ensuring room temperature stability and high mobility without unwanted transverse deviation (skyrmion Hall effect: SkHE). Achieving thermal stability typically requires multi-layered structures, which introduce dipolar coupling and enlarge skyrmions. [1] Other challenges include energy dissipation, non-optimized spin torques, and domain wall pinning, which all hinder skyrmion mobility. A promising solution is using antiferromagnetically coupled sub-layers, such as synthetic antiferromagnets (SAFs) or synthetic ferrimagnets, which ensure reduction in skyrmion size and SkHE due to neutralized magnetization and angular momentum [2, 3].

In the present work, we have delved into both SAF and ferrimagnetic multilayers to enhance skyrmion mobility while maintaining their steadfast stability. In the first part of the presentation, I will demonstrate the innovative techniques we have employed to stabilize and manipulate skyrmions electrically in SAFs without the need for an external magnetic field. [1, 4] This simultaneously simplifies device architecture and facilitates downsizing of these devices. In the second part, I will highlight the solitonic nature of these skyrmions, focusing on their efficient electrical nucleation and motion. Finally, I will show that stable, compact skyrmions in synthetic ferrimagnets can be driven in the viscous flow regime under the influence of spin-orbit torques. By simultaneous control of antiferromagnetic coupling, interfacial DMI, spin-orbit torques, and domain wall pinning of the heterostructure, we could achieve the skyrmion velocity up to 400 m/s for skyrmions with diameters ~160 nm and below while moving them in a straight trajectory. [5]

References:

1. S. Mallick et al., *Phys. Rev. Appl.* 18, 064072 (2022)
2. S. Panigrahy, S. Mallick et al., *Phys. Rev. B* 106, 144405 (2022)
3. L. Berges, S. Mallick et al., *Phys. Rev. B* 106, 144408 (2022)
4. S. Mallick et al., *Adv. Func. Mater.* 2409528 (2024)
5. S. Mallick et al., *Nat. Commun.* 15, 8472 (2024)

Bio of the Speaker: Dr. Sougata Mallick is presently an Assistant Professor (Research) at SRMIST, Kattankulathur. He earned his Ph.D. in magnetism from NISER, Bhubaneswar, and was honoured with the prestigious Outstanding Doctoral Student Award from HBNI for his thesis. Dr. Mallick pursued postdoctoral research at two of the most prestigious research groups in spintronics: Laboratoire de Physique des Solides and Laboratoire Albert Fert in Université Paris-Saclay, France. His research is focused on spintronics, particularly in skyrmions and spin-orbit torques. He has made pioneering contributions to the field of skyrmion research, demonstrating their controlled manipulation at zero magnetic field and achieving high velocities while maintaining stability and compact shapes.



Solution Processed Solar Cells- A glimpse of Organic and Perovskite Solar Cells

Manoj A. G. Namboothiry¹

¹School of Physics, Indian Institute of Science Education and Research (IISER TVM),
Thiruvananthapuram - 695551

Solution-processed semiconductors play a crucial role in developing flexible and roll-to-roll processed solar cells. However, the optical and electrical properties of the semiconductors are a matter of debate especially when they are in contact with other materials. Organic semiconductors and perovskites are the current leading solution-processed semiconductors and many research groups are working on the devices based on these systems. In this aspect, I will discuss on both organic and perovskite solar cells, the efficiency limiting factors and the current challenges. Various device characterization techniques like current-voltage measurements, external quantum efficiency measurements, and impedance and transient spectroscopies used to probe the charge carrier dynamics of the device and further correlation of the performance to the morphology will be discussed.

References:

1. Yousuf Alishan, Alvin Joseph, Anitha B Pillai, Ravari Kandy Aparna, Renjini Sarkar, Sudip Chakraborty, Sukendu Mandal, Manoj A. G. Namboothiry, Metal nanoclusters for interface engineering and improved photovoltaic performance in organic solar cells, *ACS Nano* **2024**, <https://doi.org/10.1021/acsnano.4c12256>
2. Akhil Alexander, Vishnupriya P Kamalon, Vivek V Dev, Muhammed Raees A, Sidharth Reghunathan, Pradeep R Nair, Manoj AG Namboothiry, Enhancing the efficiency and stability of perovskite solar cells through defect passivation and controlled crystal growth using allantoin, *ACS Applied Materials & Interfaces* **15 (2024)** 58406-58415

Bio of the Speaker: Prof. Manoj A. G. Namboothiry is currently a professor at School of Physics, Indian Institute of Science Education and Research (IISER TVM), Thiruvananthapuram, Kerala. He did his PhD from JNCASR, Bangalore. He has long been associated with research in the area of photovoltaic devices involving organic, organic-inorganic hybrid materials and nanocomposites. His research work is focused on making devices such as solar cells, light emitting diodes, field effect and phototransistors, and memory devices. Incorporation of plasmonic nanostructures, photocurrent spectroscopy, conducting polymer/biomolecular interface for biosensor applications are major areas of focus of his group. His current interests are in studying the photophysical and electrical properties of photovoltaic devices to understand how to improve the efficiency of the devices further.



Designing Layered Halide Perovskites for Optoelectronics: Insights from *ab initio* modelling

Dibyajyoti Ghosh¹

¹Department of Materials Science and Engineering and Department of Chemistry
Indian Institute of Technology, Delhi, India

Accelerated materials designing for light emission applications are in high demand. However, complex and interdependent structure-property-performance relations strongly limit the directed search and discovery of efficient materials. To tackle these challenges, we apply cutting-edge computational simulations that are invaluable for understanding and manipulating the functionalities and performances of a wide range of energy materials. In this talk, first I will discuss the details of charge carrier dynamics and recombination processes in layered metal halide perovskites that are leading contenders for next-generation optoelectronic devices. Using non-adiabatic molecular dynamics, I will illustrate the complex influences of dynamic structures on the excited-state carrier dynamics that strongly impact the optoelectronic performances of these materials [1-4]. Following that, my talk will focus on data-driven approaches that substantially accelerate the materials selection process for novel layered halide perovskites.[5] We will illustrate the significant influences of spacer inorganic cations on the carrier transport and recombination processes in these materials.

References:

1. Nayak et al. *J. Mater. Chem. C*, **2023**, 11, 3521
2. Ghosh et al. *J. Mater. Chem. C*, **2022**, 10, 9563
3. Ghosh et al. *J. Mater. Chem. A* **2020**, 8, 22009
4. Ghosh et al. *J. Phys. Chem. Lett*, **2020**, 11, 2955
5. Bhatt et al. *ACS Nano*, 2024, 18, 24484

Bio of the Speaker: Dibyajyoti finished his Master's in Science degree in 2012 from JNCASR Bangalore and joined the Theoretical Sciences Unit of the same institute to undertake his Ph.D under Prof. Swapan K Pati. He completed his Ph.D. in 2016 and moved to University of Bath, UK as a post-doctoral research associate for two years. He worked with Prof. Saiful Islam and Prof. Alison Walker there. Following that, from November 2018 to July 2021, Dibyajyoti was a research associate at Los Alamos National Laboratory, USA. His mentors were Dr. Sergei Tretiak and Dr. Amanda Neukirch. He joined the IIT Delhi as an assistant professor in July 2021. Dibyajyoti's group employs high-level computational simulations to investigate and manipulate the energy conversion and transport processes in optoelectronic, photocatalysts, and spintronic materials. With this fundamental knowledge, the group further applies statistical models for *in-silico* designing and the discovery of efficient environment-friendly materials for targeted applications.



Gallium Oxide Thin Film based Solar-Blind Photodetectors: Heterojunctions and Interface Engineering

Mukesh Kumar¹

¹Department of Physics, Indian Institute of Technology Ropar, Rupnagar, Punjab - 140001

Solar-blind photodetectors are an emerging technology for forest fires, territory intrusions, ozone hole monitoring, deep space exploration, satellites, and security communication [1]. A photodetector working in the <280 nm, solar-blind region, could minimize the chances of false radiation detection even under intense sun interference on the earth's surface by detecting ozone layer filtered deep UV (UV-C) terrestrial signatures. Here, we demonstrated an ultrahigh-performance and self-powered β -Ga₂O₃ thin film solar-blind photodetector fabricated on a cost-effective Si substrate using a high-temperature seed layer (HSL). The Ag nanoparticle decorated β -Ga₂O₃ photodetector exhibits a change in the polarity of the photocurrent for different UV bands. The photodetector shows a record responsivity of 250 A/W. The current reversal is rationalized by considering the charge dynamics stemming from hot electrons generated when the incident light excites a local surface plasmon resonance in the Ag nanoparticles. Paper based super-flexible, non-wettable, self-powered and high-voltage stable amorphous gallium-oxide photodetector is also fabricated and investigated in detail. The heterostructures of gallium oxide with different materials like CdS and MoS₂ are investigated for efficient charge transport. The gallium oxide thin films and grown photodetector is also investigated against extreme environment conditions for their space applications.

References:

1. Damanpreet et al. *Advanced Optical Materials*, **2021**, 9, 2002160
2. Kanika et al. *ACS Photonics*, **2018**, 5, 2391
3. Kanika et al. *Advanced Optical Materials* **2020**, 2000212
4. Kanika et al. *J. Physics D: Applied Physics*, **2019**, 52, 335103
5. Damanpreet et al. *J. Applied Physics* **2020**, 128, 065902
6. Riya et al. *Applied Surface Science* 632 (**2023**) 157597
7. Damanpreet et al. *Applied Physics Letters* **2024**, 124, 151601

Bio of the Speaker: Dr. Mukesh Kumar is an Associate Professor in the Department of Physics, IIT Ropar. He did his M.Tech. and Ph.D. in Physics from IIT Delhi, India. He worked as a postdoctoral fellow at National Renewable Energy Laboratory, CO, USA and South Dakota State Uni., SD, USA from 2010 to 2013 on nanoscale charge transport of organic solar cells and flexible thin films for next generation flexible optoelectronic devices. Before joining IIT Ropar, Dr. Kumar was working for Hysitron Inc., MN, USA. Dr. Kumar has published two book chapters, nine review articles and total more than 80 research articles in peer reviewed journals like *Energy Environmental Science*, *ACS Photonics*, *ACS Sensors*, *Applied Physics Letters*, *Small* and *Advanced Optical Materials*. Dr. Kumar has received many national and international awards like, Young Scientist Research Award from DAE, India; Bhaskara Advanced Solar Energy Fellowship from Indo-US Science and Technology Forum (IUSSTF); Faculty Research and Innovation Award, IIT Ropar. Recently, he received JSPS and prestigious Fulbright-Nehru Academic and Professional Excellence Fellowship. Dr. Kumar is a selected member of Indian National Young Academy of Science (INYAS), National Academy of Sciences, India (NASI) and Fellow of Institute of Physics (IOP). His research interest includes functional and renewable energy materials for optoelectronics and photovoltaics applications.



Density functional theory-based study of interaction of oxygen, hydrogen and water with CuInSe₂ thin-film solar-cell material

Sudhir K. Sahoo^{1,2} and Thomas D Kühne²

¹Department of Chemistry, Indian Institute of Technology Dharwad, Karnataka-580008

²Department of Chemistry, University of Paderborn, Germany

Cu (In,Ga)Se₂ (CIGS) is used as the absorber material in the highly efficient thin-film solar cell. It has been reported that the introduction of alkali metal impurities by post-deposition methods improves the efficiency of the solar cell, the world record efficiency of 23.04% is due to the treatment of Cs-metal atoms. The point defects play an important role in the semiconductor properties which eventually affect the efficiency of the solar cell. Apart from that the CIGS also undergoes various post processing methods which can introduce the defects due to elements like oxygen, hydrogen, water etc. We employed the density functional theory-based computations to study various point defects in CuInSe₂ materials. Our calculations suggest that the most stable H-point defect is when it replaces Cu-atom from its lattice whereas, in the case of O-point defects it prefers the Se-site. Further, we studied the interaction of water with CuInSe₂ surfaces with and without defects. Our calculations suggest that the water molecule prefers to adsorb molecularly rather than dissociatively in both the surfaces. Also, the defective surface needs to be calcined at a higher temperature as compared to a surface without defects to get the clean surfaces. The study is further extended to see the interaction of oxygen with the surface in collaboration with the experiment. Our DFT calculations confirm that the oxygen atoms prefer to diffuse into the subsurface layer from the surface. Since the oxygen atoms are having higher electronegativity, the electron density is accumulated over these atoms, which qualitatively explains why there is net dipole moment as observed in the experiment.

References:

1. Elizabeth et al. *ACS Applied Materials & Interfaces* **2022**, 14, 29, 34101–34112
2. Elizabeth et al. *Acta Materialia* **2020**, 200, 463-470
3. Elizabeth et al. *Physical Review Materials* **2020**, 4, 063401
4. Sahoo et al. *The Journal of Physical Chemistry C* **2018**, 122, 37, 21202-21209

Bio of the Speaker: Dr. Sudhir Kumar Sahoo

Assistant Professor, Department of Chemistry, Indian Institute of Technology Dharwad Experience: Assistant Professor (December 2022-Continuing), Department of Chemistry Indian Institute of Technology, Dharwad Postdoctoral researcher (April 2017-June 2021) Department of Chemistry, University of Paderborn Germany Education: PhD Computational Chemistry 2017 Department of Chemistry, Indian Institute of Technology, Kanpur PhD supervisor: Prof. Nisanth N. Nair MSc Chemistry (2010) Department of Chemistry, National Institute of Technology Rourkela



Excitations in semiconductors: phonon-driven phenomena

Bartomeu Monserrat¹

¹University of Cambridge, United Kingdom

Modelling the ground state properties of materials has reached predictive power over the past few decades, mostly driven by density functional theory. However, many material properties of interest appear beyond the ground state, with examples including finite temperature and electronic excitations. In turn, these play a key role in many technologies, such as light emitting diodes and solar cells.

In this talk, I will describe our work in modelling electronic excitations at room temperature. I will describe the methodology we use to describe excitons, electron-hole bound pairs that form upon photoexcitation, and their interaction with phonons. I will then provide a few examples of our recent work, highlighting exciton-phonon coupling in organic and inorganic semiconductors, and topological excitons. With each example, I will describe complementary experiments and reflect upon the interplay between theory and experiment in modelling semiconductors.

References:

1. *Nature* 629, 355 (2024)
2. *Phys. Rev. B* 102, 081122 (2020)
3. arXiv:2408.13905
4. arXiv:2406.11951

Bio of the Speaker: Bartomeu Monserrat is Professor of Materials Physics at the Department of Materials Science and Metallurgy of the University of Cambridge. He obtained a MSci in Physics from Imperial College London in 2011 and a PhD in Physics from the University of Cambridge in 2015. He then held research positions at Rutgers University (2015-17) and Cambridge (2015-19), and joined the faculty at Cambridge in 2020. Bartomeu leads a research group that develops and uses computational tools based on quantum mechanics to discover new materials. His work spans a wide range of materials and phenomena, including topological materials, superconductors, semiconductors for optoelectronic applications, and materials under extreme pressure conditions.



His scientific contributions have been recognised with multiple awards, highlighting the international Psi-K Volker Heine Young Investigator Award, the Maxwell Medal and Prize by the UK Institute of Physics, and the Young Investigator Award in Theoretical Physics by the Spanish Royal Society of Physics. Beyond research, Bartomeu is the creator and co-host of a [YouTube channel](#) teaching quantum mechanics to a global audience. The channel has over 25,000 subscribers and has received more than 1.5M views.

Generalized Dielectric-Dependent Hybrids: A New Computational Window for Bulk to Nano-structured Quantum Materials

Prasanjit Samal¹, Arghya Ghosh², Dimple Rani¹, Abhishek Bhattacharjee¹, and Subrata Jana³

¹School of Physical Sciences, National Institute of Science Education and Research,
An OCC of Homi Bhabha National Institute, Bhubaneswar 752050, India

²Department of Physics, Indian Institute of Technology, Hyderabad, India

³Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University in Torun, ul. Grudziadzka 5, 87-100 Torun, Poland

Density functional theory (DFT) is often the go-to computational method for solving the electronic structure problems of solids and materials. Although it is an exact theory, one must approximate the exchange-correlation (XC) part, which includes all the many-body interactions. The development of new XC approximations that have insightful physical content and are also accurate and efficient for solids is always desirable. Nevertheless, accurate density functionals approximations are also always the starting point of machine-learning-based functional developments, automated, and high-throughput computational workflow for solids and materials. In my talk, I discuss how our proposed new generation dielectric-dependent hybrid density functional approximations improve both the ground state and excited-state properties of materials. I will discuss the potentiality of these methods to substitute the higher-level state-of-art methods proposed from many-body perturbation theory. Lastly, I will discuss the future directions of further developments and challenges of these methods for spectroscopic properties, including phenomena related to the light-matter interactions¹⁻⁵.

References:

1. S. Jana, A. Ghosh, L. A. Constantin, and P. Samal, *Phys. Rev. B* 108, 045101 (2023)
2. A. Ghosh, S. Jana, D. Rani, M. Hossain, M. K. Niranjana, and P. Samal, *Phys. Rev. B* 109, 045133 (2024)
3. A. Ghosh, S. Jana, D. Rani, P. Samal, M. K. Niranjana (2024) [under communication]
4. S. Jana, A. Ghosh, A. Bhattacharjee, P. Samal, (2024) [under communication]
5. S. Jana, A. Bhattacharjee, P. Samal, S. Smiga (2024) [under preparation]

Bio of the Speaker: He has obtained his PhD in Physics from I.I.T. Kanpur. Then joined as a postdoctoral fellow jointly in the Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science of the University of Minnesota. He is currently working as a faculty member in the School of Physical Sciences of NISER, Bhubaneswar, where his group research focuses on various aspects of quantum materials simulations using density functional theory, machine-learning, high-throughput computational workflow, and many-body perturbation methods. He is a density functional theorist and quantum many-body physicist who works on varied range of trending research topics encompassing methodological developments through cutting edge applications.



THz magnon spintronics with non-collinear antiferromagnets

Dhanvir Singh Rana¹

¹Department of Physics, Indian Institute of Science Education and Research (IISER) Bhopal, India

The terahertz (THz) spectrum (0.1-10 THz) offers promising opportunities in the development of next-generation data processing and quantum memory technologies. These aspirations are driven by simultaneous developments in the THz spectrum and, the area of spintronics, magnonics, caloritronic, and many more. In magnetic systems, magnons- the quanta of spin waves-in a spin ordered state envisage the prospects of non-Boolean-based spin wave computation, magnon logic gates, and so on. However, magnonics has been widely explored in ferromagnets resulting in gigahertz magnons. However, the area of magnonics can be extended to ultra-low dissipation and ultrafast THz region as the antiferromagnets have magnons in this region. This offers THz radiation-based tools play a prominent role in exploring the technological utility of antiferromagnets which, so far, have played only a passive role in the emergence of magnetic devices. The THz radiation mainly couples with the magnetic-dipole moment of the spins unveiling not only the low-energy antiferromagnetic magnons but also its interplay with distinct quasiparticles such as phonons, photons, polaritons, and many more. Recently, for the first time, magnons sum and difference generation was demonstrated in YFeO₃, thus, raising the importance of algebraic operations of different THz frequency magnons. This study necessitates the exploration of antiferromagnets possessing closely spaced magnons in terahertz region (0.1-2 THz) for their potential in THz magnon algebraic logic operations. Such control over spin-waves/magnon can be contemplated in magnetoelectric/multiferroic systems, in which the spin and electric orders are entangled, resulting in electric as well as magnetic control of magnons.

In this work, I'll present our recent work in exploration of a variety of non-collinear magnets for magnon and magnon- phonon excitation modes in the THz spectral region, considering two examples. First, I'll show that A₄B₂O₉ (A=Co and B=Nb, Ta) family of non-collinear magnetoelectric antiferromagnetic exhibit i) a multitude of low-energy antiferromagnetic resonances comprised of magnons, phonons, and hybridized spin-phonon coupled modes and ii) the notion of beyond conventional magnon, that is, electromagnon. The second example is based on RCrO₃ (R=rare-earth) orthochromates in which weak magnetic moment is accompanied by sub-THz magnon modes along with complex crystal-field excitations.

Bio of the Speaker: Dhanvir Singh Rana is currently a professor at the Indian Institute of Science Education and Research (IISER) Bhopal, where he joined as faculty in 2009. He studied for Bachelor of Sciences at Himachal Pradesh University Shimla, India, and for Master of Sciences and Ph.D. in physics at Saurashtra University Rajkot, India; followed by a postdoctoral fellowship at TIFR Mumbai, India, and JSPS postdoctoral fellowship in Tonouchi lab at Osaka University, Japan. He is recipient of NASI Young Scientist Award for the year 2011. His research interests are THz spectroscopy and its applications in emergent quantum matter; antiferromagnetic spintronics, transport and magnetism of complex transition metal oxides thin film heterostructures, topological systems, etc.



In search of bulk Rashba ferroelectric semiconductor for spintronics applications

Amrita Bhattacharya¹, and Krishnaraj Kundayu²

¹Department of Metallurgical Engineering and Materials Science,
Indian Institute of Technology, Bombay, Mumbai-400076, Maharashtra, India

Ferroelectric perovskite oxides are known for their excellent technological applications such as in spintronics research i.e. as spin control devices. One such manifestation of spin control can be seen in Rashba-Dresselhaus effect in non-magnetic insulators with broken inversion symmetry. This phenomenon of spin splitting in the momentum space if it occurs in the band edges can help in realising the spin field effect transistor devices. To achieve the spin control via switching of gate voltage, existence of ferroelectric polarisation in the material is necessary. This has led to a lot of research on ferroelectric Rashba semiconductors (FERSC) and formulation of design principles necessary to search for such materials. Using first principles density functional theory based methods, we analyse the Iodate perovskites viz. AIO_3 , $\text{A}=\text{K}$, Rb , Cs , and Tl in non-centrosymmetric rhombohedral phases ($R3m$). More specifically, we study the effect of A cation in the Rashba spin splitting by taking into the account of atomic as well as geometric relaxation, spin polarization, and spin orbit coupling. Our study reveals that the Rashba splitting is inversely proportional while the band gap is directly proportional to the ionic radii of the A cation [1]. We also employ the similar analysis to identify Rashba phases in Bi based perovskites BiMO_3 ($\text{M} = \text{Al}$, Ga , In , Fe , Co , Sc , La), which reveal several exotic features. Our study also reveals persistent spin textures in BiInO_3 suitable for spin-channel applications.

References:

1. Momentum-space Spin Splitting in non-Centrosymmetric Iodate Perovskites, Krishnaraj Kundavu, and Amrita Bhattacharya, *Phys. Rev. B*, 110 (13), 134104 (2024).
2. Emergence of Rashba-Dresselhaus effect and exotic spin textures in Bi based oxide perovskites, To be communicated.

Bio of the Speaker: Amrita is currently working as an associate professor in the Metallurgical Engineering and Materials Science Department of IIT Bombay, where she has joined in December 2017. The main thrust of her research group is to employ different ab initio techniques to predict physical properties of solid-state materials, whereby she also uses density functional theory-based methods to analyze materials properties for their quintessential applications in the field of thermoelectrics, permanent magnet, correlated materials and spintronics. She has been elected as a member of National academy of Science India in 2020. She has already received several external research grants in form of DST inspire faculty award, early career research award, BRNS regular grant etc. In recognition of her research work, she has been awarded with Young Investigator Award 2020, and C-1973 research award 2023 by IIT Bombay and ACCMS and AFORD sponsored Young Woman Computational Physicist Award in National Physicists' Conclave 2024.



CAMMD Database on Electrochemical Energy Storage Materials

Satyesh Kumar Yadav^{1,2}, Vinod Sarky^{1,2}, Shivangi Keshri¹, Mannan Vali¹

¹Center for Atomistic Modeling and Materials Design, Indian Institute of Technology Madras, Chennai, Tamil Nadu 600036, India

²Department of Metallurgical and Materials Engineering, Indian Institute of Technology (IIT) Madras, Chennai 600036, India.

Several materials are reported every day that could be used in electrochemical energy storage devices. It becomes very challenging to effectively compare the performance of emerging new materials due to variation in reporting and testing procedures followed across various research groups. We developed a framework that could effectively rank performance of materials (in anode, cathode, electrolyte, separator), in various testing and processing conditions, which are substantial for a well-founded comparison. The framework enables storage of data from both experimental and theoretical/computational sources (such as DFT and ML predictions), facilitating effective comparison between them. The data extracted from publication and patent and provided by authors are stored in the database. The data extraction and curation is done by admin/editors specialized in material science and tools of data extraction. This framework benefits the contributors by organizing their vast data into a clear, structured format, ensuring easy access and long-term preservation. Web-interface for search, storage and download of data is developed.

Bio of the Speaker: Dr Satyesh Kumar Yadav is associate professor in Department of Metallurgical and Materials Engineering department at IIT Madras, he joined the department in December 2016. He completed his PhD from the University of Connecticut in 2013. He was a postdoctoral fellow at Los Alamos National Laboratory from 2013 to 2016. He earned his B.Tech degree from IIT Roorkee in the year 2008. He heads the Materials Design lab, which aims to design materials by understating the processing-structure-property relationship at the atomic level. He introduced a course on Atomistic Modelling of Materials. The course has been helping students to learn how to model materials as a set of atoms using quantum mechanics-based density functional theory (DFT).



Influence of Slurry Rheology on Electrode Laminate Properties for Enhanced Lithium-Ion Battery Performance

Sahana M. B¹, Mahender Peddi¹, Kumari Konda¹ Jyoti R. Seth², Vinay A. Juvekar², and Raghavan Gopalan¹

¹Centre for Automotive Energy Materials, International Advanced Research Centre for Powder Metallurgy and New Materials, IITM Research Park, Kanagam, Taramani, Chennai-600113, India.

²Department of Chemical Engineering Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076

The performance of lithium-ion batteries (Li-ion) is intricately linked to the structure and composition of electrode laminates, which are influenced by the slurry preparation process. This study investigates how the rheological properties of slurries composed of active materials, conductive additives, and binders affect the electrochemical performance of the batteries. By analyzing LiFePO₄-CB and LiNiCoMnO₂ (NMC) slurries, we demonstrate that the mixing sequence significantly impacts laminate properties such as porosity, tortuosity, and electronic connectivity. Our findings reveal that for LiFePO₄, with its nanometric particle size, pre-mixing carbon black with active material enhances conductivity and electrochemical performance. In contrast, for NMC with a nano-micro hierarchical structure, the mixing sequence must be tailored to the application: pre-mixing is advantageous for high-power demands, while sequential mixing improves energy density. This work highlights the importance of optimizing slurry rheology and mixing protocols to achieve the desired balance between power and energy performance in lithium-ion batteries.

References:

1. Capacity degradation of lithium-ion cell: The role of free carbon black content in the slurry and drying induced cracks in LiFePO₄ electrode, Kumari Konda et al *Journal of Energy Storage* 74 (2023) 109477
2. Effects of Nano-Micro Hierarchical Architecture Intraparticle Connectivity and Carbon Black-LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ Interaction: An Energy-Power Tradeoff In Lithium-Ion Batteries, Mahender et al *Journal of The Electrochemical Society*, 169, 020576

Bio of the Speaker: Dr. M B Sahana is a senior scientist at the Centre for Automotive Energy Materials, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI). She holds a Ph.D. from Indian Institute of Science (IISc), Bangalore, where she specialized in materials science. Following her doctoral work, Dr. Sahana completed postdoctoral research at Stockholm University, Sweden, and Wayne State University, Detroit, USA, focusing on advanced energy materials and electrochemical systems. Currently, her research is dedicated to the development of lithium-ion battery materials and technology for electric and hybrid electric vehicles. She has made significant contributions to scalable synthesis techniques for cathode materials, including LiFePO₄ (LFP) and nickel-rich oxides (NMC, NCA). Dr. Sahana has guided 4 PhD students and numerous MTech and MSc projects, authored multiple peer-reviewed publications, and played a key role in bridging the gap between laboratory-scale research and industrial applications.



Developing an in-depth understanding of promising electrode materials for the Li and Na-ion batteries

Ummar Bhat¹, Zubair Nabi¹, Dwaipayan Chakraborty¹, Nicola Seriani², Priya Johari^{1*}

¹Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Greater Noida, Gautam Buddha Nagar, Uttar Pradesh – 201314 India;

²Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy

priya.johari@snu.edu.in

The development of computational resources and methodologies has become a cornerstone in the quest to reliably predict promising electrode materials for rechargeable batteries, offering a cost-effective and time-efficient alternative to traditional experimental methods. These advancements provide valuable insights for experimentalists, guiding efforts to enhance battery performance and pave the way for next-generation, energy-efficient batteries with improved capacity and energy density, crucial for grid storage and electric vehicles. In this context, we employ first-principles density functional theory and evolutionary algorithms to conduct a comprehensive investigation of various materials. Our aim is to gain an atomistic-level understanding of the reaction mechanism and identify efficient electrode materials for Li-ion and Na-ion batteries, contributing to the evolution of cutting-edge energy storage technologies.

Bio of the Speaker: Prof. Priya Johari from Shiv Nadar University is an established researcher in India who has been working in the area of computational material science and quantum mechanical simulations for more than 15 years. Her major interest lies in studying materials that hold promise in enhancing the technology specifically in the field of energy storage/generation, opto-electronics, environment, and bio-medical. This includes prediction and rational designing of novel materials and extensive study of the known potential materials and their properties, as well as search for possible ways to tune their properties. Her group--Computational Materials Physics, actively collaborates with various experimental groups within and outside SNU.



Non-Local Interactions Governing the Local Structure and Properties of Battery Materials

Swastika Banerjee¹, Shweta Chaudhary¹, Saumya Ranjan Mahanta, Vikas Singh Thakur¹

¹Department of Chemistry, Indian Institute of Technology Roorkee, Uttarakhand-247667, India

Solid-state batteries, utilizing solid electrolytes (SEs) in place of liquid counterparts, hold significant promise for delivering high energy density and enhanced safety. However, achieving sustainability and scalability for large-scale grid storage necessitates moving beyond lithium-based systems. Designing robust battery materials, particularly SEs and compatible electrodes, remains a critical challenge. A key obstacle lies in deciphering the complex relationship between material composition and properties, which arises from intricate interactions among sublattices involving non-local electronic and nuclear dynamics. In this talk, I will present insights into electronic structure methodologies, demonstrating how a density-functional approach that incorporates non-local and many-body effects in exchange-correlation interactions enables predictive modeling of the local structure and ion diffusion properties in SEs and intercalation anodes. These findings emphasize the role of non-local electronic interactions in advancing the predictive design of solid electrolytes, electrodes, and potentially other functional materials.

References:

1. *Nat. commun.* **2021**, 12, 1, 1256
2. *J. Am. Chem. Soc.* **2022**, 144, 39, 18009
3. *J. Phys. C* **2024**, 128, 19, 7865; *Nature Commun* 2025 (just accepted)

Bio of the Speaker: Swastika Banerjee is an Assistant Professor in the Department of Chemistry at IIT Roorkee, a position she has held since March 2022. She earned her Ph.D. in Computational Materials Science from JNCASR, Bangalore, in 2017 and subsequently undertook postdoctoral research at Lawrence Berkeley National Laboratory, UC San Diego, and the University of Luxembourg. She currently leads the Computational Laboratory for Energy Application (CLEAN) at IIT Roorkee, where her research focuses on designing functional materials for energy storage, with a particular emphasis on next-generation battery technologies. Her work involves developing intercalation materials for lithium, sodium, and magnesium-ion batteries, designing solid electrolytes for solid-state batteries, and advancing computational methods for simulating materials with various applications, including catalysis, thermoelectricity, and charge transport.



Design of Functional and Sustainable Polymers assisted by Computations and Artificial Intelligence

Rampi Ramprasad¹

¹Georgia Institute of Technology & Matmerize, Inc.

Artificial intelligence (AI)-based methods and computational materials science continue to make inroads into accelerated materials design and development. Here, I will review AI-enabled advances made in the subfield of polymer informatics, with a particular focus on the design of application-specific practical polymeric materials. I will describe exemplar design attempts within a few critical and emerging application spaces, including materials designs for storing, producing, and conserving energy, and those that can prepare us for a sustainable economy powered by recyclable and/or biodegradable polymers. AI-powered workflows help efficiently search the staggeringly large chemical and configurational space of materials, using modern machine-learning (ML) algorithms to solve “forward” and “inverse” materials design problems. A theme explored throughout will be a practical informatics-based design protocol that involves creating a set of application-specific target property criteria, building ML model predictors for those relevant target properties, enumerating or generating a tangible population of viable polymers, and selecting candidates that meet design recommendations. The protocol will be demonstrated for several energy and sustainability-related applications. Finally, I will offer an outlook on the lingering obstacles that must be overcome to achieve widespread adoption of informatics-driven protocols in industrial-scale materials development.

References:

1. Huan Tran, Rishi Gurnani, Chiho Kim, Ghanshyam Pilia, Ha-Kyung Kwon, Ryan P. Lively & Rampi Ramprasad, “Design of functional and sustainable polymers assisted by artificial intelligence”, *Nature Reviews Materials* (2024)
2. Rohit Batra, Le Song and Rampi Ramprasad, “Emerging materials intelligence ecosystems propelled by machine learning”, *Nature Reviews Materials* (2020)

Bio of the Speaker: Prof. Ramprasad is the Regents’ Entrepreneur, Michael E. Tennenbaum Family Chair and Georgia Research Alliance Eminent Scholar in the School of Materials Science & Engineering at the Georgia Institute of Technology. He is also the CEO and co-founder of Matmerize, Inc. His area of expertise is the development and application of computational and machine learning tools to accelerate sustainable materials development aimed at energy production, storage and utilization. Prof. Ramprasad received his B. Tech. in Metallurgical Engineering at the Indian Institute of Technology, Madras, India, an M.S. degree in Materials Science & Engineering at the Washington State University, and a Ph.D. degree also in Materials Science & Engineering at the University of Illinois, Urbana-Champaign.

Prof. Ramprasad is a Fellow of the Materials Research Society, a Fellow of the American Physical Society, an elected member of the Connecticut Academy of Science and Engineering, and the recipient of the Alexander von Humboldt Fellowship and the Max Planck Society Fellowship for Distinguished Scientists. He has authored or co-authored over 300 peer-reviewed journal articles, 8 book chapters and 8 patents, and has delivered over 300 invited talks at Universities and Conferences worldwide. He is a member of the Editorial Advisory Boards of *npj Computational Materials*, *ACS Materials Letters* and *Journal of Physical Chemistry A/B/C*. He created and chaired the inaugural 2022 Gordon Research Conference on Computational Materials Science and Engineering.



The Quantum Materials-Neuroscience-Artificial Intelligence Interface

Shriram Ramanathan¹

¹ECE Department, Rutgers University, NJ 08854, USA

We are entering the era of quantum materials as next generation semiconductors. This is particularly interesting in the field of neuromorphic computing where highly adaptive semiconductor materials and devices are desired to emulate brain-like plasticity, learning and memory in a compact manner. In the longer term, there could be unprecedented opportunities for brain-machine interfaces. In this setting, I will describe some of our recent collaborative contributions in advancing neuromorphic hardware utilizing electric-field driven metal-insulator transitions in strongly correlated oxides, their direct interfacing with brains of awake mice for readout of synaptic transmission, and mathematical abstraction of wafer-scale electrical characteristics from devices into algorithms for energy-efficient learning in artificial neural networks. I will share experimental results wherein correlated perovskite semiconductors can demonstrate at room temperature characteristics of spin glasses that inspired early neural network models. Beyond the traditional inter-disciplinary interactions between physics and materials, I will point out why future research in quantum technologies will likely require close collaborations with neuroscience and related fields.

Bio of the Speaker: Shriram Ramanathan is the inaugural holder of the Rodkin-Weintraub Chair in Engineering at Rutgers University. Previously, he has served as a faculty member at Harvard University in Applied Physics and at Purdue University in the School of Engineering. He received his undergraduate degree from IIT Madras and PhD from Stanford University.



Computational Modeling of Semiconducting Materials for their applications in Thermoelectric and Magnetic Properties

Swapan K Pati^{1,2}

¹Theoretical Sciences Unit, School of Advanced Materials (SAMat)

²Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) Bangalore 560064

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. We also have modelled magnetic systems for finding the quantum spin liquid phase after finding the magnetic parameters and employing iterative minimization and Monte Carlo simulations. Using the BTE methods, we have computed the thermoelectric efficiency in n-type S and Te doped Ag₂Se systems and 9 Bi based half-Heusler compounds XYBi (X: Ti, Zr, Hf; Y: Co, Rh, Ir) [1]. We also have modelled TlAgSe for finding its thermal conductivity, which was synthesized and investigated experimentally [2]. I shall also discuss the possible quantum spin liquid phases in dimer-based material, Yb₂Te₅O₁₃ and hyperhoneycomb random lattices, NaYbW₂O₈ with two compositions, which were synthesized, and thermodynamical and μ -SR studies were carried out by our experimental colleague [3]. In fact, after finding the exchange constants, single ion anisotropy and biaxial anisotropy, our Monte Carlo based prediction of incommensurate phases at certain temperatures were confirmed for all the spin lattice systems. Furthermore, since the inelastic neutron scattering data is missing, we have verified our results with the experimental μ -SR data. Many more detail experimental and quantum theoretical studies are necessary to identify these as the elusive quantum spin liquid candidates.

References:

1. R. K. Biswas, S. K. Pati, Phys. Chem. Chem. Phys. (2024); S. Paul, S. Ghosal, S. K. Pati, *ACS App. Ener. Mater.* 7, 9, 595 (2024).
2. R. Pathak, S. Paul, S. Das, A. Das, S. K. Pati, K. Biswas, *Angew. Chem. Int. Ed.* 136, e202408908 (2024).
3. R. Kumar, A. J. Francis, et al. Phys. Rev. Lett. (Revision 2024); R. Kumar, A. J. Francis et. al, Phys. Rev. B (Revision Submitted 2024).

Bio of the Speaker: Professor Swapan K. Pati obtained his PhD from Indian Institute of Science, Bangalore followed by postdoctoral work at University of California, Davis, and Northwestern University, USA. He joined Theoretical Sciences Unit in JNCASR in November 2000 as an Assistant Professor and in June 2009, he became the full Professor. He has received MRSI (2006), CRSI bronze (2007) and BM Birla medals (2008); Swarnajayanthi Fellowship (2007-12), S. S. Bhatnagar award (2010) and The World Academy of Sciences award (2012). He is a recipient of J. C. Bose national fellowship in 2013, in 2018 and in 2023. He is an elected fellow of IASc (2009), NASI (2010), TWAS (2015) and INSA (2018). His research interests include designing materials for microscopic understanding and for application purposes. Some of the current projects in the lab include, modeling (i) catalytic processes for energy, (ii) Finding quantum spin liquid phase in (non) frustrated magnetic materials (iii) materials for anode/cathode for metal ion battery, (iii) generalized transport phenomena, including heat to current (thermoelectric), light to voltage (photovoltaics) and advanced transistor (FET) devices, (iv) phase transitions and new and exotic phases in dipolar Bosonic and Fermionic optical lattice systems. He is also involved in developing new theoretical tools for understanding structure–property correlations.



Exciton Dissociation by Topological Edge States

Udo Schwingenschlög¹

¹King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Exciton dissociation by edge states can enhance the power conversion efficiency of solar cells. To evaluate the potential of this mechanism for carbon nanotubes as absorber material, we show that the topology of carbon nanotubes can be characterized by winding numbers related to the orbital angular momentum. The tight-binding Hamiltonian of any carbon nanotube with CN symmetry can be represented by N tight-binding Hamiltonians of decoupled molecular chains, for which a pseudospin formulation, characterized by specific paths in a two-dimensional auxiliary space, is developed. The quantum phases are given by the N winding numbers of these paths. The paths rotate in the auxiliary space when a magnetic field of varying strength is applied along the carbon nanotube, which gives rise to quantum phase transitions.

Bio of the Speaker: Dr. Udo Schwingenschlög is a Professor of Applied Physics at King Abdullah University of Science and Technology (KAUST). Prior to joining KAUST in 2009, he worked at the International Center of Condensed Matter Physics in Brasilia, Brazil, and the University of Augsburg, Germany. His research interests in condensed matter physics and first-principles materials modeling focus on 2D materials, interface and defect physics, correlated materials, thermoelectric materials, metal-ion batteries, nanoparticles, and quantum transport.



Recent studies on spintronic and topological aspects of certain Heusler alloys

K. G. Suresh¹

¹Department of Physics, IIT Bombay

Ferromagnetic/antiferromagnetic/ferrimagnetic Heusler alloys have emerged as one of the most important classes of great interest in the fields of applied magnetism, spintronics and topological matter. Many of these alloys also show interesting thermoelectric properties such as anomalous Nernst effect as well. Among these alloys, the equiatomic alloys are particularly interesting because of diverse and exciting properties exhibited by them even with minor composition tuning. Many of these alloys exhibit very promising properties which can be exploited for applications. The inherent disorder present in these alloys often leads to electronic band structures which cause unexpected magnetic, magneto-thermal and magneto-transport properties. Of late, it has been found that many of these alloys also possess topologically protected states, spin textures etc, giving rise to considerable anomalous and topological Hall effects. Interestingly topological aspects also play a major role in some of these properties. Several novel materials and novel phenomena have been discovered as a result of extensive experimental and theoretical investigations. In this talk, I will present some of the aspects that we have studied recently on a variety of equiatomic and full Heusler alloys in which the electronic band structure was systematically tuned to synthesize novel and better materials. The talk will highlight some of the very novel aspects that have come out of our study.

Bio of the Speaker:

Educational Qualifications : PhD, IIT Madras
Professional Experience: Professor from 2011 and former Institute Chair Professor

MAJOR AWARDS/ ACHIEVEMENTS

MRSI Medal (2020)

Fellow of National Academy of Sciences, NASI (2023)

*Field of research interest : Magnetism, Spintronics,
Topological Matter*

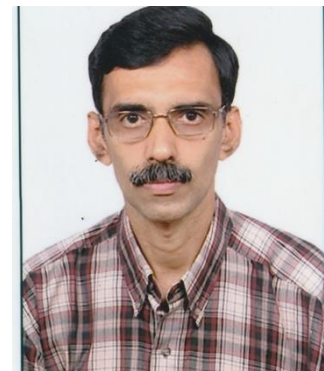
Invited Book Chapters/Invited Review articles : 3

Sponsored Projects undertaken : 15

Research Guidance : Ph. D. – 18 awarded and 3 ongoing

Papers in international journals : 245

Patents (Indian) : 1



Strategies for realizing double quantum spin Hall effect

Bahadur Singh¹

¹Tata Institute of Fundamental Research, Mumbai, India

Quantum spin Hall insulators are two-dimensional topological materials protected by time-reversal symmetry, capable of supporting a quantized spin Hall effect. A key feature of these systems is the presence of helical edge states, consisting of counterpropagating, spin-polarized modes that contribute to the quantization of spin Hall conductivity. However, perfect quantization is often hindered by spin-mixing, which arises from spin-orbit coupling or other material-specific factors. Moreover, real materials typically support no more than two helical edge states, as spin-mixing tends to gap out the edge states. In this talk, I will demonstrate how phosphorene and group Va monolayers realize atomically thin obstructed atomic insulators and transition to a state with significant spin-Berry curvature and a double quantum spin Hall effect with nearly quantized Hall conductivity [1]. Through analysis of edge state spin-texture and model Hamiltonian, I will show how generic point band inversion and spin U(1) quasi-symmetry enable spin Hall effect quantization in these materials, providing new insights and strategies for discovering materials with a quantized spin Hall effect [1-2].

References:

1. R. Verma, S.-H. Huang, B. Singh, *Physical Review B* 110, 165122 (2024)
2. R. Islam, R. Verma, B. Ghosh, Z. Muhammad, A. Bansil, C. Autieri, and B. Singh, **106**, 245149 (2022)

Bio of the Speaker: Dr. Bahadur Singh is a Faculty in the Department of Condensed Matter Physics and Materials Science at Tata Institute of Fundamental Research Mumbai. He is the Early Career Editorial Board member of the *Journal of Physics and Chemistry of Solids* [ELSEVIER, IF: 4.3]. Dr. Singh obtained his Ph.D. from IIT Kanpur, India, in 2015. His research focuses on exploring the interplay between various quantum degrees of freedom and modeling the electronic structure and spectroscopic properties of diverse quantum states of matter. He has designed, predicted, and characterized a broad spectrum of new quantum materials, including topological materials, 2D materials, charge-density wave systems, and superconductors.



Dr. Singh was the first to discover the type-II Weyl semimetal phase in LaAlGe, the ferromagnetic topological insulator phase in MnBi₈Te₁₃, and topological chiral crystals, among other novel phases. Recently, he predicted nontrivial superconductivity in materials such as RhGe, YRuO₂, and LaNiO₂, and proposed new strategies for designing materials capable of hosting quantized responses.

Floquet quasi energy spectrum of graphene and kagome lattices

Prakash Parida¹, Gulshan Kumar¹, Shashikant Kumar¹

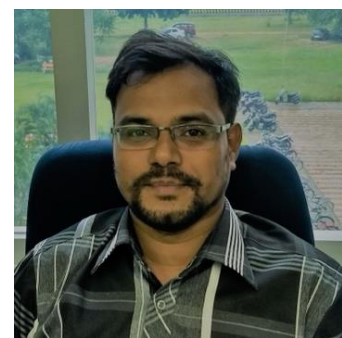
¹Department of Physics, Indian Institute of Technology Patna, Bihta, Patna, 801106, India

Using Floquet-Bloch formalism, the Floquet quasienergy spectrum of driven graphene and kagome will be discussed. Zigzag graphene nanoribbons (ZGNRs) under circularly polarized light with a frequency comparable to the system bandwidth is analyzed, revealing a method for locating monovacancy defects at edges by examining the orientation of Floquet edge states and the emergence of new Dirac points near the Fermi level. These predictions can be experimentally accessible through time- and angle-resolved photoemission spectroscopy (tr-ARPES). For kagome lattices, a generalized framework for dressed hopping potential under arbitrary field polarization is derived. Off-resonant, linearly polarized light enables precise control of hopping strengths, facilitating Dirac point merging and a transition to the Lieb like band structure with reduced bandwidth.

References:

1. G. Kumar, S. Kumar, A. Kumar and P. Parida, *Phys. Rev. B* 109, 235401 (2024)

Bio of the Speaker: He is currently a faculty member in the Department of Physics, IIT Patna. He works in the field of theoretical condensed matter physics, including topics like quantum transport, topological insulators, light-matter interaction, energy storage and harvest, 2D materials.



Harnessing Molecular Simulations for Advanced Materials Design

Sriram Krishnamurthy¹

¹Schrödinger India Pvt. Ltd., Hyderabad

Molecular simulation has become an indispensable tool for understanding and designing materials at the atomic and molecular levels, driving innovation across multiple domains of materials science. By providing atomistic insights and predictive capabilities, molecular simulations significantly contribute to the sustainable development of advanced materials. These computational techniques allow researchers to explore vast design spaces efficiently, optimizing material properties while reducing the costs and time associated with experimental synthesis and testing. This approach not only accelerates discovery but also enables the development of materials tailored to address specific challenges in technology and sustainability.

In this talk, I will showcase case studies that demonstrate the versatile capabilities of Schrödinger's molecular simulation tools - across various research domains, which enable modeling and analysis across multiple time and length-scales. By showcasing these examples, I will demonstrate how molecular simulation not only advances fundamental understanding but also bridges the gap between theoretical predictions and experimental realizations.

Additionally, I will discuss the emerging integration of molecular simulations with high-throughput computation and machine learning, outlining future opportunities to accelerate materials discovery and optimization.

Machine Learnable Representations for Materials, Molecules, and Reactions

Ananth Govind Rajan¹, Piyush Sharma¹, Raghavendra Rajagopalan¹,
Anand M. Verma¹, Shivam Chaturvedi¹, and Swastik Paul¹

¹Department 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 CO₂ from flue gas. 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 predict atomization of molecules and formation energies on dual-atom catalysts (DACs) on N-doped graphene. 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.



Discovery of Unconventional and Non-intuitive Self-assembling Peptide Materials using Experiment Driven Machine Learning

Y Nissi Talluri¹, Subramanian KRS Sankaranarayanan², H. Christopher Fry², Rohit Batra¹

¹Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, India

²Center for Nanoscale Materials, Argonne National Laboratory, USA

Prediction of secondary structure formation in peptides is challenging as it is governed by a multitude of complex molecular interactions, sequence-specific behavior and other environmental factors. Rational design strategies and computational methods, which mainly rely on hydrophobicity and structural propensity, have been put-forth to find a peptide sequence with desirable nanostructure assembly. In this work, using the example of β -sheet assembly in pentapeptides, we argue that not only such strategies are inefficient but are also biased and could indeed prevent discovery of several interesting, diverse and unconventional peptides with desired nanostructure assembly. We deployed an integrated high-throughput experimental workflow and an active learning-based AI framework to better predict the β -sheet formation propensity of peptide sequences. By focusing on sequences where machine learning (ML) predictions deviate from conventional design strategies, we synthesized and tested 268 pentapeptides, discovering 96 that successfully formed β -sheet assemblies. Our ML models outperformed traditional β -sheet propensity tables, identifying several diverse and unconventional β -sheet forming pentapeptides (e.g., ILFSM, LMISI, MITIY, MISIW, and WKIYI) that do not contain the common β -sheet former like valine. Novel chemical trends were mined by analyzing the ML models and a user-friendly web-interface is provided to make these models accessible to the community. This work highlights the value of ML-driven approaches in overcoming the limitations of current peptide design strategies.

Bio of the Speaker: Dr. Rohit Batra joined the Department of Metallurgical and Materials Engineering at IIT Madras as Assistant Professor in July 2022. Prior to this he had completed two Post-doctoral appointments, one at Center for Nanoscale Materials, Argonne National Lab, and the other at School of Materials Science and Engineering, Georgia Institute of Technology. He received his PhD in Materials Science and Engineering from University of Connecticut and B.Tech. in Metallurgical and Materials Engineering from IIT Roorkee. Before joining IIT Madras he also had a 4 month stint at Rivian Automotive LLC's R&D lab for cell manufacturing and battery development. His research interest lies in the area of combining computational and data-driven methods to design new materials. He has expertise in first-principles electronic structure methods, molecular dynamics simulations, and many machine learning based techniques, particularly geared towards the general field of chemical and materials science.



Visualizing long-range solid state amorphization in ferroic In₂Se₃

Pavan Nukala¹,

¹Indian Institute of Science, Bangalore 560012

I will discuss our recent and exciting results on in-situ transmission electron microscopy studies on T-phase, polar In₂Se₃ nanowires. Through some beautiful atomic resolution images, I'll show that the vdW layers slide with application of current (carrier wind force), eventually leading to a complete solid-state amorphization of these nanowires. I'll show in-situ videos of jerky earth quake-like response of these devices occurring due to the interaction between these defects, which eventually forms a precursor to amorphization. These insights, while on one hand may be considered to be text-book models of solid-state amorphization, have also implications in In₂Se₃ FES-FETs. I will briefly discuss our most recent foray into the transistors and show how the in situ TEM studies are relevant for these devices.

References:

1. G. Modi*, S. Parathe*, et al., Electrically driven long-range solid state amorphization in ferroic In₂Se₃, *Nature*, 635, 847, **2024**

Bio of the Speaker: Joined CeNSE, IISc in 2020 Aug Group works on materials (oxides and chalcogenides) for ferroelectric, piezoelectric and neuromorphic applications. Developing in situ microscopy capabilities here at IISc. Masters and Bachelors at IITMadras (2004-2009) in Metallurgical Engineering. Did PhD at UPenn (graduated in 2015), followed by post doc at Paris Saclay (2015-18) and Marie Curie fellow at Univ of Groningen (2018-20)



Coupling between magnetic and ferroelectric orders through lattice deformations

Daniel Cabra¹,

¹Universidad Nacional de La Plata, Argentina

We propose a microscopic magneto-electric model in which the coupling between spins and electric dipoles is mediated by lattice distortions. The magnetic sector is described by a Heisenberg model coupled directly to the lattice via a standard spin-Peierls term and indirectly to the electric dipole variables via the distortion of the surrounding electronic clouds. Electric dipoles are described by Ising variables for simplicity. We show that the effective magneto-electric coupling which arises due to the interconnecting lattice deformations is quite efficient in one-dimensional arrays. More precisely, we show using bosonization and extensive DMRG numerical simulations that by increasing the magnetic field above the spin Peierls gap, a massive polarization switch-off occurs due to the proliferation of soliton pairs. Introducing further neighbors couplings and single ion anisotropy, the system shows the "uudd" (or so-called antiphase) magnetic ordering observed in several type II multiferroic materials. We also discuss recent results for a two-dimensional generalization.



Second-principles Method for Statics and Dynamics of Ferroelectric Halide Perovskites

Ravi Kashikar¹, Sergey Lisenkov², Inna Ponomareva²

¹Department of Basic Sciences (Physics), Institute of Infrastructure Technology Research and Management, Ahmedabad, Gujarat

²Department of Physics, University of South Florida, Tampa, Florida 33620, United States

Inorganic halide perovskites of the form ABX_3 , where $A=Cs$ or Rb ; $B=Ge, Sn, Pb$ and $X=Cl, Br, I$; have gained significant attention because of their optoelectronic properties. Sn and Pb -based crystal phases are centrosymmetric, and $CsGeX_3$ ($X = Cl, Br, I$) crystalize in the polar phase. $CsGeX_3$ are the only inorganic halide perovskites where the ferroelectricity has been demonstrated experimentally. We develop an effective Hamiltonian approach to study finite temperature properties of $CsGeX_3$ and utilize this approach to probe ferroelectricity and associated phase transition in these materials. We use DFT calculations to parameterize the effective Hamiltonian. The temperature evolution of polarization predicts the phase transition from cubic to rhombohedral at 350 K, 270 K and 300 K for $CsGeCl_3$, $CsGeBr_3$ and $CsGeI_3$, respectively. Furthermore, from these simulations, the spontaneous polarization values at 10 K are $28 \mu C/cm^2$, $26 \mu C/cm^2$, and $23 \mu C/cm^2$ for $CsGeCl_3$, $CsGeBr_3$, $CsGeI_3$, respectively. In the case of thin film form, the theory introduces (i) a local order parameter, which identifies phase transitions into monodomain and polydomain phases, and (ii) a dipole pattern classifier, which allows efficient and reliable identification of dipole patterns. Our computations reveal the existence of a dynamic antipolar phase above the Curie temperature. The phase can be stabilized below the Curie temperature through quenching.

References:

1. Ravi Kashikar et al., *Nano Lett.* 24, 34, 10624–10630 (2024)
2. J. Townsend et al., *Phys. Rev. B* 109, 094121 (2024)
3. Ravi Kashikar et al. *Phys. Rev. B* 109, L020101 (2024)

Bio of the Speaker: Ravi Kashikar is an assistant professor at the Department of Basic Sciences (Physics) in the Institute of Infrastructure, Technology, Research, And Management Autonomous University by the Government of Gujarat. He completed his M.Sc. from Karnatak University, Dharwad, and his Ph.D. from the Indian Institute of Technology, Madras in 2020. He joined the computational nanoscience group at the University of South Florida as a postdoctoral associate in 2021 and later as a research assistant professor in 2022. Ravi's research experience mainly involves first-principle-based density functional calculations and tight-binding model studies for halide and oxide perovskites. Currently, he is exploring the finite temperature dynamics of halide perovskites.



Designing materials for photon-phonon conversion: From science to translation

Chandramouli Subramaniam¹, Mohammed Aslam Villan¹, Dipin Thacharakkal¹, Ananya Sah¹, Vishwanath S. Kalyani¹,

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076

Heat forms the single largest end-use of energy, accounting for ~45% of global carbon dioxide emissions. Production of environmentally benign ‘green-heat’ is imperative for sustainable development, realizing carbon-neutrality and thereby simultaneously addressing several targets under the United National Sustainable Developmental Goals (UN-SDG). Conversion of abundantly available solar energy to heat forms an important pathway to achieve this. However, this is severely limited by the choice of materials and their technological adaptability.

In this context, this work showcases nanostructured carbon florets 1-8 (NCF) as unique material exhibiting exceptionally high efficiency (~90%) towards conversion of solar energy to thermal energy. Robust coating of NCF on arbitrary substrates ranging from polymer to metals, transforms the dormant substrates into functional ones that can convert solar energy to thermal energy. Such conversion of light energy to heat results in increase in the surface temperature of any NCF-coated surface by up to 160 °C, that can be further extended beyond 350 °C using concentrated solar power. Translation of such properties into practical applications has been achieved over a wide range of domains such as (a) Water-heating for producing outlet temperature up to 85 °C with an output capacity of 75 l/day, (b) contact-less, low-power and rapid bacterial decontamination of water capable of handling bacterial concentration of 10⁶ CFU/ml, and (d) enhanced performance of supercapacitors under sub-freezing conditions. Fundamental aspects of the work, along with pragmatic applications will be discussed.

Bio of the Speaker: Dr. C. Subramaniam is currently a Professor at the Department of Chemistry, Indian Institute of Technology Bombay. He carried out his doctoral research under the supervision of Prof. T. Pradeep at IIT Madras and subsequently investigated electrical transport and vibrational signatures of carbon nanotubes with Prof. Iijima at the National Institute of Advanced Industrial Science & Technology (AIST), Japan for his postdoctoral research. Currently, his research activities focus on application-oriented fundamental research to understanding photon-phonon energy conversion pathways and thereby develop innovative materials for solar-thermal conversion, development of electrochemical energy storage systems and sensors for wearable electronics, with special emphasis on developing operando techniques for experimental understanding of heterogeneous electrified interfaces related to energy conversion, harvesting, and storage. A few selected awards and recognitions include “Young Scientist Award & Gold Medal” from the International Union of Material Research Societies (IUMRS), “Iijima Award and Medal” from the Fullerene-Nanotubes-Graphene Research Society of Japan, “Excellence in Teaching Award” and “Impactful Research Award” by IIT Bombay, and DST-SwarnaJayanti Fellowship by the Government of India. In addition to more than 75 peer-reviewed publications in reputed journals and 14 patents (Indian and International), founded NCF Green Energy Pvt Ltd that deals with coatings for solar-thermal conversion technologies. He has served as a mentor for the Integrated Clean Energy Material Acceleration Platform (IC-MAP) global initiative under the aegis of Mission Innovation Program. He is also serving as early career board member for ACS Sustainable Chemistry & Engineering and is associated with Green-Energy and Sustainability Hub (GESH) at IIT Bombay.



Surface Charges of Nanostructured Materials: A New Frontier in Hydrovoltaic Power Generation

Sudip K Batabyal¹

¹Department of Sciences, Amrita School of Physical Sciences, Coimbatore, Amrita Vishwa Vidyapeetham, India;

¹Amrita Centre for Industrial Research and Innovation (ACIRI), Amrita School of Engineering Coimbatore, Amrita Vishwa Vidyapeetham, India.

Hydrovoltaic power generation is an innovative technology that harnesses electricity from the interaction between water and surface charges of nanostructured materials. This process involves capturing energy from natural water cycles, such as rain, waves, moisture, and evaporation. We investigated an ambient condition-based hydrovoltaics power generator which can give an excellent voltage and high amount of current in an ambient condition and it is boosted further when external energy (such as solar or wind) comes into play. Different powder materials were packed in a cylindrical shape with water on the bottom and water evaporated from the top surfaces, coming with capillary action. Water evaporation-induced power generation was used in several practical applications. It is to be noted that, the device can be able to give a stable output after one year of fabrication. Our group mostly focused on activated carbon, nano clay, and metal oxide nanostructured for water evaporation-induced power generation. For a typical example, activated carbon-based 3D hydrovoltaics devices show a maximum open circuit voltage of more than 0.9 V and a short circuit current of 0.72 mA [1-4]. These hydrovoltaics devices will be useful for powering the low power IOT-based devices.

References:

1. Sujith Lal, Sudip K. Batabyal, Ambient evaporation induced electricity generation in activated carbon-water interfaced 3D hydro-voltaic device. *Journal of Power Sources*, 568, **2023**, 232951.
2. Hydrovoltaic Electricity Generation from Potato Carbon Cake: Using an Interconnected Porous Solar Steam Generator; S Lal, V Mohan, SK Batabyal; *Advanced Sustainable Systems*, **2024**, 8 (7), 2400052.
3. Integrating atmospheric water harvester with hydrovoltaics: Simultaneous freshwater production and power generation; S Lal, T Gowthaman, S Ghosh, SK Batabyal; *Separation and Purification Technology*, **2024**, 130086.
4. Streaming-Induced Hydrovoltaic Power Generation by Fluorinated Mg–Al Hydrotalcite Nanoclay; N Manikandan, SK Batabyal; *ACS Sustainable Chemistry & Engineering*, **2024**, 12, 23, 8620–8629.

Bio of the Speaker: Dr. Sudip Kumar Batabyal is a professor & chairperson in the Department of Physics, Amrita School of Physical Sciences, Coimbatore, Amrita Vishwa Vidyapeetham. Dr. Sudip has over 23 years of research experience in nanomaterials fabrication energy conversion and energy storage. His areas of expertise and research interests include semiconducting nanomaterials for energy harvesting and storage, perovskite materials, printed electronics, and electrochemistry. Sudip received his M.Sc in Physics from Vinoba Bhave University and Ph.D. in nanomaterials from Indian Association for the Cultivation of Science under Jadavpur University. Dr. Sudip worked at the Nanyang Technological University (ERI@N) as a Scientist (2010 – 2015). He Joined Amrita Vishwa Vidyapeetham in 2015. He published more than 200 international journal publications. He guided 6 Ph.D. students and currently guiding 10 Ph.D. students. He served as an editorial board member of Scientific Report and Discover energy, and edited special issues of several journals. He published a book on Carbon Quantum dots from Elsevier Science. He published his research article in many high-impact factor journals such as Nature Communication, Advanced Materials, ACS Nano, Advanced Energy Materials, etc. His work has been cited more than 8000 times, with H-index 46 and I10 index 110.



First Principles Modeling of Liquid Water: Structure, Reactivity and Optics

Ali A Hassanali¹, Edward Donkor¹, Cesare Malosso², Stefano Baroni², Solana Di Pino¹, Damian Scherlis⁴, Marta Monti¹, Giulia Galli³, Arpan Kundu³, Yu Jin³, Alex Rodriguez¹, Adu Offei Danso¹

¹The Abdus Salam International Center for Theoretical Physics (ICTP)

² Scuola Internazionale Superiore di Studi Avanzati

³University of Chicago, United States

⁴Buenos Aires University, Argentina

Liquid water plays an important role in numerous physical, chemical and biological processes. Despite long study, understanding the structural, dynamical and dielectric properties of water across the phase diagram continues to be an active area of experimental and theoretical research. In this seminar, I will give a broad and general perspective with some historical overview of the challenges in understanding the properties of water with an emphasis on the role and importance of first principles simulations. I will highlight efforts from our group [1,2] using unsupervised learning and machine learning potentials [3] to re-visit two-state models in water and the anomalous behavior of supercooled water. Recent work presenting chemical reactivity in bulk water and at interfaces [4] will also be discussed in an effort to rationalize the apparent enhanced catalysis measured experimentally in aqueous microdroplets. I will conclude my talk with some of our ongoing efforts in understanding light-matter interactions for aqueous systems.

References:

1. *J. Chem. Theory Comput.* **2022**, 18, 5, 3136–3150
2. *J. Phys. Chem. Lett.* **2024**, 15, 15, 3996–4005
3. Proceedings of the National Academy of Sciences 121 (32), e2407295121
4. *J. Am. Chem. Soc.* **2024**, 146, 46, 31585–31596

Bio of the Speaker: Ali A. Hassanali is a Senior Research Scientist in the Condensed Matter and Statistical Physics Group at the International Center for Theoretical Physics (ICTP), in Trieste, Italy. He leads an atomistic simulation group working on the theory of liquids with specific focus on understanding the properties of water across the phase diagram and in exotic thermodynamic conditions such as near biological matter and under confinement. His team develops and applies methods to study chemical reactions in water, spectroscopy and more recently, investigating how UV light interacts with water in close collaboration with several experimental groups. His research has been supported by various European grants including HORIZON 2020 on Artificial Photosynthesis and HORIZON Europe through and ERC Consolidator Grant.



Energy density and stress fields in quantum systems

Richard M. Martin^{1,2}, Nithaya Chetty³, Dallas R. Trinkle¹

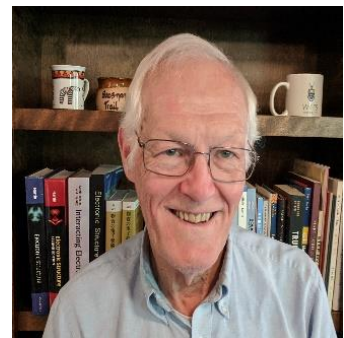
¹University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

²Stanford University, Stanford, CA 94305, USA

³University of the Witwatersrand, Johannesburg, South Africa

There has been an enduring controversy about whether or not there exist well-defined energy density and stress fields, $\epsilon(\mathbf{r})$ and $\sigma_{\alpha\beta}(\mathbf{r})$, in quantum systems. A key issue is kinetic energy since the well-known forms, $1/2|\nabla\Psi|^2$ and $-1/2\Psi\nabla^2\Psi$, lead to different densities and analogous issues arise for interactions. This work considers the ground state of a system of many interacting particles, and shows that: 1) All effects of exchange and correlation are unique functions defined at each point \mathbf{r} ; all issues of non-uniqueness involve only the density $n(\mathbf{r})$ and are equivalent to a single-particle problem with wavefunction $s(\mathbf{r}) = [n(\mathbf{r})/N]^{1/2}$. 2) Forms for these terms are determined by the nature of energy and stress. Energy has two distinct roles. Since it determines Ψ through the variational principle, the appropriate density involves the terms in the hamiltonian: $-1/2\Psi\nabla^2\Psi$ and potentials acting on the particles. This leads to DFT interpreted as equilibration of $\epsilon(\mathbf{r})$ with the same chemical potential at each point. On the other hand, energy and stress (a derivative of the energy) are determined by Ψ , and simple examples show that the only acceptable expressions involve $1/4 [|\nabla\Psi|^2 - \Psi\nabla^2\Psi]$, as derived by Pauli and others, and interactions in terms of electric fields acting between particles, not potentials. These results lead to well-defined formulations of energy density and stress fields that are physically motivated and based on a clear set of arguments.

Bio of the Speaker: Richard M. Martin is Emeritus Professor of Physics at the University of Illinois Urbana-Champaign and Adjunct Professor of Applied Physics at Stanford University. He has made important contributions to many areas of modern electronic structure, including more than 200 papers, and is the author of the book "Electronic Structure: Basic theory and practical methods" (Cambridge University Press, 2004, Second Edition, 2020) and co-author with Lucia Reining and David M. Ceperley of "Interacting Electrons: Theory and Computational Approaches (Cambridge University Press, 2016).



Anomalous magnetism induced by 4f hybridization – An overview

E. V. Sampathkumaran¹

¹Tata Institute of Fundamental Research, Mumbai-400005, India*

¹Department of Physics, IIT Roorkee, Roorkee-247667, India**

4f orbital in rare-earths (R) was historically believed to be localized well-within the ionic core. However, the fact that certain degree of 4f radial extension beyond the ionic core leads to 4f-hybridization is now well-known for Ce systems, and several novel phenomena in condensed matter physics, in particular in magnetism, have been discovered during last few decades. In this talk, I will overview this aspect of 4f-electronic structure, in particular bringing out that, even for Nd systems - such a Nd 4f hybridization leads to exceptional magnetism, as shown for Nd compounds in the AlB₂- derived ternary hexagonal series, R₂TSi₃ (T= Transition-metals), by our recent studies.

Bio of the Speaker: E.V. Sampathkumaran obtained his M.Sc (Chemistry) in Annamalai University (India) in 1976, thereafter obtaining his Ph.D at Tata Institute of Fundamental Research (TIFR), Mumbai. He retired as Distinguished Professor in 2019. Subsequently, he continued his research activities as a JC Bose Fellow and (DAE) Raja Ramanna Fellow in TIFR. He is currently a Visiting Distinguished Professor at IIT-Roorkee. He made pioneering contributions to the fields of rare-earth intermetallics and oxides, in particular on Strongly Correlated Electron Behavior (which includes Valence Fluctuation, Kondo.



Thermoelectric Properties of Topological Semimetal Cu₂ZnGeTe₄: A New paradigm to Renewable Energy

Aftab Alam^{1*}, Bhawna Sahni¹, Riddhimoy Pathak², P C Sreeparvathy¹, Tanusri Saha-Dasgupta³, Kanishka Biswas²

¹Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

²New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P. O., Bangalore, 560064, India

³Department of Condensed Matter and Materials Physics, S N Bose National Centre for Basic Sciences, JD Block, Sector-III, Salt Lake, Kolkata, West Bengal 700106, India

The study of topological quantum materials for enhanced thermoelectric (TE) energy conversion has received significant attention recently. Topological materials (including topological insulators and Dirac/Weyl/nodal-line semi-metals) with the unique combination of band structure involving linear and regular parabolic bands near Fermi level (EF) have the potential to show promising TE properties. In this talk, I will report the promising TE performance of a quaternary chalcogenide (CuZnGeTe₄) having non-trivial topological phase. At ambient condition, the compound is a narrow band gap (0.067 eV) semiconductor, with a TE figure of merit (ZT) ~1.2. Application of 5% strain drives the system to a topologically non-trivial Weyl semi-metal with the right combination of linear and parabolic bands near EF, giving rise to a reasonable ZT of 0.36. Apart from strain, alloy-engineering (Sn substituted at Ge) will also be shown to induce topological non-triviality. The present work demonstrates the potential of such unique semimetals for exceptional electronic transport properties and hence appreciable thermoelectric performance.

References:

1. Alam et al., *Phys. Rev. B* **2021**, 104, 085113.
2. Pan et al., *Adv. Mater.* **2021**, 33, 2003168.
3. Alam et al., *Phys. Rev. B* **2021**, 103, 195143.

Bio of the Speaker: Dr. Alam is a full professor at the department of physics, IIT Bombay, India. His key area of research includes materials modeling and computational materials science with an emphasis on novel functional materials. He has mentored several PhDs and postdoctoral fellows. The group has published more than 140 papers in peer-reviewed journals. He has earned several honors/awards such as young faculty award, young scientist award, early research achiever award, outstanding researcher in the field of advanced materials science etc. He has served as editorial board member for several reputed journals



Tuning magnetic anisotropy in thin film for possible application

Jyoti Ranjan Mohanty¹ Saroj Kumar Mishar, Syam Prasad P

¹Nanomagnetism and Microscopy Lab, Dept. of Physics, IIT Hyderabad

Different methods of anisotropy tuning (both intrinsic and extrinsic) in magnetic materials with higher PMA finds interesting application in magnetic memory and data storage. We are exploring a material system consisting of rare-earth and transition metal (RE-TM) alloy thin films where both the TM and RE sub-lattices couple antiferromagnetically, and hence the material shows ferrimagnetic behaviour. This material is extremely interesting because it is a soft magnetic material along with a controllable PMA with film thickness, composition, deposition methods and associated stress as well as external perturbations (ion and electron beam). Ferrimagnetic thin films consisting of RE-TM with PMA are the appropriate choice for magneto-optical data storage devices. This system offers PMA at higher thickness, avoid defect pinning, and reduced skyrmion Hall effect which aims at energy efficient devices with higher switching field compared to ferromagnet and has the advantage of magnetic contrast over antiferromagnetic counterpart. We will present potential of this system for creating controlled magnetic domain and possibility of skyrmion without the use of heavy metal. We will also discuss the ultrafast laser induced creation and switching of magnetic skyrmions in these ferrimagnetic system.

Bio of the Speaker: Prof. Jyoti Ranjan Mohanty is working as a professor at department of Physics, IIT Hyderabad. His main research interest are magnetic thin film, Interfacial magnetism, magnetic imaging, 2D materials, Multiferroics, Ultrafast Magnetism, Micromagnetic and atomistic modeling of magnetic system.



Spin-Orbit Torques in Topological Quantum Materials

Pranaba Kishor Muduli¹

¹Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India

The conventional spin-orbit torques (SOT) originating from the spin Hall effect [1,2] and/or Rashba-Edelstein effect [3] possess a symmetry in which the direction of spin current, direction of spin polarization, and direction of charge current are mutually perpendicular to each other. Hence, for an in-plane current direction, the conventional anti-damping SOT is in the plane of the device, which is not very efficient for manipulating perpendicularly magnetized-based systems used in high-density magnetic recording.

In this talk, I will discuss the observation of the non-trivial or unconventional spin-orbit torques that can produce out-of-plane spin polarization in various systems using quantum materials such as non-collinear antiferromagnets and/or low-symmetry two-dimensional materials. We also demonstrate that the PtSe₂/Ni₈₀Fe₂₀ heterostructure can generate large damping-like current-induced spin-orbit torques (SOT), despite the absence of spin-splitting in bulk PtSe₂ [4]. Using Mn₃Sn/Py, we show the observation of a large in-plane field-like torque originating from the bulk Mn₃Sn due to the magnetic spin Hall effect. The unconventional spin-orbit torques in these material systems provides immense opportunities for enabling high-density and energy-efficient magnetic recording.

References:

1. M. I. Dyakonov and V. I. Perel, *Phys. Lett. A* 35, 459 (1971).
2. J. E. Hirsch, *Phys. Rev. Lett.* 83, 1834 (1999).
3. V. M. Edelstein, *Solid State Commun.* 73, 233 (1990).
4. Richa Mudgal, et al, *Nano Lett.* 23, 11925 (2023)

Bio of the Speaker: Prof. Pranaba Kishor Muduli is a professor at the department of Physics, IIT Delhi. His research interests include spintronics and nanomagnetism with emphasis on spin torque induced magnetization dynamics. Dr. Muduli obtained his PhD degree in Physics from Humboldt University, Berlin. He received M.Tech degree in Materials science & Engineering (specialization: semiconductors) from IIT Kharagpur, India and M.Sc degree in Physics from Utkal University, India. He did postdoctoral research at the University of North Carolina, USA, Royal Institute of Technology, Sweden, and University of Gothenburg, Sweden. Dr. Muduli is a recipient of the Göran Gustafsson postdoctoral award in Sweden. Pranaba Kishor Muduli's publication record currently contains ~90 papers in high-impact international journals (with h-index of 28, and h-10 index of 57). He has published a total of >90 papers in international journals (h-index: 27). He has delivered more than 30 invited talks at reputed international conferences. He is a member of IEEE magnetic society, since 2007.



Room Temperature Dipolar Excitons in van der Waals Heterostructures

Abhishek Misra¹

¹Centre for 2D Materials Research and Innovations, Department of Physics, IIT Madras

Excitons are the bosonic system and thus the careful manipulation of their number density can lead to a range of many-body complexes. Excitons with permanent out-of-plane electric dipole moment interact via dipole–dipole interactions. Such excitons, known as interlayer excitons (IX) or dipolar excitons, further enrich the excitonic phase diagram depending on the nature of the dipole-dipole interaction. These appealing dipolar interactions have been the subject matter of intense investigations since decades using GaAs/AlGaAs quantum well structures. With the advent of van der Waals heterostructures, the realization of dipolar excitons, at least theoretically, has become rather easy. Experimentally, these have been confirmed via luminescent emission in the heterostructures of transition metal dichalcogenides. However, in these heterostructures, the IXs are not always observed as the emission is very sensitive to the lattice mismatch and the twist angle between the constituent materials. Moreover, their emission intensity is very feeble compared to corresponding intralayer excitons at room temperature. In this talk, I will discuss a possible way to stabilize these IX at room temperature. Room temperature stabilization of the dipolar excitons holds significance not only to explore many-body physics at elevated temperatures but also for their applications in the field of quantum technologies.

Bio of the Speaker: Dr. Abhishek Misra is currently an assistant professor in the department of Physics at IIT Madras since February 2018. He obtained his masters (M.Tech) and Ph.D in microelectronics from the department of Electrical Engineering, IIT Bombay, India in 2008 and 2013 respectively where he was the recipient of the best Ph.D thesis award. After his Ph.D, he worked as a principal engineer at Taiwan Semiconductor Manufacturing Company (TSMC), Taiwan until December 2014. Subsequently, he worked as a postdoctoral research associate in the department of Physics and Astronomy, University Of Manchester, UK till January 2018. After joining at IIT Madras, he is exclusively researching on the 2D Materials from growth to high performance optoelectronic devices.



Stacking and layer dependent thermal conductivity in van der Waals materials

Pramoda Kumar Nayak^{1,2}, Manab Mandal², Nikhilesh Maity³, Abhishek K. Singh³, Kanikrishnan Sethupathi²

¹Centre for Nano and Material Sciences, Jain (Deemed-to-be University), Jain Global Campus, Kanakapura, Bangalore 562112, India

²Department of Physics, Indian Institute of Technology Madras, Chennai 600 036, India

³Materials Research Centre, Indian Institute of Science, Bangalore-560012, India

Layered transition-metal dichalcogenides (TMDCs), one class of van der Waals materials possess unique thermal properties that exhibit notable distinction compared to their bulk counterparts due to the reduced dimensionality and the confinement of phonons [1]. MoSe₂ exhibits low thermal conductivity compared to other TMDCs, which makes it an excellent thermoelectric material [2]. In this talk, I will talk about the thermal conductivity of bilayer MoSe₂ around two symmetric stacking AB (0°) and AB' (60°) and some specific twist angles using the optothermal Raman technique [3]. The observed thermal conductivity values are in the range 10-30 Wm⁻¹ K⁻¹ which are well supported by our first-principles calculation results. The emergence of multiple folded phonon branches and modification in the Brillouin zone caused by in-plane rotation are accountable for the decrease in thermal conductivity. The theoretical phonon lifetime study and electron localization function analysis further reveals the origin of angle-dependent thermal conductivity in t-BL MoSe₂. In addition, I will also talk about layer-dependent thermal conductivity of 2H-polytype SnSe₂, which belongs to metal dichalcogenides (MDCs) family. Extremely low thermal conductivity values in the range 1 to 3 Wm⁻¹K⁻¹ are observed for 3L-8L SnSe₂[4]. Theoretical calculations based on the phonon Boltzmann transport equation provide strong support for the experimental findings regarding the thermal conductivity of 2H-SnSe₂ at various thicknesses

References:

1. M. Dubrovkin, B. Qiang, H. N. S. Krishnamoorthy, N. I. Zheludev, and Q. J. Wang, *Nat. Commun.* 9, 1762 (2018).
2. Peng, H. Zhang, H. Shao, Y. Xu, X. Zhang, and H. Zhu, *RSC Adv.* 6, 5767 (2016).
3. M. Mandal, N. Maity, P. K. Barman, A. Srivastava, A. K. Singh, P. K. Nayak, K. Sethupathi, *Phy. Rev. B*, 108,115439 (2023)
4. M. Mandal, N. Maity, P. K. Barman, R. Biswas, S. Mondal, V. Raghunathan, A. K. Singh, P. K. Nayak, K. Sethupathi, *Phy. Rev. B*, 110,195404 (2024)

Bio of the Speaker: Dr. Pramoda Kumar Nayak has completed his Ph.D in Physics at IIT Guwahati, India in 2007. After many years of post-doctoral experiences at various institutes across the globe, he returned to India and joined as DST Ramanujan Fellow at Dept. of Physics, IIT Madras in 2017. Currently, he is working as Associate Professor at the Centre for Nano and Material Sciences (CNMS), Jain University, Bengaluru from 2022

onwards. Besides, he is also holding an Adjunct Professor position at Dept. of Physics, IIT Madras. His research interest lies on the study light-matter interaction in 2D quantum materials and their heterostructures. He has published more than 75 international journals, 05 books, 06 book chapters, and 03 patents so far in his research career. He has received several awards and recognitions, which includes BK21Plus Research Fellowship, South Korea (2015), prestigious Ramanujan Fellowship from Department of Science and Technology, India (2017), Younger Achiever Award from Institute of Scholars (2020) and Q-pragathi award from Quantum Research Park, IISc Bangalore. He has guided 3 Ph.D and 08 Master students, completed 8 sponsored projects and his current group comprising of 02 Post-docs, 05 Ph.D. students, 01 master and 03 project associates.



Raman Gharana – Parallel Session 2

Keynote Talk 23

MXene-Organic Hybrids for Electrochemical Storage of Divalent Metal-ions

Narendra Kumar¹

¹Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi-502284,
Sangareddy, Telangana State, India
Email: narendra@chy.iith.ac.in

Organic materials are an emerging class of charge storage hosts for the development of sustainable multivalent metal-ion-based electrochemical energy storage devices in the era of post-lithium-ion batteries. However, poor electronic conductivity, dissolution and mechanical instability hamper the long-term cycling stability. A strategy based on spontaneous electrostatic assembly of perylene diimides (PDIs) onto Ti₃C₂T_x MXene is developed. Non-covalent interactions are the driving force in the formation of binder-free organic-inorganic hybrid electrodes. Ti₃C₂T_x-PDI hybrid electrode demonstrated storage of Mn²⁺, Zn²⁺, and Ca²⁺ with three-fold enhancement in charge storage capacities over pristine Ti₃C₂T_x. This research paves the way for developing MXene-organic hybrid electrodes towards development of high-capacity, high-rate multivalent metal-ion storage devices.

References:

1. S. Bhoi, S. H. Goudar, K. V. Rao, N. Kurra, *Cell Reports Phys. Sci.*, **2024**, 5, 102229.
3. S. H. Goudar, S. Bhoi, K. V. Rao, N. Kurra, *Small*, **2024**, 20, 2309905.
4. S. Yadav and N. Kurra, *Journal of Materials Chemistry A*, **2024**, 12, 32182.
5. S. Yadav and N. Kurra, *Energy Storage Materials*, **2024**, 65, 103094

Bio of the Speaker: Dr. Narendra Kurra is currently working as an assistant professor at the department of Chemistry, Indian Institute of Technology Hyderabad. He did master's from the school of chemistry, University of Hyderabad (2006-08). He was a gold medalist of 2006-08 MSc chemistry batch of University of Hyderabad. He obtained his PhD from JNCASR, Bangalore in 2013. He was a postdoctoral fellow at King Abdullah University of Science and Technology (2013-2015) and Drexel University (2015-2019), prior to becoming a Research Assistant Professor (2019-2020) at A. J. Drexel Nanomaterials Institute, USA. Dr. Narendra Kurra joined School of Chemistry, IISER-TVM, as an assistant Professor in the year 2020. After working for a year, he moved to Department of Chemistry, IIT Hyderabad. He received Teaching excellence award from IISER-TVM in the year 2021. He has been in the top 2% of highly cited researchers as per the Stanford list of highly cited researchers. He has been recognized as the "Rising Star Award" by the Research.com. His Research interests include understanding of fundamental aspects of electrode|electrolyte interfaces, nanomaterials for electrochemical energy storage applications including high rate On-chip Energy Storage and hybrid metal-ion capacitors.



Effect of Electrolyte Structure on the Mechanism and Kinetics of Solid Electrolyte Interphase Formation in Li Metal Batteries

Madhurja Buragohain and Sooraj Kunnikuruvan^{1*}

¹Department of Chemistry, Indian Institute of Technology Madras, Chennai, India

Despite their high theoretical capacity, the practical application of Li metal batteries (LMB) is severely impeded by the inherent instability of the organic electrolytes on the Li metal anodes (LMA). The high reactivity of organic electrolytes toward LMA leads to electrolyte decomposition, anode corrosion, release of flammable gasses, and safety issues due to dendrite formation.¹ Thus a stable electrode-electrolyte interphase, popularly known as solid electrolyte interphase (SEI) for anodes, is crucial.² Since modulating the properties of the SEI was found to be a promising approach for developing high-performance batteries, understanding the structure and mechanism of the formation of SEI is vital. Herein, we scrutinized the role of electrolyte structure on the mechanism and kinetics of SEI formation by analysing the reaction of the electrolytes, which are commonly used in LMB, on the surface of Li metal anode using *ab initio* molecular dynamics simulations. Furthermore, this study provides critical insights into the mechanism of formation of experimentally observed SEI components and proposes strategies for modulating the SEI structure.³

References:

1. Wu, F.; Maier, J.; Yu, Y., *Chem. Soc. Rev.*, **2020**, *49*, 1569.
2. Adenusi, H.; Chass, G. A.; Passerini, S.; Tian, K. V.; Chen, G., *Adv. Energy Mater.* **2023**, *13*, 2203307.
3. Buragohain, M.; Kunnikuruvan, S., *Manuscript under preparation*.



Mechanisms of Thermal Rectification in Semi-Stochastic Graded Graphene Microstructures

Raghavan Ranganathan¹, Simanta Lakhar², Vignesh Mahalingam¹

¹Indian Institute of Technology Gandhinagar

²Eindhoven University of Technology

Thermal rectification, similar to its electronic counterpart, is the preferential conduction of heat in one direction, and has shown promise in several frontiers of applications such as thermoelectric power generation, thermal logic circuits, and advanced thermal management devices for micro-electronics [1]. Two dimensional (2D) materials could offer a wide range of strategies or designs for generating and tuning thermal rectification (TR), which can be attributed to mechanisms such as difference in the ease of heat flow in the two opposite directions due to resonance or mismatch in the regional phonon spectra for either case, respectively, asymmetric scattering of propagating phonons depending on the direction of heat flow, and difference in the temperature-dependence of thermal conductivity in the two sides of the rectifier device [2]. For the realization of a practical and optimal thermal rectifier, a sound understanding of the underlying mechanisms of asymmetric heat transport is required.

In this work [3], we investigated the thermal rectification in periodic atomistic models of polycrystalline graphene whose grain arrangements were generated using different probability distribution functions to have different gradient grain size distributions along the heat flow direction. The reverse non-equilibrium molecular dynamics simulations, which is a key tool in this area in order to understand the asymmetric heat transport phenomena, was used to calculate the thermal conductivity and rectification of the structures equilibrated at different stress and temperature conditions. Additionally, a detailed phonon mapping was carried out to understand the underlying mechanisms based on the fluctuation-dissipation theory in order to explain the competitive interplay between two transport mechanisms, namely, (1) propagating phonon coupling and (2) temperature-dependence of thermal conductivity, that in turn, determine the degree of asymmetric heat flow in graded polycrystalline graphene. Based on a data-driven analysis, we propose the ideal parameters of a gradient grain-size structural design in graphene which can lead to an optimal thermal rectification device. Finally, strategies for rational design of 2D rectifiers will be presented.

References

1. M. Wong, C. Tso, T. Ho, and H. Lee, "A review of state of the art thermal diodes and their potential applications," *Int. J. Heat Mass Transfer*, vol. 164, p. 120607, **2021**.
2. S. Zhao, Y. Zhou, and H. Wang, "Review of thermal rectification experiments and theoretical calculations in 2D materials," *Int. J. Heat Mass Transfer*, vol. 195, p. 123218, **2022**.
3. S. Lahkar and R. Ranganathan, "Competing mechanisms govern the thermal rectification behavior in semi-stochastic polycrystalline graphene with graded grain-size distribution". *Carbon*, 218, 118638, **2024**.

Bio of the Speaker: Dr. Raghavan Ranganathan has been an Assistant Professor in the Department of Materials Engineering at the Indian Institute of Technology Gandhinagar since 2019. There, he heads the Computational Molecular Engineering Group (CMEG). He received his Bachelor of Technology degree in Metallurgical and Materials Engineering from the Indian Institute of Technology Madras and earned his Ph.D. in Materials Science and Engineering from Rensselaer Polytechnic Institute in 2016. His Ph.D. thesis elucidated atomistic mechanisms for viscoelastic damping in inorganic solids. Subsequently, he was a Postdoctoral Associate at the Massachusetts Institute of Technology for three years where he worked on the deformation behavior of semicrystalline polyethylene. Dr. Ranganathan's group works on computational approaches to study complex structure-property correlations in a wide variety of materials such as alloys, glasses, polymer composites, 2D materials and energetic materials. His group uses a variety of simulation techniques at various length and timescales ranging from electronic structure calculations using Density Functional Theory, to large-scale reactive and classical Molecular Dynamics. With the primary focus on materials phenomena at the nanoscale, his group also couples atomistic and molecular simulations with machine learning approaches to understand and model properties such as mechanical behavior, thermal and mass transport, thermodynamics and kinetics of materials and heterogeneous catalysis.



Wafer-scale production of 2D TMDs via Metalorganic Chemical Vapor Deposition

Senthil Kumar Eswaran¹, M. Vijaykumar¹, M. Kalaiarasan¹

¹2D Materials and Devices Laboratory (2DML), Sir C. V. Raman Research Park, Nanotechnology Research Centre (NRC), & Department of Physics and Nanotechnology, SRM Institute of Science and Technology (SRMIST), Kattankulathur 603203, Chennai, Tamil Nadu, India

Design and development of growth-process for the production of wafer-scale spatially homogeneous atomically-thin transition metal dichalcogenides (TMDs) is one of the key challenges to realize modern electronic devices. Recently our group has demonstrated a scalable fabrication of atomically-thin MoS₂ and WS₂ films using metalorganic chemical vapor deposition (MOCVD). We showed that the monolayer MoS₂ can be synthesized over a 2-in. sapphire wafer in a growth time as low as 4 min. Very recently, we have demonstrated the growth of Mo_{1-x}W_xS₂ ternary alloy monolayers and precise compositional tuning for the entire range of x from 0 to 1 using the gas-phase precursors. By means of Raman spectroscopy we showed that W alloying in MoS₂ lattice can lead to a tensile strain of ~0.8%. The alloying-induced tensile strain plays a key role in observing redshift in optical absorption and photoluminescence (PL) bands and resulted an unusual bandgap bowing. The coupling of tensile strain and alloying effect allowed us to tune the overall PL emission energy to as large as 185 meV. We investigated the thickness-dependent elastic properties of the MoS₂ films. Our systematic analysis from bulk to monolayer suggests that the MoS₂ exhibits nanoscale elastic-stiffening behavior with decreasing number of layers. The Young's modulus increased by a factor of ~2.7 for monolayer MoS₂ when compared with the bulk. First-principle DFT calculations affirm the nanoscale elastic-stiffening behavior of MoS₂ with decreasing number of layers.

References:

1. *APL Mater.* 7, 081113 (2019),
2. *Appl. Phys. Lett.* 118, 013102 (2021),
3. *J. Phys. Chem. Lett.*, 12, 6197 (2021).

Bio of the Speaker: Dr. Senthil Kumar is currently heading the department of Physics and Nanotechnology at SRM Institute of Science and Technology, Chennai, India. After receiving his Ph.D in physics from IIT Madras, he worked as a Postdoctoral fellow at Simon Fraser University, Canada, and as a Research Professor at Yonsei University, South Korea. Currently he is associated with the Department of Physics and Nanotechnology & Nanotechnology Research Center (NRC), SRMIST, Chennai. His current research interest includes large-scale fabrication of atomically-thin transition metal dichalcogenides (TMDs) using MOCVD process, Strain engineering, Bandgap engineering, optical spectroscopy and electrical transport properties of TMDs. Pulsed laser deposition of oxides thin films for thermoelectric applications. He has published more than 70 articles in peer-reviewed journals and a recipient of several awards including DAAD fellowship, Brain-Korea 21 fellowship, Early Career Research award (ECRA). He has received several grants including Core Research grant and early career research grant from DST SERB. Currently he is serving.



**Employing Machine Learned Functionals to Generate Potential Energy Surface for
Small molecule**

Jijila B¹, Susannal Ezhilarasi², Nirmala. V^{1*}

^{1,2} PG and Research Department of Physisc, Queen Mary's College Mylapore, Chennai,
600004, India

Recent research trend involves applying machine learning in quantum sciences to develop Density functionals, such as DeepMind's deep learning model, DM21. While the superior accuracy of DM21 has been reported in science journal, but still there is a scarcity of publications that apply pretrained DM21neural network utilizing calculations in quantum chemistry to generate potential energy surface. To address this gap, this paper computes potential energy surface using machine-learned Density Functional Approximation (DFA)-based neural density functionals (DM21, DM21m, DM21mu, DM21mc). Constructing an accurate PES using advanced theoretical methodologies like traditional Density Functional Theory (DFT) remains challenging due to the significant rise in computational cost as the step size increases. For the first time in a literature, this paper reports ML-DFA-generated PES for diatomic molecules (N₂, F₂, Cl₂) by employing a pretrained DM21m TensorFlow model with cc-pVDZ basis set. The Comparative analysis has been made with PES data derived from DM21 with those obtained from widely used DFT functionals (such as B3LYP, PW6B95, and WB97X-V). The result shows the Neural density functional – based PES computed by varying bond length and Dihedral angle was observed to be in close agreement with CCSD(T) values, when compared to one of the best performing DFT functionals (PW6B95) based on side-by-side comparison. In addition, we also analyse dipole moment, Frontier molecular properties for each molecules investigated using Machine learned functionals in PYSCF. While this paper carried out ML based DFT computations for some primary molecules, so there is a future scope for extending this work for other organic molecules.

References:

[1]B.Jijila¹, V.Nirmala¹, P.Selvarengan², D.Kavitha³, V.Arun Muthuraj⁴, A.Rajagopal⁵
Employing neural density functionals to generate potential energy surface, Journal of molecular modelling (2024).

[2] Pederson R, Kalita B, Burke K (2022) Machine learning and density functional theory. Nat Rev Phys. <https://doi.org/10.1038/s42254-022-00470-2>

Unconventional pairing in Ising superconductors: Application to monolayer NbSe₂

Subhojit Roy¹, Andreas Kreisel², Brian M. Andersen², and Shantanu Mukherjee¹

¹*Department of Physics, Indian Institute of Technology Madras, Chennai, 600036, India*

²*Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark*

The presence of a non-centrosymmetric crystal structure and in-plane mirror symmetry allows an Ising spin-orbit coupling to form in some two-dimensional materials. Examples include transition metal dichalcogenide superconductors like monolayer NbSe₂, MoS₂, TaS₂, and PbTe₂, where a nontrivial nature of the superconducting state is currently being explored. In this study[1], we develop a microscopic formalism for Ising superconductors that captures the superconducting instability arising from a momentum-dependent spin- and charge-fluctuation-mediated pairing interaction. We apply our pairing model to the electronic structure of monolayer NbSe₂, where first-principles calculations reveal the presence of strong paramagnetic fluctuations. Our calculations provide a quantitative measure of the mixing between the even- and odd-parity superconducting states and its variation with Coulomb interaction. Further, numerical analysis in the presence of an external Zeeman field reveals the role of Ising spin-orbit coupling and mixing of odd-parity superconducting state in influencing the low-temperature enhancement of the critical magnetic field.

[1] Subhojit Roy et al 2025 2D Mater. 12 015004

Symmetric spin liquids on the trellis lattice

**Sourin Chatterjee¹, Atanu Maity^{2,1}, Ronny Thomale^{2,1}, Karlo Penc^{3,1},
Yasir Iqbal¹**

¹*Department of Physics and Quantum Center for Diamond and Emergent Materials (QuCenDiEM), Indian Institute of Technology Madras, Chennai 600036, India*

²*Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Julius-Maximilians-Universität Würzburg, Am Hubland Campus Süd, Würzburg 97074, Germany*

³*Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungary*

Unlike conventional magnets, long-range magnetic orders may not be realized in some highly frustrated quantum spin systems. Rather, novel phases, such as quantum spin liquids, may emerge as ground states. Due to strong quantum fluctuations, two-dimensional spin-1/2 magnets are more prone to exhibit such phases. Being a highly frustrated two-dimensional lattice, the trellis lattice [1] may emerge as a promising candidate to explore such phases. To this end, we perform a projective symmetry group (PSG) [2] classification of symmetric quantum spin liquids on this lattice. Employing the Abrikosov fermion representation for spin, we obtain a total of 256 algebraic PSG corresponding to the invariant gauge group (IGG) Z_2 and we find a total of 128 different $U(1)$ PSGs. However, restricting up to three symmetry inequivalent nearest neighbours, we identify 5 $U(1)$ and 25 Z_2 mean field ansätze. Furthermore, we employ a $J_1 - J_2 - J_3$ Heisenberg model and studied phase diagram spinon dispersion. Moreover, we calculate the dynamical structure factor, which can be directly compared with the experimental observations.

[1] Normand, B. and Penc, K. and Albrecht, M. and Mila, F, Phys. Rev. B **56**, R5736 (1997).

[2] Xiao-Gang Wen, Phys. Rev. B **65**, 165113 (2002).

Cr-benzene Complex as a new candidate for molecular spin qubit

Soumyasree Jena^{1,*} and **Sharma S. R. K. C. Yamijala**¹

^{*}cy23r007@smail.iitm.ac.in

¹Indian Institute of Technology Madras, India.

Magnetic molecules with more than one unpaired electron exhibit zero-field splitting (ZFS), where the lowest electronic energy levels of a system split in the absence of an external magnetic field ($B = 0$). The reason for such splitting is due to the spin-spin interactions mediated by spin-orbit coupling (SOC). The ZFS Hamiltonian can be defined as:

$$\hat{H}_{\text{ZFS}} = \frac{3}{2}D_{\text{zz}}\left(\hat{S}_z^2 - \frac{1}{3}S(S+1)\right) + \frac{1}{2}(D_{\text{xx}} - D_{\text{yy}})(\hat{S}_x^2 - \hat{S}_y^2)$$

where $D = 3D_{\text{zz}}/2$ and $E = (D_{\text{xx}} - D_{\text{yy}})/2$. Here, ‘D’ and ‘E’ are the axial and rhombic zero-field splittings parameters, respectively. Many transition metal complexes exhibit ZFS. For instance, a large negative D value in such complexes is crucial for Single-Molecule Magnet (SMM) applications, while for optically addressable molecular qubits, ‘D’ should be small, allowing for control of the electron spin by microwave radiation. One can try to design molecules with a small ‘D’ by changing the ligand field strength. Recently, Cr^{4+} transition metal complexes were demonstrated as suitable candidates for spin qubits.[1], [2] The combination of strong-field aryl ligands coordinated to Cr^{4+} in a high symmetry configuration allows for a spin-optical interface with atomistic control. The theoretically calculated D parameters are found to be in good agreement with the experimental measurements. We successfully reproduced the theoretical results obtained by Sauza-de la Vega et al.[2] Specifically, we obtained a D value (3.53 GHz) that is in excellent agreement with the previous study, where we employed three multi-reference methods, namely, SA-CASSCF, MS-CASPT2, and HMS-PDFT. Further, after an extensive literature review, we modified the aryl-based ligands to acene-based ligands, specifically using benzene in our calculations. This modification gave the D-values in the range of 2.59- 5.79 GHz, making them comparable to earlier studied complexes. As a whole, we predict that Cr-benzene complexes could be potential candidates for molecular-spin qubits.

REFERENCES

- [1] S. L. Bayliss, D. W. Laorenza, P. J. Mintun, B. D. Kovos, D. E. Freedman, and D. D. Awschalom, *Optically Addressable Molecular Spins for Quantum Information Processing*, Science **370**, 1309 (2020).
- [2] A. Sauza-de la Vega, R. Pandharkar, G. D. Stroschio, A. Sarkar, D. G. Truhlar, and L. Gagliardi, *Multiconfiguration Pair-Density Functional Theory for Chromium(IV) Molecular Qubits*, JACS Au **2**, 2029 (2022).

Theoretical Insights into Inorganic Antiperovskite Nitrides (X_3NA ; $X = \text{Mg, Ca, Sr, Ba}$; $A = \text{As, Sb}$): An Emerging Class of Materials for Photovoltaics

Sanchi Monga^{1,a)}, Manjari Jain¹, Claudia Draxl² and Saswata Bhattacharya^{1,b)}

¹Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India

²Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin 12489, Germany

^{a)}sanchi@physics.iitd.ac.in, ^{b)}saswata@physics.iitd.ac.in

Antiperovskite nitrides have emerged as promising materials for optoelectronic and solar light-harvesting applications owing to their exceptional stability and unique electronic properties. However, detailed theoretical investigations into their excitonic and polaronic properties remain limited, primarily due to the high computational cost. These materials exhibit an inverted electronic structure compared to conventional perovskites and are represented by the structural formula X_3BA , where X is a cation, and A and B are different-sized anions. In this study, we employ a comprehensive state-of-the-art approach — combining density functional theory, many-body perturbation theory (GW/BSE), the Wannier-Mott model, density functional perturbation theory, and the Feynman polaron model — to systematically investigate the electronic, optical, excitonic and polaronic properties of X_3NA ($X = \text{Mg, Ca, Sr, Ba}$; $A = \text{As, Sb}$). We demonstrate that the HSE06 exchange-correlation functional is a suitable starting point for single-shot GW (G0W0) calculations, yielding band gaps in agreement with the self-consistent GW (scGW) approach and experimental results. Our electronic structure analysis reveals that these materials exhibit band gaps falling within the visible range of the solar spectrum. They possess low electron and hole effective masses and exhibit strong absorption at the optical onset, as determined from BSE@G0W0 approach, indicating their suitability for photovoltaic applications. Furthermore, we identify a significant contribution of ionic dielectric screening on the static dielectric constant. The Wannier-Mott model predicts low exciton binding energies (6-29 meV) for Sb-based antiperovskites (X_3NSb ; $X = \text{Mg, Ca, Sr, and Ba}$), implying efficient free charge carrier generation upon light absorption. In contrast, As-based antiperovskites exhibit higher binding energies. Fröhlich coupling constants suggest weak electron-phonon interactions, leading to the formation of large polarons. Remarkably, Sb-based antiperovskites exhibit superior charge carrier mobilities, as estimated using the Hellwarth polaron model, surpassing those of the benchmark photovoltaic semiconductor MAPbI₃. Our findings underscore the potential of Mg₃NSb, Sr₃NSb, Ca₃NSb, and Ba₃NSb as high-performance photovoltaic absorbers and provide valuable guidance for future experimental investigations.

References:

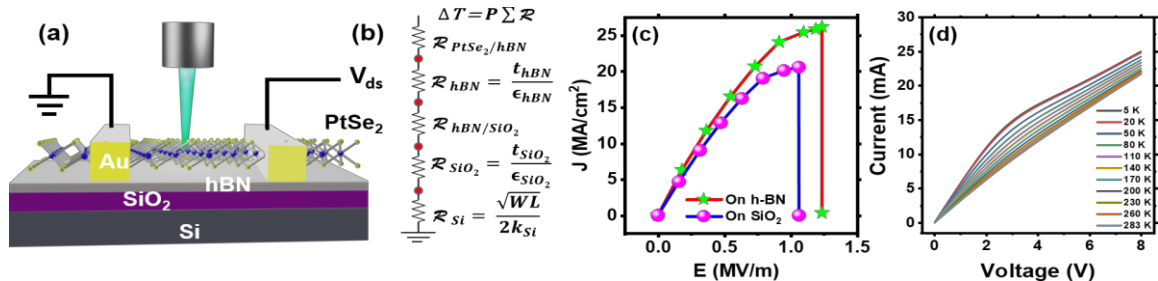
1. Monga, S., Jain, M., Draxl, C., & Bhattacharya, S. (2024). Theoretical insights into inorganic antiperovskite nitrides (X_3NA : $X = \text{Mg, Ca, Sr, Ba}$; $A = \text{As, Sb}$): An emerging class of materials for photovoltaics. *Physical Review Materials*, 8(10), 105403.

Substrate Dependent Energy Dissipation and High Field Breakdown in PtSe₂
Bubunu Biswal^{1,2}, Renu Yadav¹, Saroj Poduyal¹, P K Barman¹, B. R. K. Nanda², Abhishek Misra¹

¹Center for 2D material Research and Innovations, Dept. of Physics, IIT Madras, India, 600036 ³Center for Atomistic Modelling and Materials Design, Dept. of Physics, IIT Madras, India, 600036 Email id: abhishek.misra@iitm.ac.in & biswalbubun444@gmail.com

Platinum diselenide (PtSe₂) is an emerging 2D material with outstanding optical and electrical properties and excellent air stability. Understanding the substrate-dependent electrical transport and energy dissipation in few-layer semimetallic PtSe₂ on SiO₂ and hBN substrates is critical for optimizing its performance. In this work, the high field Current-Voltage characteristics were thoroughly investigated from the room temperature up to 5 K. There is a kink in the resistance that appears for the few layer PtSe₂ as we move from low field to high field regime, which is prominent at low temperature. This appearance of kink and the reduction of the resistance at high field is due to the local self-heating of the channel. The heat dissipation of the channel is primarily due to the heat spreading into the substrate. With the Raman thermometry measurements, we estimated the Interfacial Thermal Conductance (ITC) of PtSe₂/SiO₂ and PtSe₂/hBN interfaces and measured the maximum temperature of the channel just before the breakdown. The heat transport from the 2D channel material into the substrate is mainly contributed by the flexural phonon modes transmission of the channel material. The higher ITC value at the PtSe₂/hBN interface indicates the enhanced current carrying capacity with more efficient heat dissipation, which are crucial factors for improving the thermal management in PtSe₂-based devices.

Figure: (a) The schematic diagram of PtSe₂ device substrate and the experimental IV and Raman measurement setup. (b) The circuit diagram indicating the thermal resistance at different layers of the device. (c) The break-down characteristic of PtSe₂ on h-BN and SiO₂ substrate. (d) Low temperature IV characteristic at low and high field bias.



Designing MXene/blueP heterostructures for device application**Sarga P K¹ and Dr. Swastibrata Bhattacharyya*²**¹Department of Physics, BITS Pilani KK Birla Goa Campus, India

MXenes ($M_{n+1}X_nT_x$) are a versatile class of 2D materials combining transition metals (M), carbon or nitrogen (X), and surface functional groups (T) such as oxygen or hydroxyl. Their exceptional properties, including high electrical conductivity, mechanical stability, and chemical versatility, make them promising for diverse applications. Building two-dimensional (2D) van der Waals (vdW) heterostructures and enhancing their properties through strain engineering unlocks new applications for their constituent materials. In this study, we employ first-principles density functional theory (DFT) calculations to investigate oxygen-functionalized MXene-based heterostructures (M_2CO_2 , M= Sc, Zr, Hf) coupled with blue phosphorene (BlueP). The focus is on their structural, electronic, and optical properties under uniaxial and biaxial strain. Our findings reveal that $Sc_2CO_2/blueP$ exhibits a type-II band alignment, enabling efficient separation of photogenerated charge carriers essential for photocatalysis. $Zr_2CO_2/blueP$ and $Hf_2CO_2/blueP$ undergo a strain-induced transition from type-I to type-II band alignment, further optimizing their photocatalytic efficiency. The optical analysis confirms strong absorption in the visible spectrum, and the band alignment is well-suited for water splitting, satisfying the redox potentials required for hydrogen evolution and oxygen reduction reactions. This study establishes oxygen-functionalized MXene/blueP heterostructures as robust candidates for photocatalytic water splitting. Their strain-tunable properties and compatibility with critical photocatalytic criteria underscore their potential for advancing sustainable energy technologies.

References:

- [1] S. P., K.; K. H., J.; Bhattacharyya, S. Electronic and Interfacial Properties of 2D MXene/Blue Phosphorene Heterostructures: Impact of External Tuning Parameters and Potential for Thermoelectric Applications. *ACS Appl. Electron. Mater.* **2024**, *6* (12), 8039–8049. <https://doi.org/10.1021/acsaelm.4c01386>.
- [2] Fujishima, A.; Honda, K. Electrochemical Photolysis of Water at a Semiconductor Electrode. *Nature* **1972**, *238* (5358), 37–38.
- [3] Wang, B.-J.; Li, X.-H.; Zhao, R.; Cai, X.-L.; Yu, W.-Y.; Li, W.-B.; Liu, Z.-S.; Zhang, L.-W.; Ke, S.-H. Design of High-Performance Photocatalysts Using 2D Heterostructures Based on Functionalized MXenes. *J. Mater. Chem. A* **2018**, *6* (19), 8923–8933. <https://doi.org/10.1039/C8TA02048H>
- [4] Gao, X.; Shen, Y.; Ma, Y.; Wu, S.; Zhou, Z. Tuning Electronic and Optical Properties of 2D Heterostructures for Photocatalytic Applications. *Appl. Phys. Lett.* **2019**, *114* (22), 221601. <https://doi.org/10.1063/1.5094850>

**Phenomena of quantum magnetization plateau(s) in a class of spin $s = 1/2$
Heisenberg $J_1 - J_1 - J_2$ trimerized quantum spin chains**

Sachin Kumar¹ and Amit Kumar and S M Yusuf¹
*Solid State Physics Division, Bhabha Atomic
 Research Centre, Mumbai 400 085, India Homi
 Bhabha National Institute, Anushaktinagar,
 Mumbai 400094, India*

Quantum Heisenberg spin systems (QHSS) have been a topic of great interest in condensed matter physics due to their exhibition of a variety of intriguing phenomena of a purely quantum nature. One such phenomenon is the formation of magnetization plateaus, where the magnetization M becomes quantized at rational values of the saturation magnetization M_s during the magnetization process in QHSS. The magnetization plateau state provides an alternative way to realize the topologically nontrivial Haldane phase, which arises from the field-induced finite gap in the excitation spectra. In this work, I present the results of an investigation into the phenomenon of magnetization plateaus in a class of spin $s = 1/2$ Heisenberg $J_1 - J_1 - J_2$ trimerized quantum spin chains. The study employs the density matrix renormalization group (DMRG) method and complementary techniques, where the J -values represent the antiferromagnetic or ferromagnetic exchange interaction constants.

The occurrence of magnetization plateaus in one-dimensional spin systems is governed by the condition proposed by Oshikawa et al.: $n(s - M/M_s) \in \mathbb{Z}$,

where n is the period of the ground state, s is the magnitude of the spin. In agreement with this condition, a magnetization plateau at $m = M/M_s = 1/3$ is observed in the magnetization curve of spin $s = 1/2$ Heisenberg trimer ($n = 3$) spin chain systems. The $1/3$ quantum magnetization plateau observed in the ground-state magnetization process arises from competing exchange coupling interactions in trimer spin chains. These plateaus are also evident through the spin gap in the excitation spectra of the system. As temperature increases, thermal fluctuations begin to dominate over quantum fluctuations, narrowing the width of the plateau and eventually causing it to disappear at temperatures above a certain critical threshold. Furthermore, the presence of a next-nearest-neighbor (NNN) interaction within the trimer unit, denoted as J_3 , introduces frustration into the system. The influence of such interactions on the magnetization states is discussed in detail. The theoretical findings presented here are compared with experimentally realizable quasi-one-dimensional $s = 1/2$ Heisenberg $J_1 - J_1 - J_2$ trimerized quantum spin chain compounds and are found to agree with reported experimental results.

¹A. Vasiliev, O. Volkova, E. Zvereva, M. Markina, npj Quantum Materials 3(1) **18** (2018)

²M. Oshikawa, M. Yamanaka and I. Affleck, Phys. Rev. Lett. **78** 1984 (1997)

Ferroelectric Polymorphism and Epitaxial Strain Effect on Polarization and Electronic Structure of Cu(OH)₂

Subhajit Sau¹ and A C Garcia-Castro², G Vaitheeswaran³, and V Kanchana¹

¹Department of Physics, IIT Hyderabad, Kandi, Sangareddy, 502285, Telangana, India

²School of Physics, Universidad Industrial de Santander, Carrera 27 Calle 09, 680002 Bucaramanga, Colombia

³School of Physics, University of Hyderabad, Prof. C. R. Rao Road, Gachibowli, Hyderabad 500046, Telangana, India

Email: ph21resch01001@iiith.ac.in

Ferroic orders and their structural phase transitions play a key role in elucidating numerous unconventional phenomena in condensed matter systems. Our study examines the polymorphic ferroelectric phase transitions of Copper(II) hydroxide, considering its antiferromagnetic ground state. Through the first-principles studies and group theory analysis, we provide a systematic theoretical investigation of vibrational properties in hypothetical *Cmcm* high-symmetry phase to identify the symmetry-allowed ferroic phases. We identified a non-polar to polar (*Cmc21*) phase transition, in which the displacive transformation is primarily responsible for the phase change induced by two B_{1u} (i.e. Γ^{-2}) phonon modes within the centrosymmetric phase. The two polar structures have the same space group with different atomic arrangements, correspond to different degrees of polarization (i.e. $P_s = 3.06$ and $42.41 \mu\text{C}\cdot\text{cm}^{-2}$), emerging from the parent *Cmcm* structure. The structure corresponding to phonon branch-3, at Γ , matches with experimentally determined polar structure which is not the ground state and possess polarization of $42.41 \mu\text{C}\cdot\text{cm}^{-2}$. Here, ferroelectricity is geometric by nature and is driven by the Γ^{-2} mode in which the O- and H-sites displacements lead the polar distortion with a minor contribution from Cu-sites. Interestingly, the $3d^9$:Cu²⁺ Jahn–Teller distortion coupled with the orientational shifts of O–H atoms enhance the polarization [1]. Further we note unusual quadratic strain-polarization coupling in both polar structures. Our calculations predict this as an indirect wide bandgap semiconductor and variation of band gap as a function of epitaxial strain is also presented.

References:

[1] Subhajit Sau, Anuroopa Behatha, A C Garcia-Castro, G Vaitheeswaran, and V Kanchana, Ferroelectric polymorphic phenomena in the layered antiferromagnet Cu(OH)₂, J. Phys.:Condens.Matter 36 (2024) 315403

Platinum-adsorbed defective 2D monolayer boron nitride: a promising electrocatalyst for O₂ reduction reaction

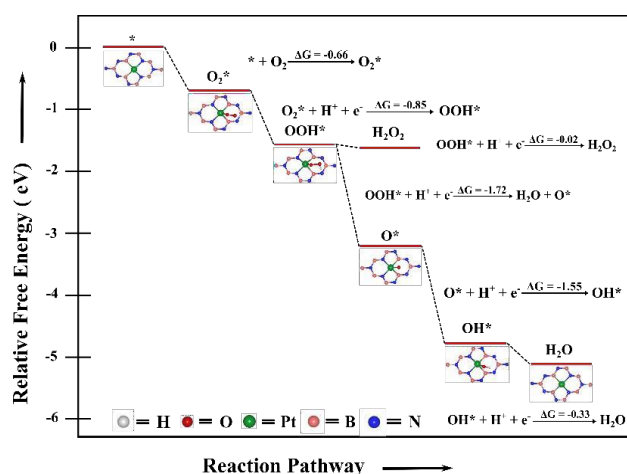
Lokesh Yadav¹ and Srimanta Pakhira²

¹Department of Physics, IIT Indore, Indore, 453552, India

²Faculty of Physics, IIT Indore, Indore, 453552, India

Presenting author: phd2101151006@iiti.ac.in

Hexagonal boron nitride (hBN) has long been considered chemically inert due to its strong covalent bonds and wide bandgap, making it unsuitable for energy conversion applications. To overcome this limitation, we have computationally designed a 2D monolayer hBN with a single nitrogen (N) and boron (B) di-vacancy denoted by VBN defective-BN (d-BN) to activate the chemical reactivity, which is an effective strategy to use d-BN for potential applications, especially in electrochemistry. Introducing a single platinum atom to the VBN defective area named Pt-d-BN functions as a single-atom catalyst (SAC), demonstrating remarkable performance in the oxygen reduction reaction (ORR). The



first principles-based dispersion-corrected periodic hybrid density functional theory (DFT-D) method has been employed to investigate the equilibrium structure and properties of the Pt-adsorbed 2D monolayer defective boron nitride (Pt-d-BN). The present study shows the semiconducting character of Pt-d-BN with an electronic band gap of 1.30 eV, which is an essential aspect of the ORR. Our results show that 2D monolayer Pt-d-BN material has high electrocatalytic activity and prefers a 4e⁻ reduction pathway, in which platinum functions as a single-atom catalyst. We have investigated dissociative and associative ORR mechanisms on the surface of 2D Pt-d-BN material. It is found that the associative mechanism is thermodynamically more favorable than the dissociative mechanism as for all the reaction pathways, free energies are negative, and all the steps of potential energy curves are downhill. This suggests that the Pt-d-BN monolayer could be a viable alternative to platinum-based electrodes in applications such as fuel cells. While practical implementation presents challenges, our study paves the way for future research and development of this material for commercial ORR catalytic applications.

References:

1. Lokesh Yadav 1. and Srimanta Pakhira 2., 2023, Platinum-adsorbed Defective 2D Monolayer Boron Nitride: A Promising Electrocatalyst for O₂ Reduction Reaction, Journal of Materials Chemistry C. 11, 15215-15232.

Distribution of charge centers in matter from geometric phases of electrons

Joyeta Saha, Sujith Nedungattil Subrahmanian, Joydeep Bhattacharjee

School of Physical Sciences, National
Institute of Science Education and
Research, A CI of Homi Bhabha
National Institute, Odisha - 752050,
India

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

References:

[1] Joyeta Saha, Sujith NS, Joydeep Bhattacharjee, "Distribution of charge centers in matter from geometric phases of electrons," *The Journal of Physical Chemistry C* 128 (42),18102-18109,2024.

Irida-Graphene: A New Two-Dimensional Electrode Material for Sodium-ion Batteries

Manpreet Kaur¹, and **T. J. Dhilip Kumar¹**

¹ Department of Chemistry, IIT Ropar, Punjab, 140001, India
 #¹manpreet.23cyz0003@iitrpr.ac.in, 9417995692

The irida-graphene monolayer's effectiveness for ion storage in sodium-ion batteries (SIBs) is evaluated using density functional theory [1]. The GGA method with the PBE functional is used to calculate exchange and correlation energy properties. It exhibits stable structural, thermal, and mechanical properties, with high conductivity confirmed through density of states and band structure analysis. The storage capacity and energy density have been assessed at 1116.7 mAhg^{-1} , and 2854.9 mWhg^{-1} respectively, for SIBs. A low energy barrier of 0.079 eV and fast Na-ion diffusion rate ($2.83 \times 10^{-4} \text{ cm}^2\text{s}^{-1}$) indicate easy ion migration as shown in Figure 1 (a) & (b). Furthermore, the voltage obtained (0.15 V), is suitable for commercial SIBs designs. Based on the theoretical investigation, irida-graphene shows excellent potential as a superior electrode for next-generation SIBs [2].

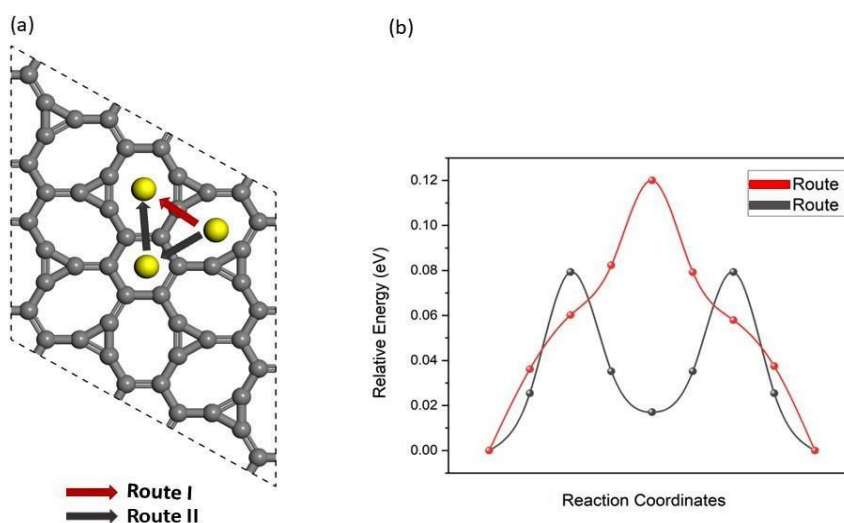


Figure 1. (a) Shows routes for Na-ion migration, and (b) displays the energy profiles for these routes.

References:

- [1] V. Dusastre and L. Martiradonna, 2017. Materials for sustainable energy, *Nat. Mater.*, 16, 15.
- [2] M. Kaur, N. Duhan and T. J. Dhilip Kumar, 2024. Irida-graphene: A new two-dimensional electrode material for sodium-ion batteries, *J. Energy Storage*, 104, 114456.

Chiral Orbital Texture and Edelstein Effect in Monolayer Janus TMDs

Pratik Sahu,^{1,2} Sashi Satpathy,^{1,2,3} and Birabar Ranjit Kumar Nanda^{1,2}

¹ Condensed Matter Theory and Computational Lab, Department of Physics, IIT Madras, Chennai-600036,

² Center for Atomistic Modelling and Materials Design, IIT Madras, Chennai-600036, India

³Department of Physics, University of Missouri, Columbia, MO 65211, USA

We investigate the orbital counterpart of the Rashba-Edelstein effect in the Janus transition metal dichalcogenides (TMDs) of the form MXX', where M is a transition metal and X, X' are distinct chalcogen atoms. We find that the inherent structural asymmetry of the Janus compounds creates chiral orbital texture in the momentum space, just like the spin texture in case of the spin Rashba effect. However, this orbital texture can be found even in the absence of the spin orbit coupling. In addition, we explore the effect near the valleys by building an analytical model based on the nearest neighbor parameters extracted from density functional theory (DFT) calculations. We list a set of parameters that control the orbital texture near the valleys for several compounds of this class. These chiral orbital and spin textures can further lead to a net accumulation of magnetic moment in response to an applied electric field i.e. Edelstein effect, offering promising avenues for novel spintronic and orbitronic devices based on these 2D materials.

References:

[1] P. Sahu, Sashi Satpathy and B. R. K. Nanda, Orbital Rashba-Edelstein effect driven by intrinsic electric field in monolayer Janus TMDs (to be submitted).

Study of sputter-grown Nitride-based memristive devices for bio- synaptic and non-volatile memory application

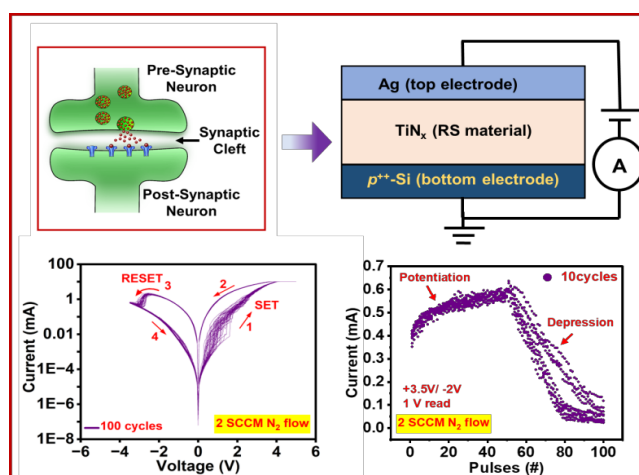
Shanu Bandyopadhyay^{1,2}, Rupam Mandal^{1,2}, Aparajita Mandal², and Tapobrata Som^{1,2*}

¹SUNAG Laboratory, Institute of Physics, Sachivalaya Marg, Bhubaneswar 751 005.

²Homi Bhabha National Institute, Training School Complex, Mumbai 400.

Due to its excellent performance, high storage capacity, low voltage, and fast operation, memristors have a lot of potential for use in memory storage applications nowadays. Apart from oxide-based memory device, nitride-based device shows promising results in storage and computing application, however there are limited works on it. In this work, we use the magneto sputtering technique to study the growth of a TiN-based memory resistive device with the following configuration: Ag/TiN/ p^{++} -Si/Ag as a function of nitrogen (N₂) flow rate. The outcome reveals a developing bipolar RS, free, non-volatile (NVM) behavior. Specifically, the N₂ flow rate has been optimized to obtain a high ON/OFF ratio, low SET RESET voltage, and good stability. Furthermore, the optimized TiN memristor demonstrates bio-synaptic functions such as depression and potentiation, which are critical for neuromorphic computing. The charge conduction process is space charge limited current (SCLC) via the N₂ vacancies, however no ohmic type conduction is observed in LRS. Therefore, TiN can be used as an electrode material and be an effective choice for memory applications.

Keywords: Memristors, Bipolar Resistive Switching (RS), Bio-synaptic.



[1] Jeon *et al.*, Low power NiN-based resistive switching memory device using Ti doping, Applied Physics Letters 109, 183507 (2016).

[2] Yang *et al.*, Effect of nitrogen-accommodation ability of electrodes in SiN_x-based resistive switching devices, Applied Physics Letters 111, 233510 (2017).

[3] Fu *et al.*, Nonlinear resistive switching features of rapid-thermal-annealed aluminium-nitride dielectrics with modified charge trapping behaviours, Microelectronic Engineering 216, 111033 (2019).

Band convergence and defect engineering synergistically revamping the carrier-phonon dynamics in $\text{Mg}_{3-x}\text{Zn}_x\text{Sb}_2$ solid solutions: An experimental and theoretical insights

S. Priyadharshini¹, V. Vijay^{1,2}, S. Kamalakannan¹, J. Archana¹, M. Navaneethan^{1,2*}

¹ Centre of Excellence in Materials for Advanced Technologies (CeMAT), Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603 203, India

² Nanotechnology Research Centre, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603 203, India

*Corresponding author

Dr. M. Navaneethan, E-mail: m.navaneethan@gmail.com, Contact E-mail: ps1206@srmist.edu.in

N-type Mg_3Sb_2 -based Zintl phase compound has attracted intensive attention for its superior thermoelectric performance, which makes it a potential candidate for medium-temperature (< 900 K) application. Herein, this work verifies the *p*-type $\text{Mg}_{1.8}\text{Zn}_{1.2}\text{Sb}_2$ solid-solution and defect engineering could be the key mechanism to reducing the κL for improving the thermoelectric performance. The carrier and phonon transport properties were studied by adding heavy element Ag at Mg-sites of $\text{Mg}_{1.8}\text{Zn}_{1.2}\text{Sb}_2$ solid-solution. As a result, the $\text{Ag}_{0.03}\text{Mg}_{1.77}\text{Zn}_{1.2}\text{Sb}_2$ sample simultaneously obtained the highest power factor of $4.56 \mu\text{W}/\text{cmK}^2$ via band convergence and defect engineering led to reduced thermal conductivity of $0.56 \text{ W}/\text{mK}$ at 753 K via the strengthening of multiscale phonon scattering. Density functional theory (DFT) indicates that the substitution of Ag into the Mg_2ZnSb_2 enhances the electron density. The substitution of Ag into the Mg_2ZnSb_2 system increases the active sites of matrix compounds. In addition, optimized carrier density and thermal conductivity resulting in a maximum zT of 0.5 at 753 K has been obtained for $\text{Ag}_{0.03}\text{Mg}_{1.77}\text{Zn}_{1.2}\text{Sb}_2$, which is 285% higher than undoped $\text{Mg}_{1.8}\text{Zn}_{1.2}\text{Sb}_2$. This work demonstrates that, heavy element substitution induces band convergence and defect engineering leads to simultaneous improvement in thermoelectric transport properties of *p*-type $\text{Mg}_{1.8}\text{Zn}_{1.2}\text{Sb}_2$ -based Zintl compounds.

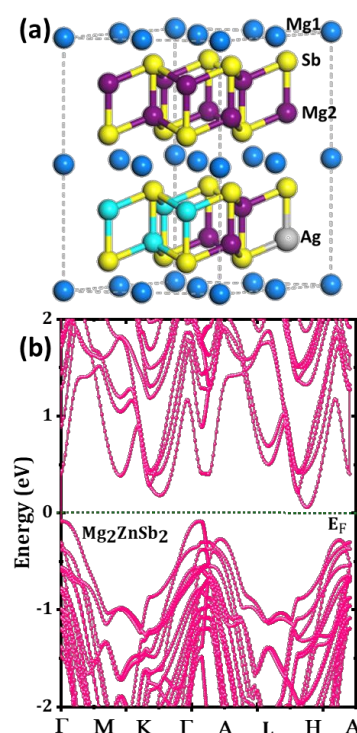


Figure: (a) Crystal structure (b) band structure of Mg_2ZnSb_2

Keywords: $\text{Mg}_{1.8}\text{Zn}_{1.2}\text{Sb}_2$; defect engineering; solid solution; band convergence; thermal conductivity.

References

- Priyadharshini, S.; Vijay, V.; Kamalakannan, S.; Archana, J.; Navaneethan, M. Realizing an Ultralow Thermal Conductivity via Interfacial Scattering and Rational-Electronic Band Reformation in *p*-Type Mg_3Sb_2 . *Appl. Phys. Lett.* **2024**, *124* (3).
- Vijay, V.; Harish, S.; Archana, J.; Navaneethan, M. Ultra-High Power Factor of *p*-Type Bi_2Se_3 for Room-Temperature Thermoelectric Applications. *Chem. Commun.* **2023**, *59* (52), 8119–8122.

Frustrated charge density wave and quasi-long-range bond-orientational order in the magnetic kagome FeGe

Arunava Kar^{1,*}, D. Subires,^{1,2} A. Korshunov,¹ C. A. Fuller,³ Y. Jiang,¹ H. Hu,¹ D. C~alug~aru,⁴ C. McMonagle,³ C. Yi,⁵ S. Roychowdhury,^{5,6} C. Shekhar,⁵ J. Stempffer,⁷ A. Jana,^{8,9} I. Vobornik,⁸ J. Dai,¹⁰ M. Tallarida,¹⁰ D. Chernyshov,³ A. Bosak,¹¹ C. Felser,⁵ B. Andrei Bernevig,^{1,4,12} and S. Blanco-Canosa^{1,12}

¹Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 20018, San Sebasti'an, Spain

²University of the Basque Country (UPV/EHU), Basque Country, Bilbao, 48080 Spain

³Swiss-Norwegian BeamLines at European Synchrotron Radiation Facility

⁴Department of Physics, Princeton University, Princeton, NJ 08544, USA

⁵Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

⁶Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhopal-462 066, India

⁷Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439

⁸CNR-Istituto Officina dei Materiali (CNR-IOM), Strada Statale 14, km 163.5, 34149 Trieste, Italy

⁹International Center for Theoretical Physics (ICTP), Strada Costiera 11, 34151 Trieste, Italy

¹⁰ALBA Synchrotron Light Source, 08290 Barcelona, Spain

¹¹European Synchrotron Radiation Facility (ESRF), BP 220, F-38043 Grenoble Cedex, France

¹²IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

[*phys.arunava20@gmail.com](mailto:phys.arunava20@gmail.com)

The intrinsic frustrated nature of a kagome lattice is amenable to the realization of exotic phases of matter, such as quantum spin liquids or spin ices, and more recently the multiple-charge density waves (CDW) in the kagome metals. Despite intense efforts to understand the mechanism driving the electronic modulations, its origin is still unknown and hindered by competing interactions and intertwined orders. Here, we identify a dimerization-driven 2D hexagonal charge-diffuse precursor in the antiferromagnetic kagome metal FeGe and demonstrate that the fraction of dimerized/undimerized states is the relevant order parameter of the multiple-q CDW of a continuous phase transition. The pretransitional charge fluctuations with propagation vector $q=q_M$ at $T_{CDW} < T < T^*(125 \text{ K})$ are anisotropic, hence holding a quasi-long-range bond-orientational order. The broken translational symmetry emerges from the anisotropic diffuse precursor, akin to the Ising scenario of antiferromagnetic triangular lattices. The temperature and momentum dependence of the critical scattering show parallels to the stacked hexatic B-phases reported in liquid crystals and transient states of CDWs and highlight the key role of the topological defect-mediated melting of the CDW in FeGe.

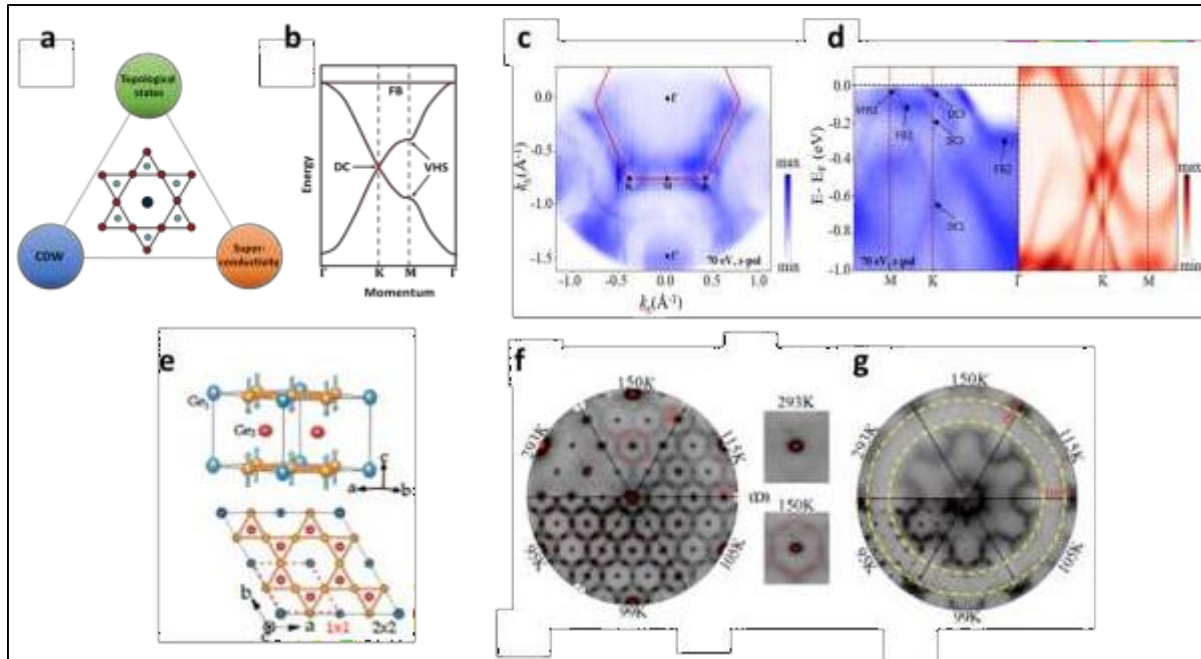


Figure: (a) Exotic Electronic orders in Kagome lattice including Superconductivity, charge density wave (CDW), and Topological state. (b) Schematic representation of the ideal band structure of Kagome lattice with Dirac cones (DC), Van Hove singularity (VHS), and flat band (FB) in momentum space. (c)-(d) Fermi surface and electronic band structure of FeGe. (blue bands from ARPES and orange bands from DFT). (e) Geometric structure of FeGe. (f)-(g) Temperature dependence diffuse scattering mapping of $(h k 2)$ and $(h k 3/2)$ planes, respectively.

References:

1. H. Tan, Y. Liu, Z. Wang, and B. Yan, Charge density waves and electronic properties of superconducting kagome metals, *Phys. Rev. Lett.* 127, 046401 (2021).
2. J.-X. Yin, B. Lian, and M. Z. Hasan, Topological kagome magnets and superconductors, *Nature* 612, 647 (2022).
3. Mielke III, C. et al. Time-reversal symmetry-breaking charge order in a correlated kagome superconductor. *Nature* 602, 245–250 (2022).
4. Teng, X. et al. Discovery of charge density wave in a correlated kagome lattice antiferromagnet. *Nature* 609, 490–495 (2022).
5. B. R. Ortiz et al., L. C. Gomes, J. R. Morey, M. Winiarski, M. Bordelon, New kagome prototype materials: discovery of KV_3Sb_5 , RbV_3Sb_5 , and CsV_3Sb_5 , *Phys. Rev. Mater.* 3, 094407 (2019).
6. D. Subires et al., Order-disorder charge density wave instability in the kagome metal $(Cs, Rb)V_3Sb_5$, *Nature Communications* 14, 1015 (2023).
7. Yin, J.-X. et al. Discovery of charge order and corresponding edge state in kagome magnet FeGe. *Phys. Rev. Lett.* 129, 166401 (2022).
8. Teng, X., Oh, J.S., Tan, H. et al. Magnetism and charge density wave order in kagome FeGe. *Nat. Phys.* 19, 814–822 (2023)

Design of Ferroelectric Double Perovskite Oxides as Photovoltaic Materials

Sathiyamoorthy Buvaneshwaran, Monirul Shaikh, Rajan Gowsalya, Trilochan Sahoo* and Saurabh Ghosh*

Department of Physics and Nanotechnology, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur 603 203, Tamil Nadu, India
e-mail: buvaneshbold@gmail.com

In ferroelectric-based photovoltaic materials, spontaneous polarization is expected to couple with the electronic and optical properties of the materials, and such materials have drawn attention as photovoltaic solar cells. Here, we utilize hybrid improper ferroelectricity to induce ferroelectric polarization in selected A-site layered and B-site rock-salt $AA'BB'O_6$ double perovskites and propose an alternate route to design ferroelectric photovoltaic semiconductors. First-principles density functional theory calculations and ab initio molecular dynamics simulations are performed to investigate the optical, electronic, and ferroelectric properties. We consider $RbLaMnWO_6$ and $RbYMnWO_6$ as model systems to pursue this study. We identify that these materials are semiconductors with a minimalist forbidden energy gap (E_g) of 2.31 and 2.14 eV, respectively. This facilitates their absorption within the visible light region, thus enabling them to be exploited for optical device applications. The optical transition occurring in $RbLaMnWO_6$ reveals the relationship between the absorption spectrum and its electronic structure. We notice a low ferroelectric switching barrier in the case of $RbLaMnWO_6$, whereas a low band gap is espied in $RbYMnWO_6$. To utilize the large visible spectra, we lower the band gap of $RbYMnWO_6$ from 2.14 to 1.67 eV by strain engineering. Similar structural, electronic, and optical properties are obtained for A-site substitution ($A = K, Na$). Further, molecular dynamics simulations show a polarization switching occurring at a temperature (T) of ~ 400 K in $RbLaMnWO_6$. This, in turn, enhances the dielectric response of $RbLaMnWO_6$ during switching and can be a potential candidate for designing optoelectronic materials where the structure-property relation can be controlled by the electric field and/or temperature.

References:

- [1] Buvaneshwaran S, et al. Phys. Chem. C 127.31 (2023)
- [2] L.J. Sonter, M.C. Dade et.al. Nat. Commun. 11, 6 (2020)
- [3] E. Despotou, Vision for Photovoltaic's in the Future (Elsevier Ltd., 2012)
- [4] T.M. Brenner Nat. Rev. Mater. 1, 15007 (2016)
- [5] C. Stimer Brazilian Journal of Phy. (2021)
- [6] Muhammad et.al. Results in Physics (2019)
- [7] J. Allibe et.al Applied Phys. Let. (2010)
- [8] R. Haumont et.al Phys.Rev. B (2008).

The Stabilization Effect of Agmatine-Salicylate Ionic Liquids on PARP-1 for Parkinson's Disease: A Perspective from DFT and MD Simulations

Priyanka¹ and M. Prakash^{1,*}

¹Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603203, Chengalpattu District, Tamil Nadu, India.

The pathogenesis of Parkinson's disease (PD), a chronic degenerative disorder, is influenced by poly(ADP-ribose) polymerase-1 (PARP-1) since its activation is a prerequisite in dopaminergic neuronal cell death.^[1] The biocompatible agmatine-salicylate ionic liquid (i.e., [Agm][Sal₂] IL) has shown promising anticancer and non-cytotoxic characteristics.^[2] The stability of the complexes is inferred to be significantly influenced by the water-mediated hydrogen bonding (H-bonding) interactions of cations and anions with aromatic amino acids in the presence and absence of water molecules, as established by density functional theory (DFT) calculations of the [Agm]²⁺ and [Sal]⁻ ions. To identify the structural stability of PARP-1 in an IL medium, a series of concentrations (mole fraction 0.20–1.00) of ILs with PARP-1 using molecular dynamics (MD) simulations are studied for 200 ns. While the oxygen atoms in the –COO⁻ group of [Sal]⁻ anions established strong H-bonding interactions with the water molecules, the dicationic [Agm]²⁺ cations formed H-bonding interactions with the residues of PARP-1. It is concluded through various analyses that PARP-1 maintains its structural stability at 0.60–0.80 mole fractions of ILs in an aqueous medium. Thus, this finding signifies [Agm][Sal₂] IL as an efficient PARP-1 stabilizer; with further in vitro studies this IL can aid in the treatments for PD.^[3]

Reference

- [1] H. Kim, S. Ham, J. Y. Lee, A. Jo, G. H. Lee, Y. S. Lee, M. L. Cho, H. M. Shin, D. Kim, O. Pletnikova, J. C. Troncoso, J. H. Shin, Y. Il Lee, Y. Lee, *OncoTargets Ther.* **2017**, *8*, 106721.
- [2] M. B. Vraneš, J. J. Panić, A. S. Tot, S. M. Ostojić, D. D. Četojević-Simin, N. Janković, S. B. Gadžurić, *ACS Sustainable Chem. Eng.* **2019**, *7*, 10773.
- [3] S. Priyanka, M. Prakash, *Adv. Theory Simul.* **2024**, 2400551. **(Cover page Dec-2024)**

Contact Email ID: priyankhasridhar05@gmail.com

Unveiling the Coexistence of Giant Rashba Splitting and Topological properties in hexagonal crystal structure

Shivendra Kumar Gupta*, and Poorva Singh† Department of Physics,
Visvesvaraya National Institute of Technology, Nagpur, 440010, India

Composite Quantum Compounds (CQCs) have emerged as a powerful platform for investigating interactions between distinct quantum phenomena. Among these, topological superconductors, axion insulators, and materials exhibiting Rashba spin physics are particularly interesting. In this study, we focus on identifying materials that intrinsically combine giant Rashba splitting with topologically nontrivial states within a single crystalline framework. Our investigation highlights three materials—RbSnBi, CsSnBi, and ZnBi—uniquely combining the above properties. RbSnBi and CsSnBi are strong topological insulators characterized by multiple band inversions and Dirac surface states. RbSnBi exhibits a Rashba splitting energy of 133 meV with a Rashba coefficient (αR) of 4.26 eV Å, while CsSnBi exhibits a Rashba splitting energy of 228 meV with Rashba coefficient αR of 6.4 eV Å—the largest reported among topological materials. Alongside this giant Rashba coefficient, CsSnBi and RbSnBi are strong topological insulators having multiple band inversion and multiple Dirac surface states in a single crystal. These extraordinary properties underline their potential for spintronics, where the coupling of spin and momentum is essential for developing high-efficiency devices. In addition, ZnBi, with its hexagonal crystal structure, emerges as a topological type II Dirac semimetal with significant Rashba splitting. ZnBi exhibits a Rashba coefficient (αR) of 2.1 eV Å and a splitting energy of 118 meV, This duality of properties positions ZnBi as a promising candidate for spintronic applications and quantum technologies. The coexistence of Rashba spin physics and topological states in RbSnBi, CsSnBi, and ZnBi establishes a new paradigm for designing materials with multifunctional properties. This work paves the way for uncovering novel quantum phenomena and highlights the immense potential of intrinsic CQCs in advancing spintronics and next-generation quantum devices.

References

- [1] S. K. Gupta, A. Kore, S. K. Sen, and P. Singh, Coexistence of giant Rashba splitting, multiple band inversion, and multiple Dirac surface states in the three-dimensional topological insulator XSnBi (X= Rb, Cs), Physical Review B 107, 075143 (2023).
- [2] S. K. Gupta, N. Singh, S. K. Sen, and P. Singh, Pressure induced Topological Dirac semimetal in XcdP (X = na, K), arXiv preprint arXiv:2312.05636(2023).

* shivendrakumarg900@gmail.com

† poorvasingh@phy.vnit.ac.in

Defect engineering in two dimensional PdTe₂ pentagonal: Tuning electronic, optical, and magnetic properties

Poonam Sharma, Vaishali Roondhe, and Alok Shukla
Department of Physics, IIT Bombay, Mumbai 400076, India

Email: pspoonamsharma44@gmail.com

Recently, the successful synthesis of the pentagonal form of PdTe₂ monolayer (p-PdTe₂) was reported [Liu et al., Nature Materials 23, 1339 (2024)]¹. In this work, we present an extensive first-principles density-functional theory (DFT) based computational study of vacancies in this material. Our study covers the evolution of the electronic, optical, and magnetic properties of various defect configurations and compares those to the pristine monolayer (p-PdTe₂). We find that VPd (VTe) is the most stable defect in the p-PdTe₂ monolayer with 0.95 (1.60) eV of formation energy in the Te-rich (Pd-rich) limit. The defects alter the electronic properties of the monolayer significantly, leading to changes in their magnetic and optical properties due to the emergence of midgap impurity states. The defect complex VPd+4Te is found to induce spin-polarization in the system with a total magnetic moment of 1.87 μ_B . The obtained low diffusion energy barriers of 1.13 eV (in-plane) and 0.063 eV (top-bottom) corresponding to VTe indicates its facile migration probability is higher in the top-bottom direction in comparison to the in-plane direction at room temperature, as revealed by AIMD simulations as well. In order to guide the experimentalists, we also simulated the scanning-tunneling microscope (STM) images corresponding to all the defect configurations. Moreover, we also computed the electron-beam energies required for creating mono-vacancies. In the optical absorption spectra of the defective configurations, finite peaks appear below the band edge that are unique to the respective defective configuration. We have also computed the excess polarizability of the defective configurations with respect to the pristine one and found that maximum changes occur in the infrared and visible regions, providing insights into the change in their optical response as compared to the pristine monolayer. Our study will open the prospects of defect engineering in this and related materials with the aim of tuning their electronic, optical, and magnetic properties from the point of view of device applications.

References:

[1] L. Liu, Y. Ji, M. Bianchi, S. M. Hus, Z. Li, R. Balog, J. A. Miwa, P. Hofmann, A.-P. Li, D. Y. Zemlyanov, Y. Li, and Y. P. Chen, A metastable pentagonal 2D material synthesized by symmetry driven epitaxy, Nat. Mater. 23, 1339 (2024).

Identification of disorder and its influence on transport properties of half-Heusler compound

Dipanwita Bhattacharjee¹, Amrita Bhattacharya² and Titas Dasgupta³

1-3 Department of Metallurgical Engineering & Material Science, IIT Bombay, 400076
Maharashtra, India Email: b_dipanwita@iitb.ac.in

Ternary inter-metallic half-Heusler (HH) compounds (XYZ) with 18 valence electron count have revealed interesting thermoelectric (TE) properties pertaining to their narrow bandgap and flexibility in undergoing doping [1]. Despite having good electronic transport properties, such materials often have inherent atomic disorders appearing in the HH structure arising during the synthesis processes. There is an ongoing controversy among the literature reports as to the most dominant disorders that are influencing the transport of such materials [2]. Therefore, one needs to understand the underlying scattering mechanism to fine-tune the material properties for its widespread application. The key focus of this work is to recognize these disorders and their influence on transport properties based on both theoretical (first- principles) and experimental perspectives through scattering-dependent mobility studies. On exploration of mobility (μ) from theoretical calculations, a high dependence on scattering due to ionized impurity, and grain boundary is observed. With the increase in simulated disorder (interstitial), the ionized impurity and polar optical phonon (POP) scattering become the most dominant scattering mechanism, limiting the total μ of the compound. To analyze the experimental transport coefficients, the Single parabolic band (SPB) model along with analytical expression of different scattering mechanisms are used to fit the experimental transport data for understanding electronic transport in the compound. A mathematical optimization (least square method of cost optimization) technique is adopted to estimate unknown material parameters and carrier concentration. Then the magnitude of defects is estimated by fitting the model to the experimental data. The defect concentration is found to decrease with an increase in annealing duration and the dominance of POP scattering in higher annealed samples gives pathways to enhance the TE properties of the HH compound $\text{ZrNiSn}_{0.98}\text{Sb}_{0.02}$ with a 67% improvement in power factor.

References:

- [1] C. Uher, J. Yang, S. Hu, D. Morelli, and G. Meisner, *Physical Review B* 59, 8615 (1999)
- [2] X. Yang, Z. Jiang, J. Li, H. Kang, D. Liu, F. Yang, Z. Chen, E. Guo, X. Jiang, and T. Wang, *Nano Energy* 78, 105372 (2020)

Evolution of Electronic Structure Theory & Experimental Realization
(EESTER) – 2025

Negative Thermal Expansion of NASICON-type $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$ Solid-State Electrolyte

Sayan Ghosh,^{1,#} C. Sudakar^{1,*}

¹*Multifunctional Materials Laboratory, Department of Physics, Indian Institute of Technology Madras, Chennai-600036, Tamil Nadu, India*

[#]presenting author: ph19d066@smail.iitm.ac.in

*Corresponding author: csudakar@iitm.ac.in

Solid-state electrolytes (SSE) are being explored extensively as an alternative to flammable organic liquid electrolytes for lithium-ion battery. Of these, NASICON-type $\text{Li}_{1.3}\text{Al}_{0.3}\text{Ti}_{1.7}(\text{PO}_4)_3$ (LATP) is a promising electrolyte for its higher ionic conductivity, better chemo-mechanical stability. However, thermo-mechanical stability of the electrolyte-electrode interface hinders the possibility of its application towards lithium-ion battery. We have explored the thermal expansion properties of LATP by temperature-dependent X-ray diffraction. It has been observed that the open structural framework of LATP exhibits an isotropic negative thermal expansion (NTE) with an estimated lattice thermal expansion along a and c axis to be $-1.07 \times 10^{-5} (\pm 0.08 \times 10^{-5}) \text{ K}^{-1}$ and $-2.56 \times 10^{-5} (\pm 0.25 \times 10^{-5}) \text{ K}^{-1}$ in the temperature range of 93 K and 303 K, respectively. The overall shrinkage of LiO_6 octahedra and phosphate librational motion have been identified as possible reason for NTE behavior along c and a -axis, respectively. This isotropic contraction results in negative volume expansion with coefficient of $-4.82 \times 10^{-5} (\pm 0.37 \times 10^{-5}) \text{ K}^{-1}$. Greater extent of distortion is found to be present in LiO_6 octahedra, estimated from temperature-dependent quadratic elongation and bond angle variance measurement. However, NTE behavior persists till 80 °C and with further increment of temperature a gradual switch over to positive thermal expansion behavior becomes observable.

First principles studies on functional mode couplings in oxide superlattices

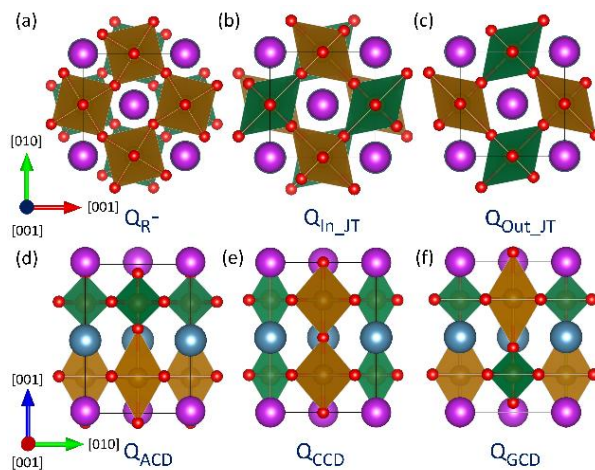
Rajan Gowsalya and Saurabh Ghosh

Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur
603 203, Tamil Nadu, India

Email: gowsalyarajan441@gmail.com

Abstract

Our research investigates the functional mode couplings in multiferroic materials with perovskite oxide superlattices, focusing on nickelates and ferrites, which are crucial for technological applications due to their unique electronic and magnetic properties [1]. In particular, the hybrid improper ferroelectric mechanism in oxide superlattices $(ABO_3)_m/(A'BO_3)_n$, (where m and $n = 1, 2$ and 3) induces microscopic polarization and also can tune the electronic structure and can tailor metal to insulator transition. Specifically, $LaNiO_3/CaNiO_3$ superlattices showed a ferromagnetic polar ground state with a half-metallic phase which is crucial for spintronics, memory storage, and memory transport [2]. On the other hand ferrite side, superlattices like $BiFeO_3/LaFeO_3$ and $BiFeO_3/CaFeO_3$ are valued for their robust magnetic properties and potential in spintronic devices. The $BiFeO_3/CaFeO_3$ superlattice, in particular, is noted for its strong magnetoelectric coupling and potential to stabilize exotic magnetic phases under strain. Utilizing first-principles calculations, we explore the structural, electronic, magnetic properties, and strain effects on $BiFeO_3/CaFeO_3$ and $LaNiO_3/CaNiO_3$ superlattices. In addition to the primary order parameters, rotation ($a^0a^0c^+$) and tilt ($a^-a^-c^0$) distortions along $a^0a^0c^+$ and $a^-a^-c^0$ and antiferroelectric distortion, we have



discovered a polar charge disproportionation mode (Q_{CD}) in (1/1) superlattice [3]. Our findings show that refining functional mode couplings makes the system much more stable and possible to get enhanced ferroelectricity, magnetoelectric coupling, and tunable electronic band topologies. These insights provide a pathway for designing multifunctional materials with tailored properties, paving the way for next-generation devices in electronics, spintronics, and energy conversion.

Reference:

[1] Shaikh, Monirul, et al. *Physical Review B* 101.5 (2020): 054101

[2] Put your JMMM aper

[3] put your BTO/CFO as submitted

Acknowledgement: S.G. acknowledges funding from DST-Core Research Grant/2023/3209

DFT Study on the Functionalization of Aluminum Nitride Nanotubes with Organic Acids for Targeted Delivery of Carmustine

Abinaya.V¹, Sneha.J¹, K. Janani Sivasankar*¹, D. John Thiruvadigal*¹,

¹Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India

*Corresponding author e-mail: johnd@srmist.edu.in, jananik@srmist.edu.in

ABSTRACT

This study investigates the structural and electronic modifications of single-walled armchair (5,5) Aluminum Nitride Nanotubes (AlNNTs) through functionalization with organic acids malic acid (MA), acetic acid (AA), and propionic acid (PA) using Density Functional Theory (DFT) calculations. Single and double-side functionalization significantly influences the nanotubes' properties, transitioning from sp^2 to sp^3 hybridization and increasing ionic character, which impacts bond lengths, bond angles, and electronic properties. Among the acids studied, malic acid functionalization leads to the most significant reduction in the band gap, enhancing electronic conductivity and reactivity, making it particularly suitable for drug delivery applications. Solvation studies reveal that functionalization improves the AlNNTs' solubility, with the double-side functionalization of malic acid showing the most pronounced effects. Interaction studies with the chemotherapeutic carmustine show strong binding energy (-0.857 eV) and favorable charge transfer, indicating a stable drug-nanocarrier complex. Further solvation analysis demonstrates that increasing water molecules reduces binding energy and enhances carmustine's desorption and solubility, thereby improving its bioavailability. These findings confirm that functionalizing AlNNTs with organic acids, especially malic acid, optimizes their structural stability and electronic properties, highlighting their potential as nanocarriers for targeted drug delivery applications.

Keywords: Aluminum Nitride Nanotubes, Density Functional Theory, Organic Acid Functionalization, Drug Delivery, Carmustine, Solubility.

References

1. Bagheri, Z. and Peyghan, A.A., 2013. DFT study of NO₂ adsorption on the AlN nanocones. Computational and Theoretical Chemistry, 1008, pp.20-26.
2. Vatanparast, M. and Shariatinia, Z., 2018. AlN and AlP doped graphene quantum dots as novel drug delivery systems for 5-fluorouracil drug: theoretical studies. Journal of Fluorine Chemistry, 211, pp.81-93.
3. Zhao, M., Xia, Y., Zhang, D. and Mei, L., 2003. Stability and electronic structure of AlN nanotubes. Physical Review B, 68(23), p.235415.

DFT STUDY ON FUNCTIONALIZATION OF BORON NITRIDE NANOTUBE WITH NON-ESSENTIAL AMINO ACIDS FOR TARGETED DELIVERY OF ALLICIN IN CANCER TREATMENT

Sneha. J¹, Abinaya. V¹, K. Janani Sivasankar*¹, D. John Thiruvadigal*¹

¹Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603 203, India

*Corresponding author e-mail: johnd@srmist.edu.in, jananik@srmist.edu.in

ABSTRACT

This study explores the structural, electronic, and solubility properties of (5,5) Boron Nitride Nanotubes (BNNT) functionalized with non-essential amino acids (cysteine, proline, and alanine) through single (X) and double-sided (2X) functionalization, using Density Functional Theory (DFT). Functionalization causes a transition from sp^2 to sp^3 hybridization, with proline leading to the largest reduction in bandgap from 4.46 eV to 3.79 eV. The total energy, binding energy, and formation energy calculations demonstrate increased stability in the functionalized systems, particularly with cysteine. The chemical potential decreases upon functionalization, especially in BNNT-2X, indicating increased reactivity. Additionally, functionalization leads to significant charge transfer, enhanced dipole moments, and increased percentage ionic character, suggesting improved interaction with biological environments. The Gibbs free energy of solvation further confirms favorable interactions with aqueous environments, with BNNT-2Cys exhibiting the most negative values, enhancing its solubility. The analysis of the interaction between BNNT2Cys and the allixin drug shows high stability, improved charge transfer, and reduced bandgap, indicating its potential for enhanced drug delivery. Collectively, these findings highlight the promise of functionalized BNNTs in applications such as targeted drug delivery, driven by their improved solubility, stability, and interaction with biological systems.

Keywords: Single-Walled Boron Nitride Nanotube (SWBNNT), Density Functional Theory (DFT), Non-essential amino acids, Interaction analysis.

REFERENCES

- [1] Zhi C, et al., Boron nitride nanotubes. *Materials Science and Engineering: R: Reports*. 70(3-6):2010 Nov 22;92- 111. <https://doi.org/10.1016/j.mser.2010.06.004>.
- [2] Saikia N, et al., Interaction of pyrazinamide drug functionalized carbon and boron nitride nanotubes with pncA protein: a molecular dynamics and density functional approach. *Rsc Advances*. 3(35):2013;15102-7. <https://doi.org/10.1039/C3RA42534G>.

EXPLORING HYDROGEN BONDING INTERACTIONS USING NEURAL DENSITY FUNCTIONAL

Susannal Ezhilarasi.S¹, Jijila², Nirmala.V^{1*} Mail: susannalsamuel1999@gmail.com

^{1,2} PG and Research Department of Physics, Queen Mary's College
Mylapore, Chennai, 600004, India

ABSTRACT:

This paper explores the hydrogen bonding phenomena through computational methods using machine learned density functional, Deepmind (DM21), which is designed to handle the fractional electron problem. Inspired by recent research article of science journal, where the DM21 functional successfully modelled in complex systems such as hydrogen chains and water clusters using open-source deep learning libraries. This study focuses on proper and improper hydrogen bonds, characterized by their distinct charge transfer mechanisms, proper hydrogen bonds involve charge transfer from lone pair of the proton acceptor to the antibonding orbital of the X-H bond, leading to bond elongation, in contrast, improper hydrogen bonds exhibit bond contraction due to charge transfer to remote parts of the donor molecule. "Fractional electron character" is an important problem in chemistry, and DeepMind has used machine learning to fix it. As per Science article [1] by the authors of Google DeepMind, a neural network based Density Functional was created by using fractional-electrons systems in the training set. Hence, we employ DeepMind21 to study the proper and improper Hydrogen bond. These phenomena are explored through optimized bond length and vibrational frequency analyses for some hydrogen bonding complexes. The computational comparisons were performed for both traditional density functional and machine learnt neural functional (DM21, DM21m) with cc-pVDZ basis set. The results obtained from the computational studies is used to calculate HOMO-LUMO energy gap, the chemical reactivity by frontier molecular orbital, Charge redistribution through Mullikan population analysis and Morokuma decomposition analysis to understand the total interaction energy through molecular fragments. The observed results of Dm21 closely agrees with CCSD(T) studies. We have computed the HOMO-LUMO energy gap, electrostatic potential (ESP) diagrams for both complex and monomer from obtained Deep Learning-based DFT computations. This study demonstrates the ability of DeepMind21 (which solved the fractional electron problem) to provide accurate and detailed insights into hydrogen bonding interactions. The findings underscore the promise of neural networks in computational chemistry [2], paving the way for more accurate and efficient studies of molecular interactions.

Reference: [1] James Kirkpatrick et al., Pushing the frontiers of density functionals by solving the fractional electron problem. *Science* 374, 1385-1389(2021). DOI:10.1126/science.abj6511

[2] Pederson R, Kalita B, Burke K (2022) Machine learning and density functional theory. *Nat Rev Phys.* <https://doi.org/10.1038/s42254-022-00470-2>

Molecular Mechanism behind Cholinium-Taurate Ionic Liquid in Stabilisation of HDAC2 for Alcohol Use Disorders: Insights from DFT and MD Simulations

S.M. Esther Rubavathy¹ and M. Prakash²

Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603 203, Chengalpattu, Tamil Nadu, India.

* e-mail: es3122@srmist.edu.in; Telephone: +91 9042377826

Abstract:

The study explores how an active pharmaceutical ingredient-ionic liquid (API-IL) Cholinium Taurate ([Cho]⁺[Tau]⁻) IL, may alter the structural and functional stability of Histone Deacetylase 2 (HDAC2), a crucial enzyme linked to alcohol use disorder (AUD) [1]. The hallmarks of AUD, a worldwide health burden, include epigenetic dysregulation, in which HDAC2 plays a major role in gene silencing and chronic neuroplastic alterations. Leveraging the unique physicochemical properties of [Cho]⁺[Tau]⁻ IL, including hydrogen bond (H-bond) formation and structural reinforcement, we explored its therapeutic potential through comprehensive computational approaches [2]. Density Functional Theory (DFT) analyses provided insights into the hydration and stability profiles of [Cho]⁺[Tau]⁻ IL, while 200-ns Molecular Dynamics (MD) simulations elucidated its interaction with HDAC2 at the molecular level. Strikingly, the [Tau]⁻ ion emerged as a key modulator of HDAC2 stability, facilitating conformational transitions in the enzyme's secondary structure, notably from turns to helices [3]. This stabilization is mediated by intricate hydration networks, water-bridged H-bonds, and diverse non-covalent interactions (NCI), as confirmed through rigorous structural analyses. Our findings highlight [Cho]⁺[Tau]⁻ IL a robust stabilizer and potential inhibitor of HDAC2, offering a novel therapeutic avenue for AUD treatment. This work underscores the promise of API-ILs in targeting epigenetic regulators and advancing strategies for AUD.

Keywords: AUD, HDAC2, DFT, MD and [Cho]⁺[Tau]⁻ IL

References:

- [1] J. P. Nelson, *Alcohol. Clin. Exp. Res.*, 38, (2014), 1167–1175.
- [2] M. Smiglak, J. M. Pringle, X. Lu, L. Han, S. Zhang, H. Gao, D. R. Mac Farlane and R. D. Rogers, *Chem. Commun.*, 50, (2014), 9228–9250.
- [3] J. Chen, S. Zhang, W. Wang, L. Pang, Q. Zhang and X. Liu, *J. Chem. Inf. Model.*, 61, (2021), 1954–1969.

A DFT Study of Doped MoSe₂ Monolayer for Improved Sensing of H₂S and HCN Gas Molecules

N. Viveka¹, C. Preferencial Kala^{*1}, D. John Thiruvadigal¹

¹Computational Materials Science and Nano Devices Simulation Laboratory,
Department of Physics and Nanotechnology,
SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India.

* Email: preferec@srmist.edu.in

Abstract

Density Functional Theory (DFT) is used to study the electronic characteristics and sensing behaviour of pure and Rh-MoSe₂ monolayers on HCN and H₂S gases. The MoSe₂ monolayer is used in transistors, photo-detectors, energy storage, and sensors because of its high surface-to-volume ratio, high electrical conductivity, and tuneable semiconducting nature. Rhodium (Rh) is a noble metal that is used as a dopant to improve the characteristics of carbon nanotube, graphene, and MoS₂ systems. Rh has high catalytic behaviour and electron mobility. The monolayer enhances the stability and adsorption when a dopant is substituted for Se. The stability of both pure and doped systems has been analysed through the binding energy and phonon band structures. The best systems are reviewed after the gases positioned at potential locations interacted with the surface. The Band structure, density of states, projected density of states, charge transfer, adsorption energy, and recovery time are all examined to analyse the electronic and sensing characteristics. Rh-MoSe₂ exhibits better adsorption for HCN and H₂S gas molecules than pure monolayer. Our results indicated that the Rh is an excellent catalyst and improves the sensing behaviour of the MoSe₂ monolayer.

References

- [1] Donarelli, M. and Ottaviano, L., 2018. 2D materials for gas sensing applications: a review on graphene oxide, MoS₂, WS₂ and phosphorene. *Sensors*, 18(11), p.3638.
- [2] Cui, H., Zhang, G., Zhang, X. and Tang, J., 2019. Rh-doped MoSe₂ as a toxic gas scavenger: A first-principles study. *Nanoscale Advances*, 1(2), pp.772-780.
- [3] Panigrahi, P., Hussain, T., Karton, A. and Ahuja, R., 2019. Elemental substitution of two-dimensional transition metal dichalcogenides (MoSe₂ and MoTe₂): implications for enhanced gas sensing. *ACS sensors*, 4(10), pp.2646-2653.

A DFT study on the drug delivery nature of Zinc Oxide nanocluster for anti-inflammatory drugs

G. Nivethitha¹, V. Sudha^{1*}

¹SRM Institute of Science and Technology, Kattangulathur-603 203, Tamil Nadu, India.

*E-mail: sudhav1@srmist.edu.in

The current study investigates the potential of (ZnO)₁₂ nanocluster as drug carrier for anti-inflammatory drugs such as aspirin and citicoline using theoretical studies. The structural optimization of Zn₁₂O₁₂ nanocage and drugs has been investigated using DFT method with B3LYP functional in both gaseous and aqueous phases. Also, LANL2DZ and 6-311++G (d, p) are the basis sets used for Zn metal and Oxygen atom respectively in Gaussian 16 package. This study evaluates the adsorption behaviour of aspirin and citicoline on a Zn₁₂O₁₂ nanocluster in gaseous phase. Further, the optimized structures in gaseous phase were also examined in the aqueous phase using Polarizable Continuum Model (PCM). Adsorption analysis focusing on interaction energies and atomic distances between the drug molecules and the nanocluster, demonstrates the potential of the (ZnO)₁₂ cluster as a drug carrier. Evaluating the solvation energy and photophysical properties of the most stable complexes in an aqueous medium could further demonstrate the suitability of the Zn₁₂O₁₂ nanocage as a biosensor and drug carrier for aspirin and citicoline. Also, various properties including thermodynamic properties, Molecular Electrostatic Potential (MEP), Natural Bond Orbital (NBO), Non-covalent interactions (NCI), and HOMO-LUMO orbital characteristics of anti-inflammatory drugs on (ZnO)₁₂ nanocage in aqueous phase were analysed. In order to reveal the drug delivery nature, the drug release profile will be simulated by protonating the complex in order to mimic the biological environment of the inflammatory cells. Hence, these findings may offer valuable insights into the potential of (ZnO)₁₂ nanocluster for effective drug delivery in biological systems.

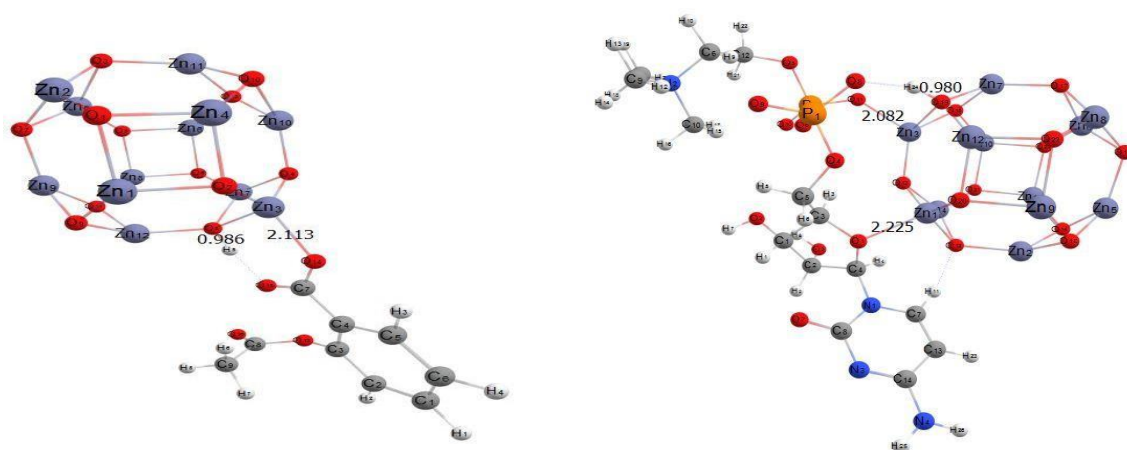


Figure 1: The optimized structures of (A) Zn₁₂O₁₂-Aspirin and (B) Zn₁₂O₁₂-Citicoline Complexes in aqueous phase.

Keywords: Drug delivery, Drug carrier, Zn₁₂O₁₂ nanocluster, Aspirin, Citicoline

Reference:

[1] Mohammad Taghi Baei, Ali Ahmadi Peyghan, Quantum chemical analysis on hydrogenated Zn₁₂O₁₂ nanoclusters, *Comptes Rendus Chimie*, 2013, 16, 122–128.

DFT+NEGF Insights on Thermoelectric Transport Properties of GeTe/arsenene vdW Heterostructure: Interface Engineering

Sakthi Balaji A¹, Akash Ramasamy¹, Hariharan R M^{1*}, John Thiruvadigal D¹

¹ Computational Materials Science and Nanodevices Simulation Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India

*Corresponding author: hariharr@srmist.edu.in

Abstract

Stacking two-dimensional materials into van der Waal heterostructures (vdWH) is a promising choice for thermoelectric devices. Applying the first-principles method with NEGF formalism, we examined the structural, electronic study, and thermoelectrical transport features of the GeTe/arsenene 2D vdW heterostructure and its constituent monolayer. Heterostructures are constructed by combining GeTe with arsenene (AS) monolayers through vdW stacking using the Coincident site lattice (CSL) theory. The stability of these vdWHs is proven by the parameters of interlayer distances, binding energies, and dynamical stability. The stable heterostructure exhibits an indirect bandgap (0.41 eV) with a band-type-II profile. A two-probe device model of the armchair (AC_vdWH) is constructed to examine the thermoelectric transport properties. The negative Seebeck coefficient of the systems depicts an n-type character. Our findings predict that n-type AC_GeTe/arsenene vdWH with a high ZT value of 4.4 at 400 K, will be the promising choice for low-temperature thermoelectric device applications.

Keywords: GeTe/AS vdWH, DFT+NEGF, Type-II band alignment, Seebeck coefficient, and figure of merit (ZT)

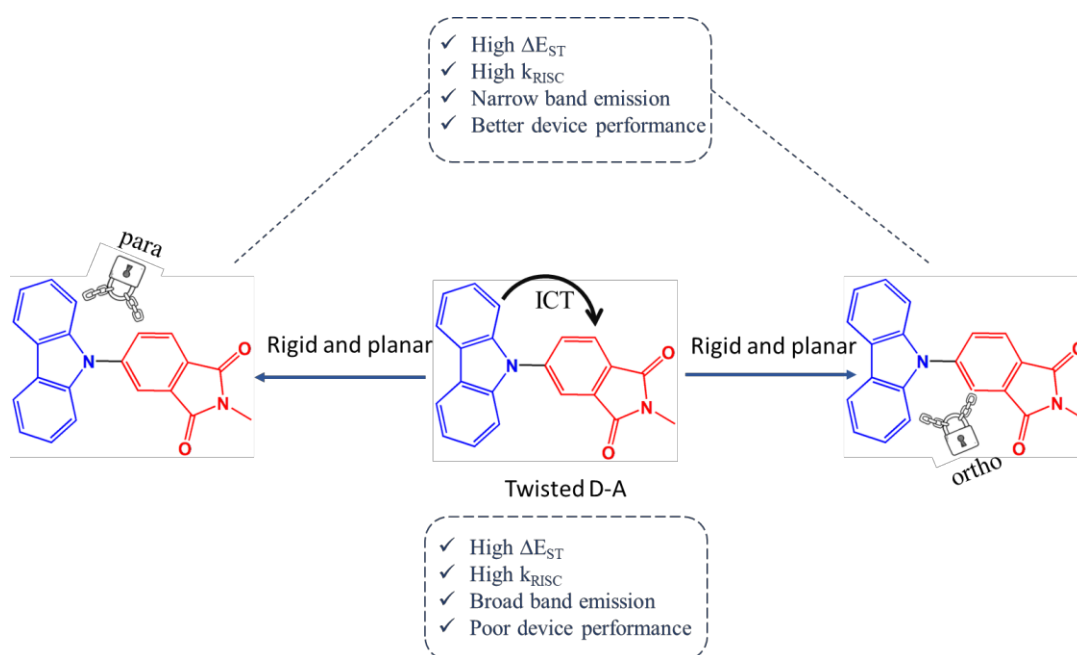
References:

1. P. Zhang, F. Zhao, P. Long, Y. Wang, Y. Yue, X. Liu, Y. Feng, R. Li, W. Hu, Y. Li, Sonication-assisted liquid-phase exfoliated α -GeTe: a two-dimensional material with high Fe 3+ sensitivity, *Nanoscale* 10(34) (2018) 15989-15997
2. C. Kamal, M. Ezawa, Arsenene: Two-dimensional buckled and puckered honeycomb arsenic systems, *Physical Review B* 91(8) (2015) 085423.
3. A. Sidike, B. Zhang, J. Dong, G. Guo, H. Duan, M. Long, Realization of high thermoelectric performance of black phosphorus/black arsenic hybrid heterojunction nanoscale devices by interface engineering, *Physica B: Condensed Matter* 673 (2024) 415357.

The Role of Backbone Rigidification in Thermally Activated Delayed Fluorescence: A Structure-Property Analysis

L. N. S. Laya Pagadala and Mahesh Kumar Ravva
Department of Chemistry, SRM University-AP, Amaravati, India 522240

Thermally activated delayed fluorescence (TADF) exploits twisted intramolecular charge transfer states to harvest triplet excitons in OLEDs through the twisted configuration of donor and acceptor units. However, the highly twisted conformation of TADF molecules results in limited device lifetimes. In this work, we have designed rigid and planar fused TADF emitters based on indolocarbazole as a donor with various acceptors. The newly designed molecules have been thoroughly studied using density functional theory and time-dependent density functional theory methods. Furthermore, we have studied their excited state properties. Results obtained from these simulations will help establish the intricate relationships between molecular structure and key photochemical properties, including intersystem crossing rates, reverse intersystem crossing rates, radiative decay rates, and charge transfer.



Reference:

- (1) Kuila, S.; Miranda-Salinas, H.; Eng, J.; Li, C.; Bryce, M. R.; Penfold, T. J.; Monkman, A. P. Rigid and Planar π -Conjugated Molecules Leading to Long-Lived Intramolecular Charge-Transfer States Exhibiting Thermally Activated Delayed Fluorescence. *Nat Commun* **2024**, *15* (1), 9611. <https://doi.org/10.1038/s41467-024-53740-1>.

Superior Anchoring behaviour of Calcium Polysulfides through the Integration of ZIF-8 MOF as a substantial cathode in Ca–S Battery: A DFT study

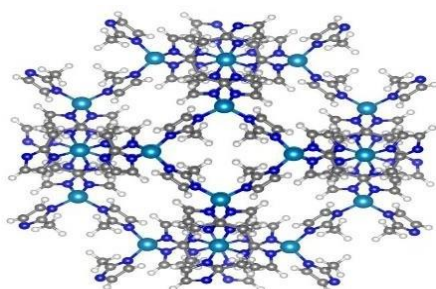
S. Saral Sessal¹, V. Sudha^{1*}

¹ Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603 203, Tamil Nadu, India

E-mail: ss6992@srmist.edu.in; Telephone: 8524983528

In the current scenario, Calcium ion batteries (CIBs) have gained attention due to the abundant and relatively lower cost of calcium than lithium. Also, the divalent nature of calcium acquires a high capability to be combined with sulfur cathodes resulting in the high energy–density calcium sulfur batteries. Meanwhile, to overcome the challenges of sulfur batteries including the polysulfide shuttle effect, volume expansion, and dissolution of active materials, considerable efforts have been implemented with the introduction of an anchoring material. The metal-organic framework is widely used in metal-sulfur batteries as an electrode due to its structural adaptability, and functional tunability at the molecular level which paves the way to rapid ionic mobility, and improved electronic conductivity. In the present research, DFT calculations have been performed using the Vienna ab initio Simulation Package (VASP). Firstly, ZIF–8 Unit cell containing 276 atoms was optimized by employing PAW pseudopotential and GGA–PBE exchange–correlation functional. DFT+U method was adopted along with DFT-D3 dispersion correction for all the adsorption studies. For computational efficiency, ZIF-8 primitive cell (204 atoms) structure have been considered and the adsorption behaviour of different polysulfides such as CaS₈, CaS₆, CaS₄, CaS₂ and CaS over the optimized ZIF-8 primitive cell were examined. Further, the band structure calculation, PDOS study, charge transfer analysis, and MD simulation studies have been carried out to understand the anchoring ability of ZIF–8 in calcium – sulfur battery.

A.



B.

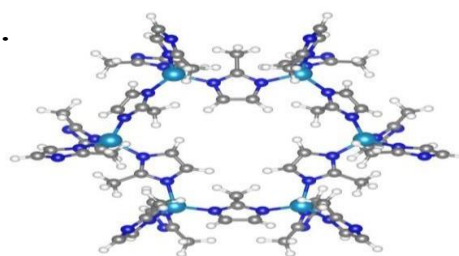


Figure: Optimized structures of A) ZIF–8 Unit cell and B) ZIF–8 Primitive cell

Keywords: Calcium- sulfur battery, shuttle-effect, ZIF-8 MOF, anchoring cathode

Reference

[1] Li, C., Zhang, X., Zhang, Q., Xiao, Y., Fu, Y., Tan, H. H., ... & Wu, Y. *Computational and Theoretical Chemistry*, **2021.1196**, 113110.

Electronic Structure and Magnetic Properties of $S = 1/2$ Alternating Spin Chain System $\text{KCuGa}(\text{PO}_4)_2$

R.C Moharana,¹ ***V. K Singh**,¹ **S. Gayen**,² **T Chakrabarty**,³ **S. K Panda**,² **S Chattopadhyay**^{4*}
and **B. Koteswararao**¹

¹ *Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517506, India*

² *Department of Physics, Bennett University, Greater Noida, Uttar Pradesh 201310, India*

³ *Division of Sciences, Krea University, Sri City, Andhra Pradesh 517646, India*

⁴ *UGC-DAE Consortium for Scientific Research, Mumbai Centre, India*

Email: ph24d003@iittp.ac.in, Ph20d504@iittp.ac.in

Abstract: The correlation between low dimensionality and spin interactions can foster the emergence of unique and exotic states within quantum magnets. In this study, we explore the structural, magnetic, and heat capacity properties, along with density functional theory + Hubbard U (DFT + U) electronic structure calculations on the Cu-based compound $\text{KCuGa}(\text{PO}_4)_2$, which has $S = 1/2$ alternating spin chains with J_1 and J_2 couplings. The nearest-neighbor (NN) coupling J_1 forms spin dimers, and the second-NN coupling J_2 constitutes spin chains. The interactions between Cu^{2+} ($S = 1/2$) ions are predominantly antiferromagnetic (AFM) in nature, as evidenced by the Curie-Weiss temperature $\theta_{\text{CW}} \approx -8$ K. The magnetic data analysis based on alternating chain simulations gives out the spin gap of 10 K with the ratio of exchange interaction strengths $(J_2/J_1) = 0.40$. Theoretical electronic structure calculations also estimate the relative strength of exchange couplings through the total energy method and by evaluating hopping integrals. The ratio of exchange couplings derived from DFT calculations aligns well with the values obtained from our experimental findings.

References:

- [1] D. C. Johnston R. K. Kremer, M. Troyer, X. Wang, A. Klümper, S. L. Bud'ko, A. F. Panchula, P. C. Canfield. 2000. Thermodynamics of spin $S=1/2$ antiferromagnetic uniform and alternating-exchange Heisenberg chains. *Phys. Rev. B*, 61, p. 9558–9606.
- [2]. X. H. Chen, R. Z. Guo, Y. X. Huang, Y. Pan, J. X. Mi., 2021. Crystal structure and magnetic properties of the magnetically isolated zigzag chain in $\text{KGaCu}(\text{PO}_4)_2$. *Dalton Trans.*, **50**, p. 7835–7842.

Facile synthesis of large area single crystal MoS₂ for photodetector

Gowthami S¹ and Pramoda K Nayak^{1,2}

¹Centre for Nano and Material Sciences (CNMS), Jain (Deemed-To-Be University), Jain Global Campus, Kanakapura, Bangalore 562112, India

²Department of Physics, Indian Institute of Technology Madras, Chennai 600 036, India

E-mail: gowthami.s@jainuniversity.ac.in

Abstract: Two-dimensional (2D) materials, particularly semiconducting transition metal dichalcogenides (TMDs), are gaining attention for their potential in electronics and optoelectronics [1]. Among these, molybdenum disulfide (MoS₂) in its 2H phase is distinguished by its thermodynamic stability and notable properties, including a tunable bandgap, high carrier mobility, and excellent light absorption [2]. These qualities make 2H-MoS₂ ideal for applications like field-effect transistors, photodetectors, and solar cells [3]. In the present work, we report a cost-effective method for synthesizing large-area single-crystal 2H-MoS₂ with a 13 mm diameter and 1 mm thickness. The process involves high-pressure compaction of MoS₂ powder, followed by thermal annealing at 1000°C for 24 hours in an inert argon atmosphere. This scalable method produces high-quality crystals with minimal defects, making it suitable for industrial use. X-ray diffraction (XRD) analysis reveals a prominent peak around $2\theta \approx 14^\circ$, corresponding to the (002) reflection of the 2H crystal structure. The sharp diffraction peaks indicate high crystallinity and phase purity, crucial for optimizing the material's performance. Raman spectroscopy shows peaks at $\sim 377\text{ cm}^{-1}$ and $\sim 407\text{ cm}^{-1}$, corresponding to the characteristics E_{2g}¹ and A_{1g} modes of 2H-MoS₂, respectively. The increased separation ($\sim 30\text{ cm}^{-1}$) between E_{2g}¹ and A_{1g} modes suggests the formation of bulk 2H-MoS₂. In addition, the photoluminescence (PL) spectrum shows peaks at 1.75 eV and 2.06 eV, corresponding to the A and B excitons, confirming the bulk nature of the material. Room-temperature photocurrent measurements show a photocurrent (I_{photo}) of 47 μA and a dark current (I_{dark}) of 43 μA at $\pm 10\text{ V/cm}$, resulting in a photoresponsivity (R) of $\sim 82\text{ }\mu\text{A/W}$. These findings indicate the persistent photoconductivity effect, suggesting the material's potential for photodetectors and light sensors. Overall, the synthesized 2H-MoS₂ crystals exhibit excellent optoelectronic properties, confirming their potential for scalable production and future applications in photosensitive devices at room temperature.

References:

- [1] Chhowalla, M., Shin, H. S., Eda, G., Li, L. J., Loh, K. P., & Zhang, H. (2013). The chemistry of two-dimensional layered transition metal dichalcogenide nanosheets. *Nature chemistry*, 5(4), 263-275.
- [2] Czerniak-Łosiewicz, K., Gertych, A. P., Świniarski, M., Judek, J., & Zdrojek, M. (2020). Time dependence of photocurrent in chemical vapor deposition MoS₂ monolayer—intrinsic properties and environmental effects. *The Journal of Physical Chemistry C*, 124(34), 18741-18746.
- [3] Furchi, M. M., Polyushkin, D. K., Pospischil, A., & Mueller, T. (2014). Mechanisms of photoconductivity in atomically thin MoS₂. *Nano letters*, 14(11), 6165-6170.

Theoretical Investigation of Ba_3XO ($X = Si, Ge, Sn$): Exploring Structural, Electronic, and Elastic Properties in Inverse Perovskites

A. Thameemul Ansari¹, K.P. Mohamed Jibri¹, C. Kanagaraj¹, J. Archana², M. Navaneethan^{1*2}

¹Nanotechnology Research Centre, SRM Institute of Science and Technology, KTR Campus, Chengalpattu Tamilnadu-603-203.

²Centre of Excellence in Materials and Advanced Technologies, SRM Institute of Science and Technology, KTR Campus, Chengalpattu Tamilnadu-603-203.

Abstract

Inverse perovskites Ba_3XO ($X = Si, Ge, Sn$) are an intriguing class of materials characterized by unique structural, electronic, and elastic properties, making them promising candidates for thermoelectric applications. In this study, first-principles calculations are employed to investigate the structural stability, electronic band structure, and elastic properties of these compounds, providing insights into their thermoelectric potential. The materials adopt a distinctive $O-A_6$ octahedral framework, where cations occupy the face-centred positions, leading to soft lattice dynamics and an ideal electronic interaction. The electronic structure analysis, performed using density functional theory, revealed the presence of both heavy and light electronic bands near the valence band maximum, which significantly influence the thermoelectric properties. The band gaps were determined to be 0.64 eV for Ba_3SiO , 0.60 eV for Ba_3GeO , and nearly zero for Ba_3SnO . Notably, Ba_3SnO exhibits metallic behaviour, with its conduction bands primarily dominated by contributions from $Ba-5d$ states. These findings highlight that the electrical conductivity, a critical factor for thermoelectric efficiency, is strongly dependent on the choice of the X-site anion. Elastic property calculations, including elastic constants, bulk modulus, and Poisson's ratio, confirm the mechanical stability of the compounds. $Ba_3Si_{0.5}Sn_{0.5}O$ demonstrates an optimal balance of stiffness and ductility, reflected in a Poisson's ratio of 0.246, favourable for thermoelectric performance. Analysis of Debye temperatures (214.9 K to 224.7 K) and Grüneisen parameters highlights significant phonon scattering, contributing to reduced lattice thermal conductivity which is essential for thermoelectric materials. This study provides a detailed understanding of the interdependence between the structural, electronic, and elastic properties of Ba_3XO ($X = Si, Ge, Sn$). The results underscore the exceptional thermoelectric potentials of $Ba_3Si_{0.5}Sn_{0.5}O$, which combines enhanced electronic transport with reduced lattice thermal conductivity, offering a pathway for efficient thermoelectric energy conversion.

References:

- [1] He, Xinyi, et al. "Inverse-Perovskite Ba_3BO ($B= Si$ and Ge) as a High Performance Environmentally Benign Thermoelectric Material with Low Lattice Thermal Conductivity." *Advanced Science* 11.10 (2024): 2307058.
 - [2] Pöhls, and Arthur Mar. "Thermoelectric properties of inverse perovskites A_3TtO ($A= Mg, Ca$; $Tt= Si, Ge$): Computational and experimental investigations." *Journal of Applied Physics* 126.2 (2019).
-

Role of structural disorder on the electronic and magnetic properties of Cr₃Al

Pooja Vyas^{1,*}, R. Philip², S. Manni², and Aftab Alam¹

¹Department of Physics, Indian Institute of Technology Bombay, Mumbai-400076, Maharashtra, India.

²Department of Physics, Indian Institute of Technology Palakkad, Kerala-678623, India.

*Email: poojavyas1251995@gmail.com

Abstract: High-performance spintronic devices demand materials such as half-metals or spin gapless semiconductors (SGS) that exhibit a peculiar electronic band structure that is suggestive of high spin polarization. Apart from ternary and quaternary Heusler alloys, in recent years, binary DO3-type Heusler alloys are also been examined from a spintronics viewpoint [1-4]. From this Heusler family, we have theoretically investigated and tried to unveil the structural, electronic, and magnetic properties of Cr₃Al, a comparatively less explored binary compound. It is observed that the DO3-structured Cr₃Al behaves as a metallic ferrimagnet at equilibrium with a net magnetic moment of 2.77 μ_B /f.u. and transits to an SGS at an expanded lattice constant. Experimental [5] magnetic measurements on bulk single- and polycrystalline Cr₃Al predict a very small net magnetic moment ($\sim 10^{-3}$ μ_B /f.u.), and the X-ray diffraction data confirms the absence of (111) and (200), the two order-dependent reflection peaks. Since the discrepancy in the net moment and the absence of peaks are associated with an A2-type structural disorder, the theoretical investigations taking this disorder into account substantially reduces the net magnetic moment to 0.71 μ_B /f.u. Further, the electronic studies predicts a spin gapless semiconducting behaviour for the ground state A2 disordered structure, hinting towards a possibility for Cr₃Al of being a potential candidate for spintronic applications.

References:

- [1] W. Q. Zhao, X. F. Dai, X. M. Zhang, Z. J. Mo, X. T. Wang, G. F. Chen, Z. X. Cheng, and G. D. Liu, *IUCrJ*, **6**, 552 (2019).
- [2] G. Y. Gao and K-L Yao, *Appl. Phys. Lett.*, **103**, 232409 (2013).
- [3] Z. Boekelheide, T. Saerbeck, Anton P. J. Stampfl, R. A. Robinson, D. A. Stewart, and F. Hellman, *Phys. Rev. B*, **85**, 094413 (2012).
- [4] Z. Boekelheide, D. A. Stewart, and F. Hellman, *Phys. Rev. B*, **86**, 085120 (2012).
- [5] R. E. Philip, R. Kumar, and S. Manni, *AIP Conf. Proc.*, **2995**, 020151 (2024).

First Principles Calculations of Argyrodite Compounds Ag₉XSe₆ (where X = Al, Ga and In) for Thermoelectric Applications

Ramesh Hariharan¹, K P Mohamed Jibri¹, C Kanagaraj¹, Muthuramalingam Prakash², Mani Navaneethan^{1*}

¹ Nanotechnology Research Centre, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India.

² Computational Chemistry Research Laboratory, Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India .

Email : hariharr1@srmist.edu.in and navaneem@srmist.edu.in

Abstract:

Argyrodites compounds are widely used in the applications of energy storage devices and energy conversion methods. Thermoelectric materials convert the heat energy into electricity. The characteristics of Phonon Liquid Electron Crystal (PLEC) of argyrodites, phonon travels through the liquid like lattice. Although scattering occurs by disturbing phonon propagation and carriers easily conducts into the rigid lattice with higher mobility. This liquid like sublattice shows the Ag ion migration leads to low thermal conductivity. Due to this characteristic of Ag argyrodite, it is experimentally difficult to understand the molecular properties of these materials. Thus, we have employed atomistic simulation-based calculations to understand the structure, stability and electronic properties of argyrodite materials Ag₉XSe₆ (X = Al, Ga, In). The calculated formation energies of Al, Ga and In complexes are -5.83eV, -5.14eV, -4.48eV, respectively. Further to understand the bonding and electronic properties of all complexes, band gap, DOS, PDOS and Bader charge transfer analyses have been carried out. Our study will provide valuable information about the nature of bonding and structural defects of Ag₉XSe₆ crystalline materials for the high- performance thermoelectric materials.

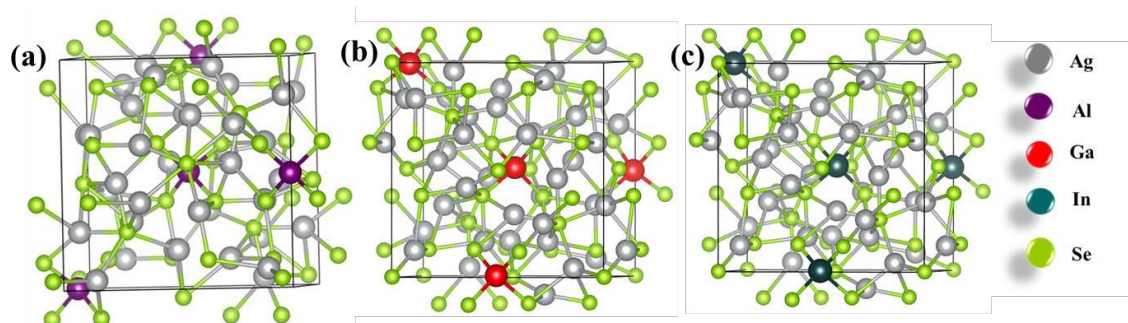


Figure 1: Optimized geometries of (a) Ag₉AlSe₆ (b) Ag₉GaSe₆ (c) Ag₉InSe₆ complexes.

References:

1. Lin, S., Li, W., Li, S., Zhang, X., Chen, Z., Xu, Y., Chen, Y., & Pei, Y. (2017). *Joule*, 1(4), 816–830.
2. Li, W., Lin, S., Weiss, M., Chen, Z., Li, J., Xu, Y., Zeier, W. G., & Pei, Y. (2018). *Advanced Energy Materials*, 8(18).
3. Andriyevsky, B., Barchiy, I. E., Studenyak, I. P., Kashuba, A. I., & Piasecki, M. (2021). *Scientific Reports*, 11(1).
4. Liu, J. Y., Chen, L., & Wu, L. M. (2022). *Nature Communications*, 13(1).

Selective Targeting of KRAS Mutations via Machine Learning-Assisted Molecular Docking and Dynamics Simulations

G. Hema, M. Prakash*

Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603 203, Chengalpattu, Tamil Nadu, India.

Email: hemagopal1999@gmail.com / prakashm4@srmist.edu.in

Abstract:

KRAS is one of the most frequently mutated oncogenes in human cancers, with significant implications in pancreatic, colorectal, and lung cancers. Mutations such as G12D, G12V, and G13C result in a constitutively active KRAS protein, driving uncontrolled cell growth and resistance to treatment. Despite its critical role, KRAS has long been considered "undruggable" due to its smooth surface and lack of deep binding pockets, which complicates the design of effective inhibitors.^[1] While recent advancements have shown promise, current therapies remain limited, especially for mutations beyond G12C. This research aims to address this challenge through a fully computational approach, integrating machine learning (ML) with molecular docking and molecular dynamics simulations to discover selective inhibitors for KRAS mutations.^[2] ML models will be trained on datasets containing known KRAS inhibitors and structural information of the KRAS protein. These models will predict potential ligands and their binding affinities for various KRAS mutant forms. The predicted ligands will then undergo molecular docking simulations to identify their optimal binding poses, followed by molecular dynamics simulations to assess the stability and interaction profiles of these compounds within the mutated KRAS structures. By focusing on mutation-selective inhibitors, this research provides a novel computational pipeline for drug discovery, reducing the need for traditional experimental methods and accelerating the process of identifying effective therapeutic candidates.^[3]

References:

- [1] P. Gomez-Gutierrez, J. Rubio-Martinez, J. J. Perez, *J. Chem. Inf. Model.* **2023**, *63*, 6412.
- [2] A. Fraissenon, C. Bayard, G. Morin, S. Benichi, C. Huguin, S. Protic, L. Zerbib, S. Ladraa, M. Firpion, T. Blauwblomme, O. Naggara, M. Duruisseau, M. Delous, C. Boitel, P.-P. Bringuier, L. Payen, C. Legendre, S. Kaltenbach, E. Balducci, P. Villarese, V. Asnafi, A. Bisdorff, L. Guibaud, G. Canaud, *N. Engl. J. Med.* **2024**, *391*, 334.
- [3] R. Yadav, M. Sharma, N. Agrawal, *Comput. Bioinforma. Multidiscip. Appl.* **2021**, 155.

Screening of Anion in Ionic Liquid - Graphene Interface for the Energy Storage Applications: First Principles Approach

Chockalingam Gopalakrishnan[#] and Muthuramalingam Prakash^{*}

Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur – 603203, Chengalpattu District, Tamil Nadu, India.

[#]e-mail: gopi4017189@gmail.com; ^{*}prakashm4@srmist.edu.in; Telephone: +91 90808 23391

Graphene is a 2D material which is widely used in energy harvesting application, also it is well known for its zero band gap. Along with graphene, ionic liquids (ILs) are widely used as electrolytes due to the excellent ionic conductivity and stable electrochemical window.[1,2] Here, we made an effort to analyze the changes in electronic structure of graphene with various adsorbed ILs (collectively called as GRAPHIL). In this study, we have taken series of ILs with organic/inorganic fluorinated and non-fluorinated anions and common MIM cation.[3,4,5] To get more insights on the complex structure, stability, selection of a suitable density functional theory (DFT) method is important to study the interfacial influence of IL at the graphene surface. Here, the interaction of ILs such as $[\text{MIM}]^+ [\text{X}]^-$ (where, X=OAc, AlCl_4 , PF_6 , BF_4 , Cl, OTf, Tf_2N and DCA) with graphene is studied. We found that the physisorption mechanism of ILs on the graphene surface is mainly driven by the anions through different mode of interaction. Furthermore, energy-minimized structure, adsorption energy, projected density of states, band structure and charge transfer indicates that the interaction between GRAPHIL is dominated by non-covalent forces. Interestingly, the electronic and quasi-metallic behavior are governed by tuning of anion of ILs. Our findings reveals that, chemical composition of elements and size of the anions plays the vital roles in strength of interaction between the GRAPHIL. Our study can provide valuable microscopic-level information to predict potential supercapacitor materials for energy storage applications.

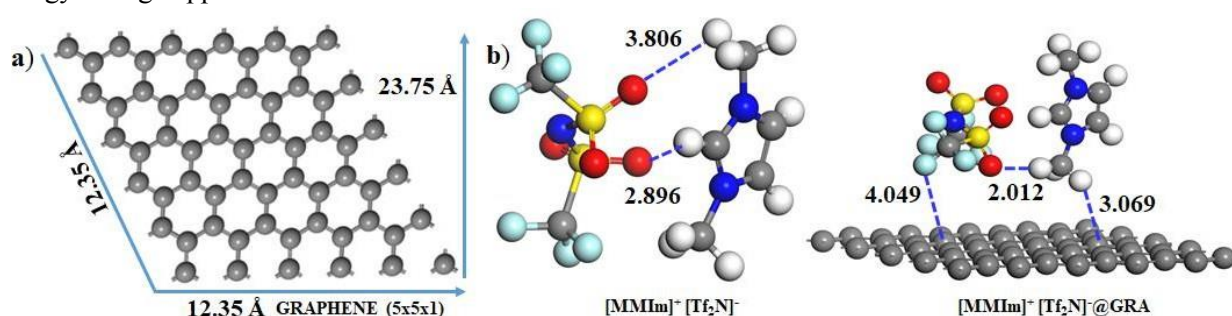


Figure .1 a) Mono layer of graphene surface (5x5x1). b) Energy minimized geometry of $[\text{MIM}]^+[\text{Tf}_2\text{N}]^-$ and $[\text{MIM}]^+[\text{Tf}_2\text{N}]^- @\text{Graphene}$

References

- [1] M. Armand, F. Endres, D.R. MacFarlane, H. Ohno, B. Scrosati, *Nat. Mater.* 8 (2009) 621–629.
- [2] M. Watanabe, M.L. Thomas, S. Zhang, K. Ueno, T. Yasuda, K. Dokko, *Chem. Rev.* 117 (2017) 7190–7239.
- [3] K. R. Maiyelvaganan, S. Kamalakannan, M. Prakash, *J. Appl. Surf. Sci.*, 495 (2019) 143538.
- [4] S. Kamalakannan, M. Prakash, G. Chambaud, M. Hochlaf, *ACS Omega.* 3 (2018) 18039–18051.
- [5] K. R. Maiyelvaganan, M. Prakash, R. M. Kumar, *Theor. Chem. Acc.*, 1209 (2022) 113601.

Identification of Dual Inhibitors Targeting VEGFR2 and HDAC: A Computational Study

N. Giri Lakshman, M. Prakash*

Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603203, Chengalpattu District, Tamil Nadu, India.

Email: girilakshman2704@gmail.com & prakashm4@srmist.edu.in

The family of receptor protein tyrosine kinases (RTKs) known as vascular endothelial growth factor receptors (VEGFRs) controls tumor-induced angiogenesis. Each VEGFR family has unique characteristics and has been identified as a promising tumour therapy target. In addition, histone deacetylase (HDAC) enzymes play an indispensable role in biological processes such as gene regulation, transcription, cell proliferation, angiogenesis, migration, differentiation, and metastasis, suggesting that HDAC inhibitors may have therapeutic value. Therefore, it's necessary to discover novel approaches to enhance clinical results and reduce the harmful effects of VEGFR2 and HDAC inhibitors¹. Due to their excellent pharmacodynamics, low toxicity, and anti-resistant actions, VEGFR dual-target inhibitors are gaining popularity as a viable treatment option, synergising with other medicines in tumour formation and progression. A group of VEGFR2/HDAC dual inhibitors with hydroxamic acid and N-phenylquinazolin-4-amine moieties was discovered earlier². Pharmacophores of both inhibitors were recently synthesised to assess the inhibitory effects of phenylurea hydroxamic acids against VEGFR2 and HDAC³. Also, inhibitors were developed and evaluated based on earlier reported pazopanib-based HDAC and VEGFR dual inhibitors⁴. Herein, a novel series of dual inhibitors were identified, screened, and evaluated based on previously reported FDA-approved drugs. Molecular docking and molecular dynamics studies will be conducted to understand the interactions between ligands and the targeted protein. The protein-ligand complexes will be subject to free energy and entropy calculations during the binding mechanism of the ligand in the cavity.

References

- [1] Y. Liu, Y. Li, Y. Wang, C. Lin, D. Zhang, J. Chen, L. Ouyang, F. Wu, J. Zhang, and L. Chen, 2022. *J Hematol Oncol.*, 2022, 15, 89.
- [2] F. W. Peng, J. Xuan, T. T. Wu, J. Y. Xue, Z. W. Ren, D. K. Liu, X. Q. Wang, X. H. Chen, J. W. Zhang, Y. G. Xu, and L. Shi, 2016. *Eur. J. Med. Chem.*, 109, 1.
- [3] J. Zang, X. Liang, Y. Huang, Y. Jia, X. Li, W. Xu, C. J. Chou, and Y. Zhang, 2018. *J Med Chem.*, 61, 5304.
- [4] S. Lee, S. W. Wang, C. L. Yu, H. C. Tai, J. Y. Yen, Y. L. Tuan, H. H. Wang, Y. T. Liu, S. S. Chen, and H. Y. Lee, 2021. *Bioorg. Med. Chem.*, 2021, 50, 116454.

Unveiling Topological Phenomena and Spin Hall Conductivity in NaCdBi

Arka Bhowmick¹ and V Kanchana¹

¹Department of Physics, IIT Hyderabad, Kandi, Sangareddy, 502285, Telangana, India

Email: ph23resch11005@iith.ac.in

Abstract: Topological materials are a unique quantum state of matter, defined by their distinctive edge or surface states, which arise from the topological properties of bulk wave functions. In this study, we examine the structural and electronic properties of the orthorhombic compound NaCdBi[1]. Without spin-orbit coupling (SOC), NaCdBi exhibits semimetallic behavior, but the inclusion of SOC induces splitting between the valence and conduction bands. This SOC-induced band splitting leads to the emergence of Dirac-like surface states near the bulk gap, classifying NaCdBi as a topological material. To confirm its non-trivial topological nature, we calculated the Z_2 invariants and found NaCdBi to be a strong topological material with $(\nu_0; \nu_1\nu_2\nu_3) = (1; 000)$. Moreover, its bulk electronic structure features Dirac points at the high-symmetry X point, protected by crystal symmetries, including time-reversal, inversion and nonsymmorphic symmetry. NaCdBi also exhibits substantial spin Hall conductivity, attributed to the pronounced spin Berry curvature near degenerate nodes and spin-orbit coupling-induced band splitting. These properties make NaCdBi a promising candidate for applications in spintronics and electronics devices. Its topologically protected boundary states, which are immune to backscattering from non-magnetic impurities and defects, further enhance its functional stability and application potential.

References:

[1]Shao, Dexi, Zhaopeng Guo, Xianxin Wu, Simin Nie, Jian Sun, Hongming Weng, and Zhijun Wang. "Topological insulators in the NaCaBi family with large spin-orbit coupling gaps." *Physical Review Research* 3, no. 1 (2021): 013278.

Thermoelectric properties of layered $\text{Bi}_2\text{YO}_4\text{Cl}$: a cageless rattler host structure

Namrata Das¹, Subhajit Sau¹ and V Kanchana¹

¹Department of Physics, IIT Hyderabad, Kandi, Sangareddy, 502285, Telangana, India

Email: namratadas147@gmail.com

Abstract: The rising demand for sustainable energy solutions has intensified the pursuit of advanced thermoelectric materials capable of efficient energy conversion. Layered compounds are of particular interest due to their ability to decouple electrical and thermal conductivity, thereby enhancing performance. Our study systematically explores the structural, electronic, and transport properties of the layered $\text{Bi}_2\text{YO}_4\text{Cl}$ compound using first-principles theory and Boltzmann transport equations, focusing on the underlying mechanisms of its low lattice thermal conductivity. This compound exhibits a unique cageless rattler mechanism, which significantly contributes to its low lattice thermal conductivity (κ_l). Unlike conventional rattlers confined in cages, the loosely bound 'Cl' atoms in $\text{Bi}_2\text{YO}_4\text{Cl}$ acts as rattler and achieve similar effects in reducing κ_l . Additionally, the low Debye temperature ($\theta_D = 284.10$ K) and the presence of flat frequency bands in the phonon dispersion supports the low lattice thermal conductivity. The phonon dispersion also features topological optical phonons, which can introduce additional scattering channels and potentially influence thermal conductivity. Our results indicate that $\text{Bi}_2\text{YO}_4\text{Cl}$ is an indirect bandgap semiconductor with a band gap of 2.5 eV. Electronic structure properties hint at promising transport properties benefiting from the emergence of flat bands at the top of the valence band. Our calculations yield an optimal figure of merit (ZT) of 0.33 for p-type and 0.13 for n-type doping along the c-axis at $T = 900$ K.

References:

- [1] Yadav, Neetu, and Rajamani Nagarajan. "Optical bandgap variation and photo-Fenton property evolution in Fe- doped $\text{Bi}_2\text{YO}_4\text{Cl}$." *Solid State Sciences* 139 (2023): 107154.
- [2] Yu, Jinxing, Shufang Chang, Li Shi, and Xiaoxiang Xu. "Single-crystalline $\text{Bi}_2\text{YO}_4\text{Cl}$ with facet-aided photocarrier separation for robust solar water splitting." *ACS Catalysis* 13, no. 6 (2023): 3854-3863.

Exploring Spin Hall Conductivity and Magneto transport in the Rare-Earth Topological Antiferromagnetic Dirac Semimetal: GdCuSn

Sonali Srotaswini Pradhan¹ and V Kanchana¹

¹Department of Physics, IIT Hyderabad, Kandi, Sangareddy, 502285, Telangana, India

Email: sonalisrotaswini@gmail.com

Abstract: Magnetic topological materials, with their intricate electronic structures, have garnered significant interest due to their ability to exhibit unique phenomena such as spin Hall conductivity and large magnetoresistance. These attributes hold great potential for advancing data storage technologies and magnetic sensor applications. Using first-principles calculations, we present an in-depth analysis of the structural, magnetic, electronic, and dynamic properties of the rare-earth equiatomic (1:1:1) intermetallic compound GdCuSn. This compound adopts a C-type antiferromagnetic ground state with a Neel temperature of 27 K [1], as determined by examining various spin configurations using the Heisenberg spin model within a mean-field framework. The electronic band structure reveals a nodal surface along the $k_z = \pi$ plane, stabilized by the interplay of time-reversal symmetry and non-symmorphic twofold screw-rotation symmetry. Notably, this non-centrosymmetric compound hosts Dirac points, which are rare in structures lacking inversion symmetry. Additionally, a pronounced spin Hall effect, driven by spin Berry curvature, underscores its non-trivial topological character. We further investigate the longitudinal and transverse magnetoresistance under varying magnetic fields, linking these behaviors to the topology of the Fermi surface. Phonon dispersion calculations confirm the compound's dynamic stability and identify a nodal surface within the $k_z = \pi$ plane of the phononic spectrum in the bulk Brillouin zone.

References:

[1] Ryan, D. H., Cadogan, J. M., Krylov, V. I., Legros, A., Rejali, R., & Boyer, C. D. (2017). The magnetic structures of GdCuSn, GdAgSn and GdAuSn. *Journal of Physics: Condensed Matter*, 29(49), 495804.

Azole-Based Diarylethene Photoswitches for Molecular Solar Thermal Energy Storage: A Computational Study

THILLAIARASI SUKUMAR¹, MAKESH KUMAR RAVVA¹, BASWANTH ORUGANTI²

¹Department of Chemistry, SRM University-AP, Mangalagiri, 522240, India

²School of Mathematics and Natural Sciences, Chanakya University, Bengaluru, India

Abstract: Diarylethene photoswitches featuring azole units combined with benzoheteroarene π -linkers have gained significant research interest in recent years due to their potential to achieve higher photocyclization efficiencies compared to conventional dithienylethenes switches give interesting results for advancing Molecular Solar Thermal energy (MOST) storage system. To evaluated thermal electrocyclization and cycloreversion reactions to determine energy storage densities (~ 0.30 MJ kg⁻¹) and storage times (≥ 10 hours) under ambient conditions. Findings indicate that dithiazolyl and dioxazolyl switches, featuring linkers such as indole and benzothiophene, achieve favorable energy storage density. Analysis reveals that variations in energy storage efficiency stem from differences in the aromaticity of the diaryl core and π -linker, along with non-covalent interactions. These results demonstrate that azole-based photoswitches can enhance MOST performance, achieving large free energy and energy density values while ensuring stable, photoreactive conformations.

References:

- [1] F. Hemauer, U. Bauer, L. Fromm, C. Weiß, A. Leng, P. Bachmann, F. Düll, J. Steinhauer, V. Schwaab, R. Grzonka, A. Hirsch, A. Görling, H. P. Steinrück, C. Papp, *ChemPhysChem* 2022, 23, e202200199.
- [2] E. M. Arpa, B. Durbeej, *Chemistry--Methods* 2023, 3, e202200060.
- [3] B. Oruganti, P. Pál Kalapos, V. Bhargav, G. London, B. Durbeej, *J. Am. Chem. Soc.* 2020, 142, 13941– 13953.

Strain tuning of TlN for thermoelectric applications

Zayid Ahmed, Karthik HJ and Swastibrata Bhattacharya

Department of Physics, Birla Institute of Technology and Science Pilani, K. K. Birla Goa Campus,
Goa, 403726, India

Abstract: Topological materials represent a unique class of materials characterized by topologically protected conducting edge states and insulating bulk states, offering promising potential for thermoelectric applications due to their non-dissipative transport properties. In this study, we propose strain-dependent tuning of thermoelectric properties in Thallium Nitride, a novel topological material. Using ab initio density functional theory and Boltzmann transport theory, we calculate electronic properties, thermoelectric coefficients and the thermoelectric figure of merit under different strain conditions. Additionally, we investigate the impact of spin-orbit interactions on the electronic and thermoelectric properties under varying strain conditions. Strain analysis provides dual benefits: it reveals the effects of fabrication-induced strain on thermoelectric performance and enables precise tuning of thermoelectric coefficients, including the Seebeck coefficient, electrical conductivity, and thermal conductivity. These findings highlight the potential of strain engineering in optimizing thermoelectric materials for advanced applications.

References:

- [1] G. Kresse and J. Furthmüller. 1996. Efficiency of Ab-Initio Total Energy Calculations for Metals and Semiconductors Using a Plane-Wave Basis Set, *Computational Materials Science*, 6, 15-50
- [2] J. P. Perdew, K. Burke and M. Ernzerhof. 1998. Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett.* 80, 890
- [3] P. E. Blöchl. 1994. Projected Augmented Wave Method, *Phys. Rev. B*, **50**, 17953
- [4] V. Wang, N. Xu, J.-C. Liu, G. Tang and W.-T. Geng. 2021. VASPKIT: A User-friendly Interface Facilitating High-throughput Computing and Analysis Using VASP Code, *Comput. Phys. Commun.*, 267, 108033
- [5] M. Khazaei, A. Ranjbar, Y.-G. Kang, Y. Liang, R. Khaledialidusti, S. Bae, H. Raebiger, V. Wang, M. J. Han, H. Mizoguchi, M. S. Bahramy, T. D. Kühne, R. V. Belosludov, K. Ohno and H. Hosono. 2022. Electronic Structures of Group III–V Element Haeckelite Compounds: A Novel Family of Semiconductors, Dirac Semimetals, and Topological Insulators, *Adv. Funct. Mater.*, **32**, 2110930.
- [6] Nzar Rauf Abdullah, Botan Jawdat Abdullah, and Vidar Gudundsson. 2022. Electronic and optical properties of metallic nitride: A comparative study between the MN (M = Al, Ga, In, Tl) monolayers, *Solid State Communications*, Volume 346, 114705
- [7] Georg K.H. Madsen and David J. Singh. 2006. BoltzTraP. A code for calculating band-structure dependent quantities, *Computer Physics Communications*, Volume 175, Issue 1, 1 July, Pages 67-71

Ab-initio calculation of Lattice Thermal Conductivity of Janus Graphene

Rishab Sahoo,¹ Zimmi Singh,¹ and Sankha Mukherjee^{1,*}

¹Department of Metallurgical and Materials Engineering, IIT Kharagpur, Kharagpur, 721302, India

*E-mail: sankha@metal.iitkgp.ac.in

Unlike other two-dimensional Janus materials such as MoSSe, VSiGeN₄, hydrohalogenated graphene, MoSSe-WSe₂ etc, which rely on either asymmetric functionalization, stacked heterojunctions or differential adsorption of elements across monolayer for their opposing properties on either side of the atomic planes, Janus graphene presents an ‘intrinsic’ symmetry breaking to account for the effect which roots from its corrugated, non-planar structure. Thermoelectric (TE) materials with a high thermoelectric figure of merit (zT) are an effective way to reduce energy consumption while ensuring sustainability and mitigating damage to the environment. Maximizing the efficiency of TE materials requires a low value of lattice thermal conductivity (κ_{lat}). The optimum combination of thermoelectric coefficients required for a high value of zT is observed to be unique to semiconductors. In semiconductors, thermal conductivity is predominantly due to contribution from lattice owing to their low charge carrier concentration. The bandgap of the material calculated through the GGA approximation using PBEsol ultrasoft pseudopotential, establishes it as a semiconductor. Through this paper, we aim to study the phonon transport in the newly discovered 2D material, Janus graphene, within the framework of the Peierls-Boltzmann Transport Equation (PBTE) and show its candidacy as a TE material based on that. With the increasing emphasis on use of 2D materials for nanoelectronic applications with the advantage of device miniaturization, exploring a potent material like Janus graphene could be crucial in the design of TE devices.

References:

- [1] Linfeng Yu, Jianhua Xu, Chen Shen, Hongbin Zhang, Xiong Zheng, Huimin Wang, Zhenzhen Qin, and Guangzhao Qin. Janus graphene: A two-dimensional half-auxetic carbon allotrope with a nonchemical Janus configuration. *Phys. Rev. B* 109, L121402 (2024).
- [2] A.-Y. Lu, H. Zhu, J. Xiao, C.-P. Chuu, Y. Han, M.-H. Chiu, C.-C. Cheng, C.-W. Yang, K.-H. Wei, Y. Yang et al., Janus monolayers of transition metal dichalcogenides, *Nat. Nanotechnol.* 12, 744 (2017).
- [3] S.-W. Ng, N. Noor, and Z. Zheng, Graphene-based two-dimensional Janus materials, *NPG Asia Mater.* 10, 217 (2018).
- [4] L. Zhang, J. Yu, M. Yang, Q. Xie, H. Peng, and Z. Liu, Janus graphene from asymmetric two-dimensional chemistry, *Nat. Commun.* 4, 1443 (2013).
- [5] L. Ju, M. Bie, X. Zhang, X. Chen, and L. Kou, Two-dimensional Janus van der Waals heterojunctions: A review of recent research progresses, *Front. Phys.* 16, 13201 (2020).
- [6] S.-D. Guo, W.-Q. Mu, J.-H. Wang, Y.-X. Yang, B. Wang, and Y.-S. Ang, Strain effects on the topological and valley properties of the Janus monolayer VSiGeN₄, *Phys. Rev. B* 106, 064416 (2022).

Polymorph exploration of niobium oxynitride using first-principles calculations

Deepak Upadhyay* and Prafulla K Jha

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

*deepakupadhyay888@gmail.com

Abstract: The niobium based oxynitride NbON has received significant attention due to its interesting optical and electronic properties¹. In this study the high pressure behavior of niobium oxynitride (NbON) was studied using density functional theory (DFT) up to 100 GPa. The enthalpy and geometry of the structures was derived from periodic DFT calculations at finite temperature (T= 0 K) using meta-GGA r2SCAN functional², with an appropriate van der Waals corrections (D3 method). At ambient pressure NbON crystallize in monoclinic baddeleyite phase³ (P2₁/c) which is isostructural with monoclinic zirconia (ZrO₂) and TaON. The enthalpy difference suggested that the ambient-pressure phase (P2₁/c) transforms to orthorhombic (Pnma) cotunnite-type structure via an orthorhombic-I (Pbca) structure. The phonon dispersion curves (PDC) of baddeleyite phase indicates the stability at ambient pressure as there are no imaginary frequencies in entire Brillouin zone (BZ). Interestingly the PDC of cotunnite phase is also stabilized at ambient pressure that might be suggested the possible existence of cotunnite phase at ambient conditions.

References:

- [1] P. Yadav, Anil C. A., B. S. Naidu 2025. Illustrating the potential of oxynitrides: harnessing solar power for efficient water splitting *Sustainable Energy Fuels*, 2025, Advance Article
- [2] J. W. Furness, A. D. Kaplan, J. Ning, J. P. Perdew and J. Sun, 2020 Accurate and Numerically Efficient r2SCAN Meta-Generalized Gradient Approximation *J. Phys. Chem. Lett.*, 11, 8208–8215.
- [3] S. Kozaki et. al. 2024 High-pressure X-ray study of NbON oxynitride: direct transition from baddeleyite to cotunnite structure *Chemistry Letters*, 53, 6.

Computational Modelling of Single-Molecule Magnet (SMM) behavior in 1D nanotubes and 3D Metal-Organic Framework by embedding Dyprocenium-based SMM in their voids

Kusum Kumari, Saurabh Kumar Singh*

Department of Chemistry

Indian Institute of Technology, Hyderabad

Email: sksingh@chy.iith.ac.in

Abstract: SMMs are the class of compounds that retain magnetization in the absence of a magnetic field with open magnetic hysteresis of purely molecular origin and have applications in high-density data storage devices and spintronics. Lanthanide-based SMMs are particularly attractive because of their high stability and giant magnetic anisotropy, which result in large energy barriers (U_{eff}) and magnetization-blocking temperatures (T_B). Although these SMMs are highly promising for information storage device applications, their integration into real devices for an end-user application requires sufficient resilience upon grafting or absorption on one/two and three-dimensional architectures to access individual molecules as magnetic bits for the read-and-write processes. Inspired by prior works,¹ the study uses periodic Density Functional Theory (pDFT) and multireference calculations to model hybrid SMM@MOF and SMM@BNNT assemblies. **a) SMM@MOF:** The high-performing $[\text{Dy}(\text{Cp}^*)_2]^+$ SMM ($U_{\text{eff}} = 2200$ K) was encapsulated into the triangular voids of Zr-based MOFs (NU-1000, PCN-222-Zn). Additionally, the SMM was attached to MOF nodes, enabling a novel way of nanostructuring SMMs within MOFs. **b) SMM@BNNT:** Highly axial $\text{Ln}\equiv\text{N}$ units ($\text{Ln} = \text{Dy}, \text{Tb}$) with a giant barrier of ~ 2700 K were deposited into BNNTs with varying diameters (BNNT (n,0), n=8,9). DFT tools like ETS-NOCV, NCI, charge difference density, and pDOS plots revealed significant interactions between SMMs and the MOF/BNNT hosts. CASSCF calculations confirmed the retention of SMM behavior post-encapsulation, showcasing MOFs and BNNTs as promising platforms for

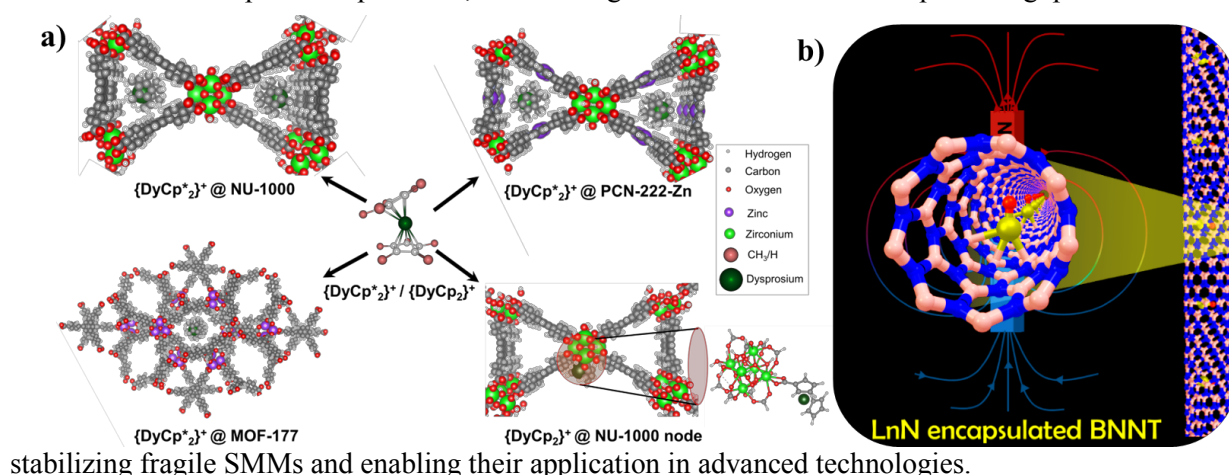


Figure: a) Encapsulation of $\{\text{DyCp}_2\}^+$ SMM into MOFs. b) $\text{Ln}\equiv\text{N}$ deposition in BNNTs.

References:

1. D. Aulakh, L. Liu, J. R. Varghese, H. Xie, T. Islamoglu, K. Duell, C.-W. Kung, C.-E. Hsiung, Y. Zhang, R. J. Drout, O. K. Farha, K. R. Dunbar, Y. Han and M. Wriedt, *J. Am. Chem. Soc.*, 2019, **141**, 2997–3005.

Unveiling the Role of Surface Redistribution of High-Index Cu₂O on CO₂RR

Priyanka Ghosh¹, Biswarup Pathak*

¹Department of Chemistry, Indian Institute of Technology Indore, Indore 453552, India

*Email: biswarup@iiti.ac.in

Abstract: Electrochemical CO₂ reduction reaction (CO₂RR) to commercially valuable chemicals is considered as a promising technology to mitigate the carbon content. In this regard, copper oxide-based catalysts are reported to produce high value multicarbon (C₂₊) products such as ethanol, ethane, n-propanol etc. at lower overpotentials than Cu nanoparticles (1). Recent investigations reveal the rapid oxygen depletion process of Cu₂O catalyst under electrocatalytic condition is the key factor for selective C₂₊ product formation (2). Furthermore, this reconstruction induced by grain boundary or crystal defects are more favorable in case of high-index Cu₂O surfaces due to presence of larger number of coordinatively unsaturated active sites compared to low-index surfaces (3). Therefore, in this work, by means of ab initio molecular dynamics simulation on high index Cu₂O surfaces [(200), (210) and (211)] and their oxide-derived forms up to third subsurface, we have investigated how surface reconstruction can impact the coordination environment as well as oxidation state of surface Cu atoms. This work provides novel insight into high index Cu₂O surface redistribution and its effect on CO₂RR which can accelerate future experimental studies.

References:

- [1] Christina W. Li and Matthew W. Kanan, 2012. CO₂ Reduction at Low Overpotential on Cu Electrodes Resulting from the Reduction of Thick Cu₂O Films. *Journal of the American Chemical Society*, 134, p.7231-7234.
- [2] Federico Dattila, Rodrigo Garcia-Muelas, and Nuria Lopez, 2020. Active and Selective Ensembles in Oxide-Derived Copper Catalysts for CO₂ Reduction. *ACS Energy Letters*, 5, p.3176-3184.
- [3] Wenli Fu, Zhen Liu, Tanyuan Wang, Jiashun Liang, Shuo Duan, Linfeng Xie, Jiantao Han and Qing Li, 2020. Promoting C₂₊ Production from Electrochemical CO₂ Reduction on Shape-Controlled Cuprous Oxide Nanocrystals with High-Index Facets. *ACS Sustainable Chemistry & Engineering*, 8, p.15223-15229.

Interaction Study of Toxic gases with Nickel decorated α -CN: A First Principles Study Heli

Mistry^{1*}, Shardul Vadalkar², Keyur N. Vyas¹, Prafulla K. Jha¹

¹*Department of Physics, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat - 390002, India.*

²*Department of Applied Science & Humanities, Sardar Vallabhbhai Patel Institute of Technology, Vasad, Gujarat – 388306, India.*

*Presenting author: hailey.mistry13@gmail.com

Abstract: Toxic gases such as carbon monoxide (CO), nitric oxide (NO) and ammonia (NH₃) pose serious health and environmental risks^[1]. While existing toxic gas monitors are costly, two-dimensional (2D) materials have shown promise for gas sensing applications due to their high surface-to-volume ratios and sensitivity.^[2] Among these, α -CN has been identified as a potential candidate for gas adsorption mechanisms. This study investigates the adsorption performance α -CN surface with the decoration of nickel (Ni)-atom for CO, NO, and NH₃ toxic gases using state of art density functional theory (DFT) based first principles calculations. The results indicate that the Ni-decoration significantly enhances the adsorption performance of α -CN, as evidenced by highly negative adsorption energies. Therefore, the calculated recovery times are extremely long, suggesting that Ni-decorated α -CN is more suitable for the removal of these toxic gases rather than as a sensor. The structural and electronic properties, including projected density of states (PDOS), band structure, charge density diagrams and transfer mechanisms, have been thoroughly analyzed. Additionally, sensing properties such as work function has been evaluated to validate the effectiveness of the material.

References:

- [1] D. Upadhyay, B. Roondhe, A. Pratap, P. K. Jha, *Appl. Surf. Sci.* **2019**, 476, 198–204.
- [2] K. Zhang, J. Robinson, *MRS Adv.* **2019**, 4, 2743–2757.

V-decorated Graphdiyne for Efficient Hydrogen Storage- Insights from DFT

Heera T Nair^{1*}, Prafulla K Jha¹, and Brahmananda Chakraborty²

¹Department of Physics, The M. S. University of Baroda, Vadodara-390002, Gujarat, India.

²Bhabha Atomic Research Centre, Mumbai-400085, India

*E-mail: heeratnair18@gmail.com

Abstract: Hydrogen serves as a desirable substitute for fossil fuels because it is a very clean and sustainable fuel. Using Density Functional Theory, we investigated the hydrogen storage capacity of synthesized 2D carbon allotrope, ‘Graphdiyne’ (GDY)[1]. Since pristine GDY exclusively bonds the hydrogen molecules by van der Waals interactions, it is not ideal for storing hydrogen under ambient conditions. The adsorption energy can be increased by decorating GDY with metal atoms, especially Transition metals, where the Kubas interaction [2] helps in binding hydrogen to the adsorbent. We, therefore, explored the possibilities of enhancing the hydrogen storage capacity of GDY by adsorbing Vanadium on GDY. Without V, we noticed that the binding energy for hydrogen on GDY was -0.16eV, which improved when V was bound. The V-decorated GDY exhibits a gravimetric weight percent of 4.88%, capable of holding up to six H₂ molecules. The system demonstrates a binding energy of -0.35 eV meeting the DOE requirements. Projected Density of States analysis reveals that charge transfer from the Vanadium 3d orbitals to the hydrogen 1s orbital stabilizes this interaction. Additionally, the thermal stability of the V-decorated GDY system was evaluated using ab initio Molecular Dynamics (AIMD) simulations confirming its feasibility for practical applications. This enhanced system demonstrates promising characteristics for hydrogen storage, paving the way for advancements in clean energy technologies.

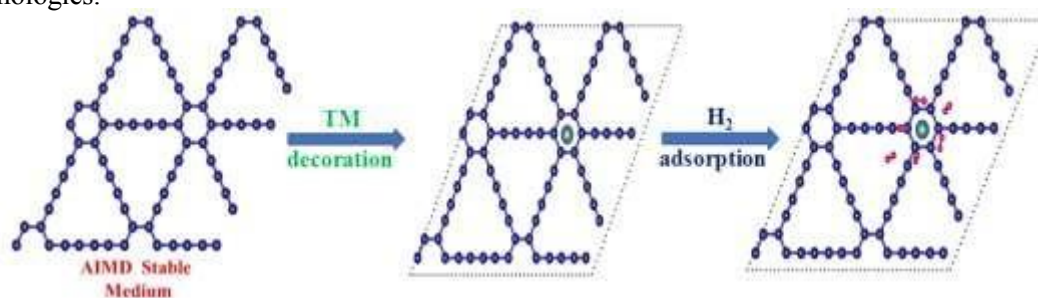


Fig.1. (a) Pristine Graphdiyne (GDY) (b) GDY+V (c) H₂ adsorption on GDY+V

References:

- [1] Gouging Li, Yuliang Li, Huibiao Liu, Chem. Commun., 46 (2010)3256-3258.
- [2] Gregory J Kubas, Chemical Reviews, 107 (2007) 4152-4205.

Topological signatures of Triply Degenerate nodal point Fermions in TbPtBi Heusler Alloy

Bhautik R Dhorì* and Prafulla K Jha

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

*bhautikdhorì6421@gmail.com

Abstract: Triply degenerate nodal point (TDNP) Fermions, lacking elementary particle counterparts, have been theoretically anticipated as quasiparticle excitations near specific band crossing points constrained by distinct space-group symmetries instead of Lorentz invariance^[1,2]. Here, based on *first-principles* calculations and symmetry analysis, we demonstrate the presence of TDNP fermions in TbPtBi Heusler alloy^[3]. Furthermore, we predict that these Fermions are situated away from the Γ high-symmetric point along the C_3 axis, extremely close to the Fermi level, and primarily not coexisting with another quasi-particle excitation, is critical to explore the intrinsic properties of this TDNP fermion, it is still a big challenge and has not been achieved up to now. We show that TbPtBi harbors peculiar Fermi arcs and surface states on the (111) and (001) crystal facets, owing to the coexistence of threefold rotational and time reversal symmetry. We also show that the these TDNP fermions characteristics can be engineered by tuning the pressure environment. Our work provides a prototype material platform for experimental detection through angle-resolved photoemission spectroscopy or scanning tunneling spectroscopy and practical spintronic applications. It illustrates that “condensed matter cosmos” can uphold more captivating particles simultaneously.

References:

- [1] Bradlyn, Barry, et al. "Beyond Dirac and Weyl fermions: Unconventional quasiparticles in conventional crystals." *Science* 353.6299 (2016): aaf5037.
- [2] Lv, B. Q., et al. "Observation of three-component fermions in the topological semimetal molybdenum phosphide." *Nature* 546.7660 (2017): 627-631.
- [3] Chen, Jie, et al. "Large anomalous Hall angle in a topological semimetal candidate TbPtBi." *Applied Physics Letters* 118.3 (2021).

Machine Learning Force Field-Accelerated Prediction of Lattice Thermal Conductivity in Strained WS₂ Monolayer

Zarna D. Ponkiya^{1,*}, Adisak Boonchun² and Prafulla K. Jha¹

¹Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, Gujarat, India-390002

²Department of Physics, Faculty of Science, Kasetsart University, Thailand 10900

*zponkiya137@gmail.com

Abstract: Thermal transport is a fundamental property of condensed matter, in which heat is transmitted through microscopic collisions of particles such as phonons and electrons. While Density Functional Theory (DFT) is a powerful tool for simulating thermal properties, its computational cost can be significant, especially for complex materials. Our study proposed a convenient strategy to evaluate the phonon dispersion and lattice thermal conductivity (K_L) of WS₂ monolayer and strained WS₂ monolayers by combining on-the-fly machine learning force field (MLFF) and phonon Boltzmann transport equation [1]. We found MLFF predicted phonon dispersion and the room temperature K_L of WS₂ ($99.4 \text{ Wm}^{-1}\text{K}^{-1}$) monolayer agree well with DFT calculated values. Further, the MLFF predicted K_L falls perfectly with temperature as DFT-based values [2]. MLFF is found to be much efficient over DFT in terms of time and resources consumption to calculate these thermal properties. This highlights the high accuracy and efficiency of MLFF in predicting thermal properties. Using this approach, we extended our predictions to room-temperature K_L of biaxially strained WS₂ monolayers (2% to 20%), finding instability at 21% strain due to imaginary phonon frequencies. The K_L decreases non-monotonically with increasing strain in WS₂, from $99.4 \text{ Wm}^{-1}\text{K}^{-1}$ at 0% to $44.5 \text{ Wm}^{-1}\text{K}^{-1}$ at 20%. This trend is similar to other 2D transition metal dichalcogenides (TMDs) [3]. The minimum K_L of $11.1 \text{ Wm}^{-1}\text{K}^{-1}$ was found at 16% strain. We analyzed the harmonic and anharmonic properties of the strained WS₂ monolayer and observed an overall impact of decreasing phonon group velocity and phonon lifetime, while the increasing trend of specific heat with strain, induces the resultant reduction trend of the K_L in the strained WS₂ monolayer. Considering remarkable advancements in 2D materials, the proposed methodology offers an efficient approach for investigating thermal properties in these materials.

References:

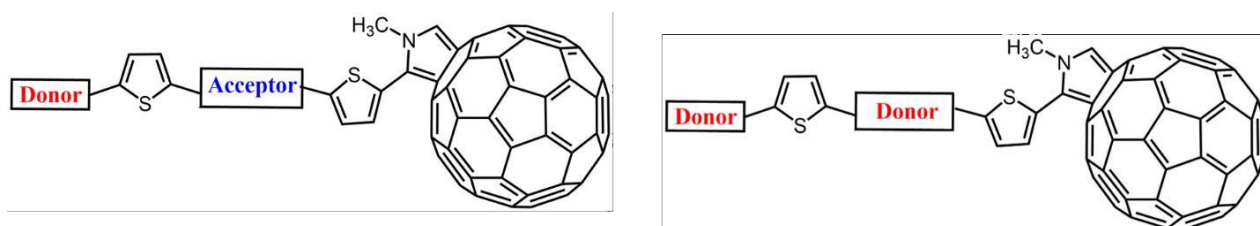
- [1] Jinnouchi, R., Karsai, F., Verdi, C., and Kresse, G., 2020. On-the-fly active learning of interatomic potentials for large-scale atomistic simulations. *The Journal of Physical Chemistry Letters*, 11(17), pp.6946-6955.
- [2] Zulfiqar, M., Zhao, Y., Li, G., Li, Z., and Ni, J., 2019. Intrinsic thermal conductivities of monolayer transition metal dichalcogenides MX₂ (M = Mo, W; X = S, Se, Te). *Scientific Reports*, 9(1), p.4571.
- [3] Yuan, K., Zhang, X., Li, L., and Tang, D., 2019. Effects of tensile strain and finite size on thermal conductivity in monolayer WSe₂. *Physical Chemistry Chemical Physics*, 21(1), pp.468-477.

Rational Design of D- π -A- π -A(C60) and D- π -D- π -A(C60) Architectures: Electric Field-Mediated Charge Transfer Dynamics for Single-Component Organic Solar Cells

Hemalatha Maricherla and Mahesh Kumar Ravva

Department of Chemistry, SRM University-AP, Amaravati 522240

In this study, we designed molecular dyads featuring a D- π -A- π -A(C60) and D- π -D- π -A(C60) architecture to investigate photoinduced electron transfer properties. The system was analysed using various donor and acceptor units to comprehensively understand the charge transfer dynamics. The investigation extended to studying the photoinduced electron transfer process under the influence of an external electric field. We conducted a systematic evaluation of several key parameters: electronic coupling, reorganization energies, and free energies associated with different charge transfer states. These parameters were assessed both in the presence and absence of an external electric field. The findings from this comprehensive analysis provide valuable insights for the rational design of novel single-component organic solar cells.



References:

- (1) Wang, X.; Wang, H.; Zhang, M.; Pullerits, T.; Song, P. Charge-Separated States Determined Photoinduced Electron Transfer Efficiency in a D-D-A System in an External Electric Field. *J. Phys. Chem. C* **2023**, *127* (6), 2805–2817.

Prediction of SJTM Observables in Putative PDW State in Cuprates

Monikana Gope and Peayush Choubey

Department of Physics, Indian Institute of Technology Roorkee, Roorkee-247667, Uttarakhand, India

In high temperature superconductors such as (BSCCO), the coexistence of competing electronic phases such as pair density wave (PDW) and charge density wave (CDW) is a unresolved mystery. PDW and CDW arise from different mechanisms, exhibit spatial modulations and change superconducting modulation in different ways. To probe these modulations at the atomic scale, we employ scanning Josephson spectroscopy to directly measure the local superconducting gap and the Josephson critical current. Scanned Josephson Tunnelling Microscopy (SJTM) is a variant of scanning tunnelling microscopy (STM) which measures Josephson and quasiparticle tunnelling current between a superconducting tip and a superconducting sample. As SJTM works as a direct local probe of superconducting gap order parameter $\Delta(\mathbf{r})$, it is most suitable for detecting intertwined order parameters characterized by periodically modulating $\Delta(\mathbf{r})$ and other density wave parameters.

Here, we have used tJ model, which captures the strong electron correlations and the interplay between electron hopping, exchange interactions and strong correlation effects in cuprate superconductors. With a particular amount of doping and fixed temperature PDW state can be stabilized as a metastable phase [2]. First, we have calculated critical current in the lattice space in a PDW and 'PDW+dSc' state with a s-wave tip, and I_c and $|I_c|^2$ shows different modulation in the two different states. Later, we would formulate a Wannier function based theory of SJTM observables and validate it for d-wave superconducting state of unconventional superconductors and predict various SJTM signatures of PDW state in them.

References:

1. Hamidian, M H et al. "Detection of a Cooper-pair density wave in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$." *Nature* vol. 532,7599 (2016): 343-7. doi:10.1038/nature17411.
2. Wang, Shuqiu et al. "Scattering interference signature of a pair density wave state in the cuprate pseudogap phase." *Nature communications* vol. 12,1 6087. 19 Oct. 2021, doi:10.1038/s41467-021-26028-x.

Topological phases of Honeycomb system with broken in-plane mirror symmetry

Arkamitra Sen¹ and Ritwik Das² and Indra Dasgupta^{*}

^{1,2}School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata, India

^{*}Senior Professor, School of Physical Sciences, IACS, Kolkata, 700032, India

¹arkasm2017@gmail.com

Abstract: Topological phase transitions can be driven by varying magnetic moment direction in buckled honeycomb lattice with broken in plane mirror symmetry(M_z). In these buckled honeycomb lattice the Chern number that serves as the topological invariant happens to jump alternatively from +1 to -1 as we change the in-plane magnetic moment direction of the atom sitting at the A/B sub-lattice. This phenomenon can be described via a simple 4-band tight-binding model respecting all the symmetries of the system and writing out each term of the tight-binding model accordingly. The tight-binding model with its symmetries are presented along with the numerical computation of Chern number by looking at the hybrid wannier charge center flows.

References:

- [1] Ritwik Das, Subhadeep Bandyopadhyay, and Indra Dasgupta, In-plane magnetization orientation driven topological phase transition in OsCl_3 monolayer, *Electronic Structure*, 6(2), 025005 (2024).

Effect of spin-orbit coupling in non-centrosymmetric Heusler family (half-Heusler, inverse-Heusler and quaternary-Heusler)

Anupam Mondal¹, Kunal Dutta² and Indra Dasgupta^{*}

¹amondalxb@gmail.com

^{1,2}School of Physical Science, Indian Association for the Cultivation of Science, Kolkata, India

^{*}Senior Professor, School of Physical Sciences, IACS, Kolkata 700032.

Abstract: In noncentrosymmetric systems, the nonvanishing gradient of the electrostatic potential results in a momentum-dependent magnetic field $\mathbf{\Omega}(\mathbf{k})$ in the rest frame of the electron. The coupling of this field with the spin of the electron lifts the spin-degeneracy of the bands in an otherwise nonmagnetic system. Depending on the symmetry^[1], $\mathbf{\Omega}(\mathbf{k})$ may have both linear and higher-order \mathbf{k} -dependent terms. The momentum-dependent field that locks the electron's spin direction to its momentum not only removes the spin degeneracy of the bands but also leads to complex spin textures in the reciprocal space. Spin textures depending on the symmetry may display Rashba^{[2],[4]},^[3], Dresselhaus^[1], persistent^[2], radial, Zeeman, band splitting with vanishing spin polarisation(BSVSP)^[4] or more complex spin configurations in the momentum space.

Heusler materials with no inversion symmetry exhibiting unusual electronic and magnetic properties have always attracted considerable experimental and theoretical attention with a view to harnessing these unconventional properties into possible device applications. Using first principle electronic structure calculation we have shown Heusler alloys display noble spin textures. The outcomes of our first-principles calculations, further supplemented by the formulation of low-energy $\mathbf{k} \cdot \mathbf{p}$ model Hamiltonians, have successfully revealed the presence of the linear Dresselhaus effect localized at the X point, which exhibits D_{2d} symmetry and Rashba effect, characterized by the coexistence of both linear and nonlinear terms, occurring at the L point, which has C_{3v} point group symmetry, in non-centrosymmetric Heusler family. Moreover, we have identified and characterized the presence of nontrivial Zeeman spin splitting at the non-time-reversal invariant W point for noncentrosymmetric Heusler family. In this work, we also explore a particularly fascinating phenomenon referred to as band splitting with vanishing spin polarization (BSVSP).

References:

- [1] Kunal Dutta, Subhadeep Bandyopadhyay, and Indra Dasgupta. Effect of spin-orbit coupling in noncentrosymmetric half-heusler alloys. Phys. Rev. B **108**, 245146, (2023).
- [2] K Dutta, I Dasgupta. [Persistent Spin Textures in Nonpolar Chiral Systems](#). arXiv preprint arXiv:2412.03229, 2024
- [3] S. Bandyopadhyay, A. Paul, and I. Dasgupta, Origin of Rashba-Dresselhaus effect in the ferroelectric nitride perovskite LaWN₃, Phys. Rev. B **101**,014109 (2020).
- [4] S. Bandyopadhyay and I. Dasgupta,Orbital-dependent spin textures in ferroelectric Rashba systems. Phys. Rev. B **103**, 014105 (2021).

Unlocking the Optoelectronic Potential of AGeX_3 (A = Ca, Sr, Ba; X = S, Se): A Sustainable Alternative in Chalcogenide Perovskites

Ayan Chakravorty, Surajit Adhikari, and Priya Johari

Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Greater Noida, Gautam Buddha Nagar, Uttar Pradesh 201314, India
Contact Email: ac900@snu.edu.in, sa731@snu.edu.in, priya.johari@snu.edu.in

The quest for environmentally benign and stable optoelectronic materials has intensified, and chalcogenide perovskites (CPs) have emerged as promising candidates owing to their non-toxic composition, stability, small bandgaps, large absorption coefficients, etc. However, a detailed theoretical study of excitonic and polaronic properties of these materials largely remain underexplored due to high computational demands. Herein, we present a comprehensive theoretical investigation of Germanium-based CPs, AGeX_3 (A = Ca, Sr, Ba; X = S, Se), which adopt distorted perovskite structures (β -phase) with an orthorhombic crystal structure (space group : $pnma$) by utilizing state-of-the-art density functional theory (DFT), density functional perturbation theory (DFPT), and many-body perturbation theory [GW and Bethe-Salpeter equation (BSE)]^[1-5]. Our calculations reveal that these materials are thermodynamically and mechanically stable, with bandgaps ranging from 0.646 to 2.001 eV - suitable for optoelectronic devices. We analyze the ionic and electronic contributions to dielectric screening using DFPT and BSE methods, finding that the electronic component dominates. The exciton binding energies range from 0.03 to 73.63 meV, indicating efficient exciton dissociation under ambient conditions. Additionally, these perovskites exhibit low to high polaronic mobilities (1.67–167.65 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$), exceeding many lead-free CPs and halide perovskites due to reduced carrier-phonon interactions. This unique combination of wide tunable bandgaps, low exciton binding energies, and enhanced charge-carrier mobility suggests AGeX_3 as a potential material for next-generation optoelectronic applications. These compounds are stable, high-performing, and eco-friendly, showing great promise for experimental realization and device integration.

References:

- [1] Hedin, L. New Method for Calculating the One-Particle Green's Function with Application to the Electron-Gas Problem. *Phys. Rev.* **1965**, *139*, A796–A823.
- [2] Hybertsen, M. S.; Louie, S. G. First-Principles Theory of Quasiparticles: Calculation of Band Gaps in Semiconductors and Insulators. *Phys. Rev. Lett.* **1985**, *55*, 1418–1421.
- [3] Albrecht, S.; Reining, L.; Del Sole, R.; Onida, G. Ab Initio Calculation of Excitonic Effects in the Optical Spectra of Semiconductors. *Phys. Rev. Lett.* **1998**, *80*, 4510–4513.
- [4] Rohlfing, M.; Louie, S. G. Electron-Hole Excitations in Semiconductors and Insulators. *Phys. Rev. Lett.* **1998**, *81*, 2312–2315.
- [5] Gajdoš, M.; Hummer, K.; Kresse, G.; Furthmüller, J.; Bechstedt, F. Linear optical properties in the projector-augmented wave methodology. *Phys. Rev. B* **2006**, *73*, 045112.

Effect of Metal based Anion in Ionic Liquid@UiO-66 MOF for Selective CO₂ Capture and Separation: A Computational study

Mohandas Sanjiv Kumar¹ and Muthuramalingam Prakash²

Computational Chemistry Research Laboratory (CCRL), Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur-603 203, Chengalpattu, Tamil Nadu, India.

* e-mail: sm4768@srmist.edu.in; Telephone: +91 6382097583

Abstract:

The carbon capture from flue gases is an important step to fight global warming and climate issues due to the fact that CO₂ is considered to be a main cause for global warming [1]. In past decade researches were carried out to identify a potential candidate for CO₂ capture and separation from the flue gas. Ionic Liquids (ILs) and metal organic framework (MOF) are two well-known materials in the field of CO₂ capture [2,3]. In this work we have selected UiO-66, a Zirconium based MOF with several ILs which has common cation as [EMIM]⁺ and various anions such as [Cl]⁻, [AlCl₄]⁻ and [FeCl₄]⁻. To understand the effect of metal based anion in CO₂ capture and its selectivity over other gases, selected ILs were impregnated in *Octahedral (Oh)* and *Tetrahedral (Td)* pores of UiO-66 [3]. It is found from calculations that the selectivity of CO₂ increases with increase in spatial confinement. Heat of adsorption of CO₂ is relatively higher for [EMIM]⁺ [AlCl₄]⁻ @ UiO-66 composite. Selectivity of CO₂/CH₄ and CO₂/N₂ was evaluated for selected ILs@UiO-66 composites. Our study will depict a molecular level understanding towards effective CO₂ capture and its separation.

Keywords: CO₂, global warming, MOF, ILs, UiO-66 and Confinement.

References:

- [1] X. Xia, G. Hu, W. Li, S. Li, *ACS Appl. Nano Mater.*, 2 (2019), 6022–6029.
- [2] A. Thomas, M. Prakash, *Appl. Surf. Science*, 491 (2019) 491, 633-639.
- [3] A. Thomas, M. Prakash, *J. Phys. Chem. C*, 124 (2020), 26203–26213.
- [4] L. Valenzano, B. Civalleri, S. Chavan, S. Bordiga, M. H. Nilsen, S. Jakobsen, K. P. Lillerud, C. Lamberti, *Chem. Mater.*, 23 (2011), 1700–1718.

Exploring Spin textures and Modulating Spin-Splitting in Layered Perovskites: A First-Principles Computational Approach

Shantanu Pathak^{1, a)} and Saswata Bhattacharya^{1, b)}

¹Department of Physics, Indian Institute of Technology Delhi, New Delhi, 110016, India

^{a)}shantanu.pathak@physics.iitd.ac.in

^{b)}saswata@physics.iitd.ac.in

Noncentrosymmetric materials (lacking inversion symmetry) exhibit electronic energy bands splitting by the Spin-Orbit Coupling (SOC) effect. This effect is responsible for non-trivial spin configurations and emergent quantum mechanical phenomena. Persistent spin texture (PST) refers to the ability of certain materials to uphold a consistent spin configuration across momentum space. This characteristic is anticipated to contribute to significantly prolonged carrier spin lifetimes, holding great potential for spintronics applications. Here, we predict this property in a noncentrosymmetric orthorhombic family of layered organic-inorganic lead halide perovskites. In the material, the PST property is enforced by nonsymmorphic space group symmetry. We study this behavior in A_2BX_4 (A = organic ammonium cations, B = Pb, X = I) perovskites using density functional theory (DFT). We investigate spin-dependent electronic structures and demonstrate the appearance of spin configurations as PST driven by spin-orbit coupling. We observe large spin-splitting at the conduction band minimum around ~ 3.3 eV $\cdot\text{\AA}$ and PST around the conduction band minima and valence band maxima in the k_x - k_y path for our materials. This spin splitting occurs due to the contributions of Pb-5d and I-4p orbitals in the upper valence band and lower conduction band of the material. The two-band k p model is used to analyze spin configurations in terms of PST and validate the results obtained using DFT. Further, we study the tuning of spin splitting by applying strain or stress on the materials. Our findings expand the variety of materials that can be employed for spintronics applications.

Back-to-Back Successful Transformation of Domain Wall Pair and Skyrmion in a Specially Designed Racetrack for Memory Storage Application

Mani Bharathi Manickavasagam¹, Hari Prasanth Perumal, Priyanka Babu¹, Perarasan T¹, Praveen P¹, Jaivardhan Sinha^{1*}

¹Spintronics and Nanomagnetism Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Nanotechnology, Kattankulathur, Chennai, Tamil Nadu, India – 603203

(*e-mail: jaivardr@srmist.edu.in)

To address the growing demand for ultra-dense storage and high-speed processing, Spintronics, an innovative field that leverages the spin of electrons, has emerged as a crucial technology. In the 2000s, various works had been reported that utilizes the chiral spin textures such as domain wall (DW) pairs and skyrmions for the memory applications[1-2]. In this work, we investigate the reversible conversion of DW pair and skyrmion in a typical junction geometry consisting of a wider track packed in between the three narrow tracks on either side using micromagnetic simulations (OOMMF)[3]. For this study, we initially relaxed the DW pairs on each of the left narrow tracks of the designed system. Their dynamics and conversion process are studied by introducing the system with spin transfer torque which is the result of application of current density of 4×10^{10} A/m² along the -x axis. This moves the spin textures along +x axis. We study them in the system that has material parameters of Pt/Co[4]. Our results show that the successful reversible back-to-back conversion between DW pairs and skyrmions is possible when the suitable strength of current density is applied to the system. When the spin textures have the form of DW pairs, their topological charge remains as “0” and when they attain the form of skyrmions, they gain the topological charge of “-1”. Similarly, when they travel as DW pairs in the narrow tracks, their velocity reaches to 400 m/s, but when they traverse as skyrmions in the wider track, their net velocity raises to 450 m/s. A similar work where the DW pairs are initially stabilized on the right narrow tracks, their dynamics and conversion when the system is subjected to the same strength of current density but along the +x axis is also explored.

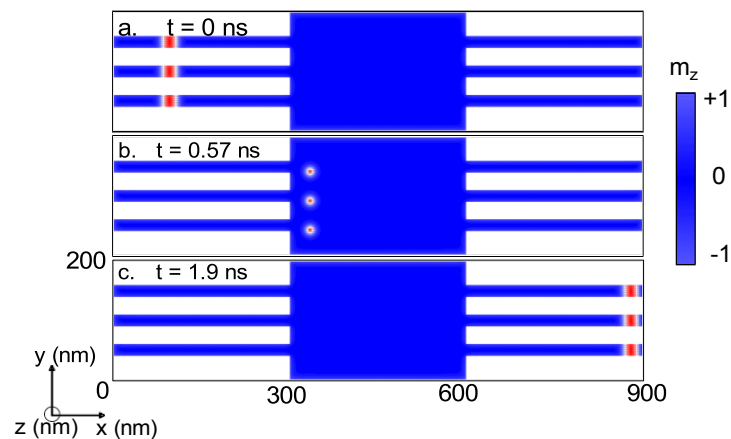


Figure 1: Dynamics and conversion of spin textures in the specially designed system (a-c).

References:

- [1] S. S. Parkin., Science., (2008)
- [2] Yan Zhou *et al.*, Nat. Commun. 5, 4652 (2014)
- [3] Marijan Beg *et al.*, IEEE Trans. Magn. 58, 1 (2022)
- [4] Hari Prasanth P., *et al.*, ACS Appl. Electron. Mater. 5, 7, 3641 (2023)

AB-stacked bilayer β_{12} -borophene as a promising anode material for alkali metal-ion batteries

Ankita Narwal,^{1,2} Subhadeep Banerjee,^{1,3} and Sharma S. R. K. C. Yamijala^{1,2,3,4,*}

1. Department of Chemistry, Indian Institute of Technology Madras, Chennai, 600036 India.
2. Centre for Atomistic Modelling and Materials Design, Indian Institute of Technology Madras, Chennai 600036, India.
3. Centre for Quantum Information, Communication, and Computing, Indian Institute of Technology Madras, Chennai 600036, India.
4. Centre for Molecular Materials and Functions, Indian Institute of Technology Madras, Chennai 600036, India.

* yamijala@iitm.ac.in

Abstract: As the lightest 2D- material, monolayer borophene exhibits a specific charge capacity of 1860 mAh g⁻¹ for Li-ion batteries, which is four times higher than that of graphite and is one of the highest specific charge capacities ever reported for 2D anode materials. Additionally, it showed high mechanical strength and a low diffusion barrier. However, monolayer borophene suffers from stability issues in its free-standing form, which restricts its real-life applications. Inspired by the recent experimental investigations, which proved the higher stability of bilayer borophene polymorphs (BBPs) over their monolayer counterparts, in this work, we investigated the dynamical and thermodynamical stabilities of both AA and AB-stacked BBPs in their β_{12} phase using first-principles calculations. Between the two stacking patterns, we found that only the AB-stacked β_{12} -BBP is both energetically and dynamically stable, and we further investigated its potential as a high-performance anode material for alkali metal ion batteries. Our investigations show that AB-stacked β_{12} -BBP exhibits good electrical conductivity before and after metal atom (Li/Na/K) adsorption onto it. Further, AB-stacked β_{12} -BBP adsorbs the metal atoms strongly with adsorption energies ranging between -0.89 to -1.44 eV, indicating that there is a lesser possibility of forming dendrites on this anode. Similarly, it has a low diffusion energy barrier (\sim 0.13–0.49 eV) for metal atoms, meeting the fast charge/discharge rate requirements. Moreover, it exhibits a reasonably low average metal-insertion voltage (0.43 to 0.65 V) and a specific charge capacity of 330–413 mAh g⁻¹ that is comparable to graphite. All the above findings suggest that the AB-stacked bilayer β_{12} - borophene can be a potentially favorable anode material.

Effect of Graphene Electrode Functionalization on Machine Learning aided Single Nucleotide Classification

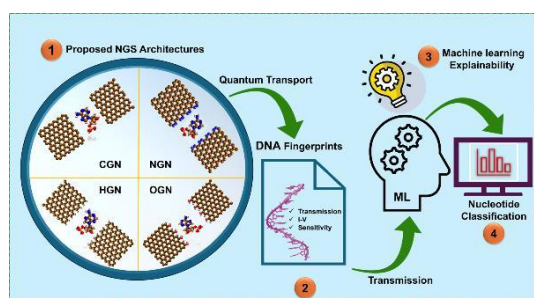
Mohd Rashid,¹ Milan Kumar Jena,¹ Sneha Mittal,¹ Biswarup Pathak¹

¹Department of Chemistry, Indian Institute of Technology (IIT) Indore, Indore, Madhya Pradesh, 453552, India

E-mail: phd2301131003@iiti.ac.in; biswarup@iiti.ac.in

Abstract

Solid-state nanogap-based DNA sequencing with quantum tunneling approach has emerged as a promising avenue due to its potential to deliver swift and precise sequencing outcomes. Nevertheless, despite significant progress, experimentally achieving single base resolution with a high signal-to-noise ratio remains a daunting challenge. In this work, we have utilized a machine learning (ML) framework coupled with quantum transport method to assess and compare the nucleotide identification performance of graphene nanogap functionalized with four different edge-saturating entities (C, H, N, and OH). The optimized ML model, especially the random forest classifier (RFC), demonstrates high accuracy (>90%) in classifying unlabeled nucleotides from their transmission readouts with four functionalized graphene nanogaps. Additionally, the minor variance in the accuracy of nucleotide classification across the nanogaps highlights that RFC can capture the role of electrode-nucleotide coupling dynamics on their transmission function. Moreover, we have also conducted conductance sensitivity (%) and current-voltage ($I - V$) analysis of each functionalized nanogap. Among the edge-saturating entities, the nitrogen atom terminated graphene nanogap is found to be the most sensitive for distinguishing DNA nucleotides. Our quantum transport combined ML study provides a useful perspective by conducting a comparative analysis of the role of edge-saturating entities in single-molecule DNA sequencing.



Reference:

- [1] Jena, M. K.; Pathak, B., **2023**. Development of an Artificially Intelligent Nanopore for High-Throughput DNA Sequencing with a Machine-Learning-Aided Quantum-Tunneling Approach. *Nano Lett.* 23 (7), 2511–2521.
- [2] Jena, M. K.; Roy, D.; Mittal, S.; Pathak, B., **2023**. Artificially Intelligent Nanogap for Rapid DNA Sequencing: A Machine Learning Aided Quantum Tunneling Approach. *ACS Mater. Lett.* 5 (9), 2488–2498.
- [3] Mittal, S.; Jena, M. K.; Pathak, B., **2024**. Integration of Artificial Intelligence and Quantum Transport toward Stereoselective Identification of Carbohydrate Isomers. *ACS Cent. Sci.* 10 (9), 1689–1702.

Electronic and phonon studies of B-site ordered double perovskites Nd_2BTiO_6 (B = Zn, Ni)

Bommareddy Poojitha*, Vineeta Yadav, Rudra Sekhar Manna

Department of Physics, IIT Tirupati, AP 517619, India.

*Presenting author, e-mail: poojitha@iittp.ac.in

Double perovskites (DP), with the chemical formula $\text{A}_2\text{BB}'\text{O}_6$ (A, B, B': rare earth or transition metal cations) exhibit a rich variety of physical and chemical properties, making them interesting in fundamental as well as applications point of view. In these types of materials, the structural flexibility of incorporating various types of rare earth and transition metals at both B- and B'-sites offers the tunability of magnetic ordering and possibly induce exotic magnetic ground states [1-2]. Among DPs, Ti-based double perovskites gain attention for their interesting dielectric, magnetic, and magneto-resistive properties as well as technological applications [2-4].

In this work, we have investigated electronic, magnetic, and vibrational properties of double perovskite Nd_2BTiO_6 (B = Zn, Ni). The polycrystalline compounds were synthesized by using solid state reaction method. Rietveld refinement results of X-ray diffraction pattern reveals that the compounds are stabilized in monoclinic structure with space group $P2_1/n$. The optical band gap is found to be 3.9 and 4.1 eV, respectively for B = Zn and Mg from UV-VIS absorption spectra. No magnetic ordering is observed down to 2 K for B = Zn and antiferromagnetic (AFM) ordering is observed B = Ni below 17 K. Notably, magnetic field dependent magnetization at 2 K exhibits non-linear behaviour, arising from crystal-field effects of Nd^{3+} ions in these compounds. Density functional theory calculations are performed using Vienna *ab initio* simulation package (VASP) software to determine the ground state of Nd_2BTiO_6 (B = Zn, Ni) by employing the GGA+*U* approach. Comparison of calculated ground state energies of different spin configurations, “NM, FM ($\uparrow\uparrow\uparrow$), AFM ($\uparrow\downarrow\uparrow\downarrow$), AFM1 ($\uparrow\uparrow\downarrow\downarrow$)”, revealed that the G-type AFM is the most stable configuration for these compounds.

[1] K. Pajskr *et al.*, Phys. Rev. B **93**, 035129 (2016).

[2] W. Z. Yang *et al.*, J. Appl. Phys. **107**, 124102 (2010).

[3] G. Tse *et al.*, Comput. Condens. Matter **9**, 35 (2016).

[4] M. Goto *et al.*, Bull. Chem. Soc. Jpn. **96**, 1269 (2023).

Inverse design of cathode materials for metal-ion batteries using Variational Auto-Encoder neural network architecture

Pritish Joshi^{1*}, Tanmoy Paul¹

¹*Research Institute for Sustainable Energy, TCG-CREST, Kolkata, West Bengal, India*

* prishranjan.joshi@tcgcrest.org

The demand for lithium-ion batteries has grown in recent years, driven by the drastic growth of the electric vehicle (EV) industry and portable electronics. However, lithium's limited abundance and high cost have given rise to a shift toward sodium-ion batteries as a more sustainable alternative. Regardless of the chemistry, discovering novel electrode materials, particularly cathode materials with high energy density and extended lifecycle, remains a significant challenge. Although first principles (ab initio) calculations are widely employed for accelerating materials discovery, their high computational cost and time requirements make them inefficient for large-scale exploration. Deep neural network models offer a promising alternative in this context, combining predictive accuracy with efficiency. Recognizing their potential, we developed a pipeline for the inverse design of cathode materials for Li- and Na-ion batteries using Variational Auto-encoders (VAEs) [1] coupled with Density Functional Theory (DFT).

Our VAE model, trained on a diverse dataset of cathode materials, generates potential candidates by sampling a property-conditioned latent space. These candidates exhibit high accuracy in structure, composition, and properties. The predictions predominantly include layered transition metal oxides of lithium and sodium featuring one or more transition metals. The designed compounds were structurally relaxed through spin-polarized GGA+U [2] DFT calculations with appropriate Hubbard 'U' values for transition metals. Additionally, Density of States (DOS) calculations validated the band gaps of the optimized structures, yielding promising results for future applications.

Acknowledgments:

This work is financially supported by the SERB SRG grant (SRG/2023/001641). The support and the resources provided by 'PARAM Brahma Facility' under the National Supercomputing Mission, Government of India at the Indian Institute of Science Education and Research (IISER) Pune are gratefully acknowledged.

References:

- (1) Kingma, D. P.; Welling, M. Auto-Encoding Variational Bayes. arXiv [stat.ML], 2013.
- (2) Dudarev, S. L.; Botton, G. A.; Savrasov, S. Y.; Humphreys, C. J.; Sutton, A. P. Electron-Energy-Loss Spectra and the Structural Stability of Nickel Oxide: An LSDA+U Study. Phys. Rev. B Condens. Matter 1998, 57 (3), 1505–1509.

Strain induced electronic and magnetic transition in S=3/2 ferromagnetic spin chain compound SbCrSe₃

Sk. Soyeb Ali

Department of Physics, Bennett University, Greater Noida, UP 201310, INDIA

Email: E22SOEP0076@bennett.edu.in

The study of two-dimensional (2D) magnetic materials and their pressure driven electronic and magnetic transitions are growing research field in modern condensed matter physics. In this context, recently ferromagnetic Cr-based compounds such as CrGeTe₃, CrI₃, have been investigated experimentally and theoretically for their possible spintronics applications. Here, we theoretically studied the electronic and magnetic properties of a relatively less explored Cr-based chalcogenide, namely SbCrSe₃ where 2D layers of magnetic Cr³⁺ ions form a triangular lattice. In this work, we employed density functional theory including Hubbard U (DFT+ U approach) in conjunction with constrained random-phase approximation (cRPA) where the later was used to estimate the strength of U . Our findings at ambient pressure show that the system exhibits a semiconducting ferromagnetic ground state with a gap of 0.5 eV and large Cr moments that corresponds to nominal S=3/2 spin-state. To understand the nature of magnetism, we calculated the inter-site magnetic exchange coupling strength using magnetic force theorem. The exchange interaction calculation shows, 1st nearest-neighbor (NN) interatomic exchange coupling (J_1) is found to be weak ferromagnetic (FM), while 2nd NN coupling (J_2) are relatively strong ferromagnetic (FM), making this system a candidate for 1D non-frustrated ferromagnetic spin-chain family of materials. Based on orbital resolved interactions, we demonstrated the reason behind two different types of interactions among 1st and 2nd NN despite their very similar bond lengths. We observe a significant spin-orbit coupling effect, giving rise to a finite magneto crystalline anisotropy, and Dzyaloshinskii-Moriya (DM) interaction. Further, we found that by applying uniaxial strain along crystallographic a and b-axis, SbCrSe₃ exhibits a magnetic transition to a semi-conducting AFM ground state and give rise to novel phenomenon angle dependence of exchange coupling. We also showed that the Neel temperature of AFM ground state could be significantly enhanced by applying compressive strain. Thus, our findings can enrich the versatility of SbCrSe₃ and make it a potential application.

**This work has been carried out in collaboration with Dr. Swarup Kr. Panda (Bennett University, Greater Noida, India).*

Pressure Induced electronic and magnetic transition in antiferromagnetic NiS: A combined DFT+U and Monte-Carlo study

Shovan Gayen

Department of Physics, Bennett University

Email: e22soep0056@bennett.edu.in

Employing first-principle density functional theory + Hubbard U (DFT+U) approach and classical Monte Carlo simulations, we investigated the lowest energy electronic structure in hexagonal NiS which exhibits a semi-metallic antiferromagnetic ground state at ambient condition. We derived a spin model Hamiltonians consisting of Heisenberg exchange interactions (J_{ij}) up to the third nearest neighbours, Dzyaloshinskii–Moriya *interactions* (DMI), and single ion anisotropy (K). Our calculations show that the 3rd nearest neighbour (NN) and 1st NN J_{ij} are strongly antiferromagnetic, while the 2nd NN J_{ij} is weak ferromagnetic. Further the effect of spin-orbit coupling (SOC) is also found to be significant, leading to a finite DMI and K . The classical Monte-Carlo result nicely capture the experimental specific heat, magnetic susceptibility etc, giving credence to our derived spin-model. The application of external pressure is demonstrated to be an effective tool to exhibit electronic and magnetic transition in NiS. We found that tensile stress gives rise to a metal-insulator transition, while compressive stress provides the ways to collapse local magnetic moment on Ni site. The dominant exchange couplings are calculated for various values of pressure and the route for enhancing transition temperature is proposed based on Monte-Carlo study. Our results is expected to enrich the understanding of electronic structure and magnetism in NiS.

* The work has been carried out in collaboration with Dr. Swarup Panda, Bennett University.

Unravelling Electronic Structure, Bonding and Magnetic Properties of Dysprosocene Single Molecule Magnets

Ibtesham Tarannum¹ and Saurabh K Singh¹

¹Department of Chemistry, IIT Hyderabad, Kandi, Sangareddy, Telangana, India-502285 e-mail: sksingh@chy.iith.ac.in

Abstract: Single-molecule magnets (SMMs) are a form of nanomagnet that can potentially retain magnetization at low temperatures. The application of SMM ranges from storage devices to quantum computing. Due to their large magnetic anisotropy, Dy(III) ions, with total orbital angular momentum ($J = 15/2$), are crucial in SMM research. Over the past decade, researchers have focused on enhancing Dy(III)-based SMM's performance by designing ligands that create optimal crystal fields, maintaining high local symmetry, and suppressing detrimental Raman and QTM processes¹. In this work, we have studied and characterized six sandwich complexes of Dy(III) with aromatic carbocyclic ring viz. $[\text{Dy}(\text{C}_m\text{R}_m)_2]^{n\pm}$ (where $\text{R} = \text{H}, \text{SiH}_3, \text{CH}_3$; $m = 4 \text{ to } 9$; $n = 1, 3$). These complexes were studied using Density Functional Theory (DFT) and Ab initio methods to compute the spin Hamiltonian (SH) parameters using the ORCA suite. This work shows that dianionic cyclobutadiene ligands $[\eta^4\text{-Cb}]^{2-}$ are more effective than Cp ligands for designing highly anisotropic SMMs. The stronger electrostatics and covalency in the $[\text{DyCb}_2]^-$ complex result in a giant barrier height, exceeding the U_{cal} value of ~ 2333 K reported for $[\text{DyCp}_2]^+$. Given the importance of cyclobutadiene dianion $[\eta^4\text{-Cb}]^{2-}$ ligands in Dy(III)-based SIMs, we explored whether alternative ring systems like $(\text{N}_4)^{2-}$, $(\text{P}_4)^{2-}$, $(\text{As}_4)^{2-}$, $(\text{P}_2(\text{CH})_2)^{2-}$ and $(\text{As}_2(\text{CH})_2)^{2-}$ could replicate the axial ligand field effects of $[\text{Dy}(\eta^4\text{-Cb})_2]^-$. Inspired by Scheer et al.'s isolation of the homoleptic $[\text{FeP}_4]^{2-}$ complex, we studied five Dy(III) sandwich complexes $[\text{Dy}(\text{E}_4)_2]^-$ ($\text{E} = \text{N}, \text{P}, \text{As}$) to investigate Dy–ligand bonding and the influence of soft or heavy atoms on magnetic anisotropy. Among these, $[\text{Dy}(\text{N}_4)_2]^-$ showed the highest anisotropy with a calculated energy barrier (U_{cal}) of ~ 2332 K, presenting a promising carbon-free alternative to organometallic dysprosocenium complexes.

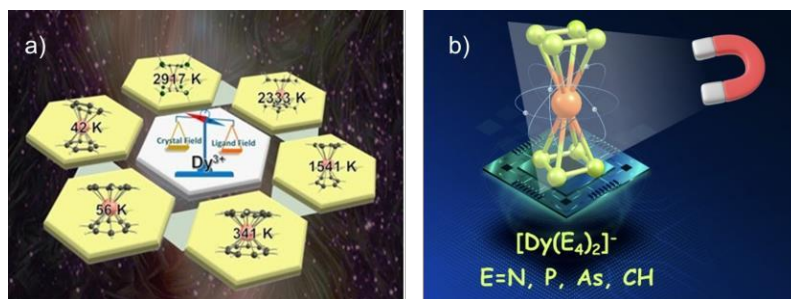


Figure 1: a) Organometallic sandwich dysprosium complexes $[\text{Dy}(\text{C}_m\text{R}_m)_2]$ b) Dy(III) sandwich complexes alternative ring systems like $(\text{N}_4)^{2-}$, $(\text{P}_4)^{2-}$, $(\text{As}_4)^{2-}$, $(\text{P}_2(\text{CH})_2)^{2-}$ and $(\text{As}_2(\text{CH})_2)^{2-}$.

References:

[1] D. N. Woodruff, R. E. P. Winpenney and R. A. Layfield, *Chem. Rev.*, 2013, **113**, 5110-5148.

Unveiling the Electrocatalytic Activity of Metallophthalocyanine based Covalent Organic Frameworks towards CO₂ Reduction Reactions

Kahkasha Parveen¹ and Srimanta Pakhira^{1,2*}

¹Department of Physics, IIT Indore, Indore, 453552, India.

²Centre for Advanced Electronics (CAE), IIT Indore, Indore, 453552, India.

*E-mail: kahkashap52@gmail.com

Abstract: The increasing energy demand has accelerated the development of clean and reliable energy sources. In recent years, there has been significant interest in developing novel materials with high efficiency and durability of electrochemical energy conversion. Transition metal macrocyclic metallophthalocyanine (MPc)-based catalysts, characterized by their unique 2D structures have shown great potential due to their high tailorable structures and molecular functionalities, enhancing their performance as electrocatalytic materials in energy conversion applications such as carbon dioxide reduction reactions (CO₂RR). Herein, using the periodic Density Functional Theory (DFT) calculations, the intrinsic electronic properties and electrocatalytic activity of MPc-based 2D monolayer COFs containing thiomorpholine and dithiine linkages (named CoPc-DNDS-COF and CoPc-DSDS-COF respectively) were examined for CO₂RR. The results of the electronic properties reveal the semiconducting nature of both the COFs with an energy band gap of 1.49 eV and 1.64 eV for the DNDS and DSDS COFs, which is due to the vacant d-orbital and the low electronegativity of sulfur, providing an opportunity to modulate the electronic properties of both the sulfur-containing heterocycles COFs. Next, using the eight different pathways leading to the production of CH₄, the CO₂RR mechanism of both COFs was examined using the same hybrid DFT B3LYP-D3 method. The exploration of the reaction mechanism demonstrated that the DNDS surface efficiently reduced CO₂ into CH₄ through the *CHO intermediate pathway with a change in Gibbs free energy (ΔG) of -2.28 eV, while the surface of DSDS was more prone towards CO desorption ($\Delta G = 0.68$ eV) rather than *CO intermediate ($\Delta G = 0.76$ eV) undergoing further hydrogenation. Thus, the study provides valuable insights into the strategic design of highly efficient electrocatalysts converting CO₂ into valuable C₁ products and holds an important role in understanding the mechanisms involved in electrocatalytic CO₂ reduction through different pathways.

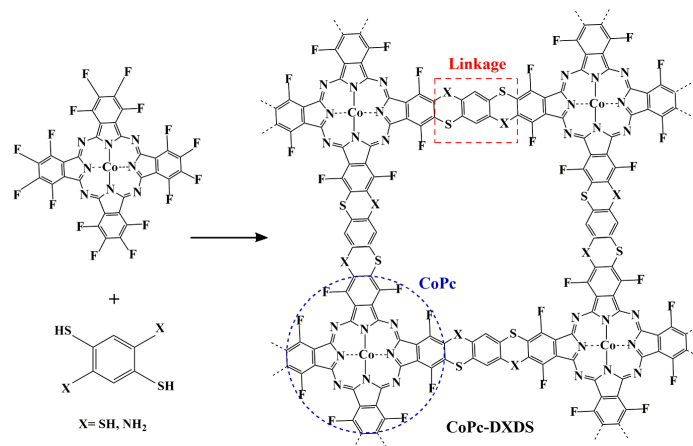


Figure 1: The chemical structure of CoPc-DXDS-COF materials, where X stands for SH and NH₂ group.

References:

- [1] Kahkasha Parveen. and Srimanta Pakhira, 2024. Designing Organic Bridging Linkers of Metal-Organic Frameworks for Enhanced Carbon Dioxide Adsorption, 48, 13700-13714.

Computational Modelling of Electron Transport through the Spin Cross-Over (SCO) complex $[\text{Co}(3,4\text{lutidine})_4\text{X}]^+$ (X=F, Cl, Br)

Basantia Saswat Abhilash¹, Saurabh Kumar Singh², and Archak Purkayastha³

¹Centre of Interdisciplinary Program, ²Department of Chemistry, ³Department of Physics

Indian Institute of Technology Hyderabad, Kandi, Telangana 502285

email address: sksingh@chy.iith.ac.in, archak.p@phy.iith.ac.in

Abstract: Spin-crossover (SCO) materials exhibit reversible transitions between low-spin (LS) and high-spin (HS) states under external stimuli¹, making them ideal for molecular electronics. Inspired by Daniel Aravena and Eliseo Ruiz's 2011 study² on spin filtering in Fe(II) SCO molecules, we investigated similar properties in Co-based complexes. Specifically, we examined the effect of substituting the bromide ligand in $[\text{Co}(3,4\text{-lutidine})_4\text{Br}]^+$ with various halogen and neutral ligands on SCO properties. Transition temperatures ($T_{1/2}$) were calculated, and electronic transport behavior of in $[\text{Co}(3,4\text{-lutidine})_4\text{Br}]^+$ was studied using the DFT+NEGF framework² in QUANTUM ATK software. The analysis included spin-Hamiltonian parameters, such as zero-field splitting (D) and g-tensor values. Our findings underscore the impact of ligand substitution on SCO behavior and transport properties, advancing their potential use in molecular spin filters, switches, and sensors.

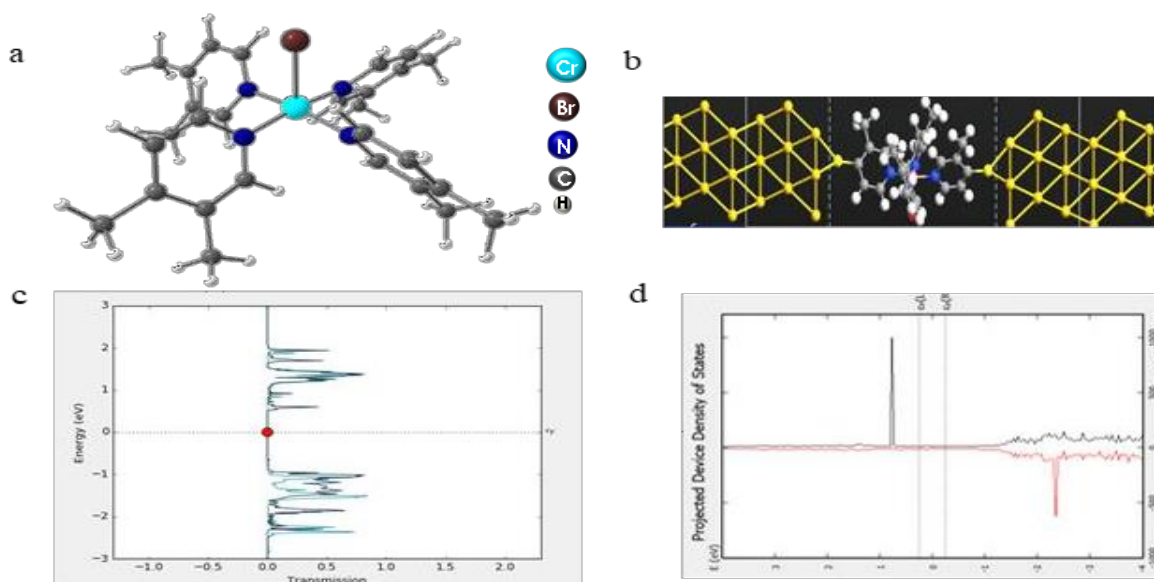


Fig.1 (a) DFT optimized structure of $[\text{Co}(3,4\text{-lut})_4\text{Br}]^+$ (b) Schematic model of molecular junction (c) Transmission spectra of molecular junctions (d) Projected Device DOS of molecular junction

References:

- (1) Aravena, D.; Ruiz, E. 2012. Coherent Transport through Spin-Crossover Single Molecules. *J. Am. Chem. Soc.*, 134 (2), 777–779
- (2) Kahn, O. 1996. Spin-Crossover Molecular Materials. *Curr. Opin. Solid State Mater. Sci.*, 1 (4), 547–55.



Janus van der Waals Heterostructures: Unlocking Ultra-High Thermoelectric Efficiency in SnS₂ and its Janus monolayer based Systems

Karthik HJ¹ and Swastibrata Bhattacharyya¹

¹Department of Physics, BITS Pilani KK Birla Goa Campus, India

Abstract: Two-dimensional materials have emerged as a groundbreaking class of materials for efficient thermoelectric applications, owing to their exceptional properties. Among these, tin-based transition metal dichalcogenides have garnered substantial attention due to their abundance, cost-effectiveness, environmentally friendly nature, and exceptional electronic, mechanical, and thermal properties. This study focuses on the SnS₂-Janus SnSSe hetero-bilayers (HBs), a van der Waals heterostructure, to explore their electronic and thermoelectric potential. Employing first-principles calculations combined with semi-classical Boltzmann transport theory, we conducted a comprehensive investigation into the thermodynamic and mechanical stability of SnS₂-SnSSe HBs. Our analysis confirms the stability of the HB, providing a solid foundation for its application in thermoelectric devices. A significant aspect of this study is the calculation of the electron relaxation time and mobility, achieved through deformation potential theory. In addition to electronic properties, we examined critical thermal parameters such as modal heat capacity, phonon group velocity, phonon mean free path, and phonon lifetime. These properties are crucial for understanding and optimizing lattice thermal conductivity (LTC). Our findings reveal that the SnS₂-SnSSe HB exhibits an ultra-low LTC of 3.85 W/mK at 300 K. This remarkable reduction in thermal conductivity is attributed to the low group velocity of low-lying acoustic phonon modes and the short mean free paths, both of which effectively suppress heat conduction. The reduced thermal conductivity, coupled with excellent electronic transport properties, significantly enhances the thermoelectric figure of merit (ZT). Specifically, we report exceptional ZT values of 3.6 for p-type doping and 3.2 for n-type doping at 900 K. Furthermore, the underlying mechanisms of charge and heat transport, elucidated through our study, provide valuable insights for designing advanced thermoelectric materials. The unique combination of tunable electronic properties, low thermal conductivity, and robust stability makes the SnS₂-Janus SnSSe HB a material of great potential for energy harvesting and waste heat recovery technologies paving the way for future innovations in sustainable energy technologies.

References:

  Karthik HJ. and Swastibrata Bhattacharyya, 2024. Janus van der Waals Heterostructures: Unlocking Ultra-High Thermoelectric Efficiency in SnS₂-Based Systems. International School and Conference on Evolution of Electronic Structure Theory and Experimental Realization, 1, p.1.

Exploring Frustration in the Hollandite Lattice and Its Connection to the 3D Triangular Lattice

Abhishek Hota^{1,2} and Saptarshi Mandal^{1,2}

¹Institute of Physics, Sachivalaya Marg, Bhubaneswar 751005, India

²Homi Bhabha National Institute, Training School Complex, Anushakti Nagar,
Mumbai 400094, India

Email: abhishek.hota@iopb.res.in

Abstract: Geometrically frustrated lattices are known for hosting exotic magnetic phases. In this work, we explore the frustration in the Hollandite lattice and its connection to the 3D triangular lattice, aiming to understand their role in magnetic behavior. The Hollandite lattice consists of planes parallel to the x - z plane, interconnected along the y direction. Each unit cell contains eight sites in a triangular arrangement, with repetition along the y axis creating unique connectivity. This local triangular geometry contributes to the lattice's frustration, making it a compelling system for studying magnetic properties. We first examine the classical J_1 - J_2 zigzag ladder chain, a minimal frustrated model. The competition between nearest-neighbor (J_1) and next-nearest-neighbor (J_2) interactions results in various magnetic phases. Analytical solutions and numerical simulations reveal frustration-induced spin configurations. By comparing a flattened 2D version of the Hollandite lattice with the 2D triangular lattice in Mathematica, we found both lattices share the same topology. Given the known spin-liquid phase in the triangular lattice, we aim to explore this phase in the Hollandite lattice through interpolation. We also aim to investigate the symmetry reduction from the hexagonal space group $P6/mmm$ to the tetragonal space group $I4/m$, providing a geometric understanding of the phase transition between these lattice structures. This work will bridge the understanding of two prominent frustrated systems, offering insights into their shared and unique magnetic properties and guiding future studies of lattice-driven emergent phenomena.

References:

1. S. Mandal, A. Andreanov, Y. Crespo, and N. Seriani, 2014. Phys. Rev. B 90, 104420.
2. Y. Crespo, A. Andreanov, and N. Seriani, 2013. Phys. Rev. B 88, 014202.
3. Atanu Maity and Saptarshi Mandal, 2018. J. Phys.: Condens. Matter 30, 485803.

Deciphering the Insulating Behavior of pentavalent Ir-based perovskite oxide: Interplay of Spin-Orbit Coupling and Hubbard U

Singdha Sagarika Behera¹ and Priyadarshini Parida¹

¹Department of Physics, KIIT University, Bhubaneswar, 751024, India

Email: 2381156@kiit.ac.in

Abstract: The family of iridates, among numerous spin-orbit linked systems, has garnered significant attention due to the presence of diverse crystal geometries and varying Ir valencies within the same family [1,3]. This ternary Ir-based metal oxide adopts a perovskite structure and has sparked interest in both applied and basic science communities due to the unique phase state formed by strong spin-orbit and Coulomb interaction [1,2]. This study investigates the structural, electronic, and magnetic properties of NaIrO₃, a pentavalent post-perovskite compound with Ir in a d⁴ electronic configuration, within the GGA+PBE framework using fully relativistic pseudopotentials to incorporate spin-orbit interactions via the Quantum ESPRESSO package. The structural parameters of NaIrO₃ were optimized through the variable cell relaxation method and fitted to the Birch-Murnaghan equation of state. The structure comprises distorted IrO₆ octahedra, sharing their corners along the c-axis and edges along the a-axis to create IrO₃ sheets [2]. The stabilization of the non-magnetic state of Ir occurs even in the absence of spin-orbit coupling (SOC) using the minimum energy principle. A comparison of electronic properties with and without the Hubbard correction (U) and SOC reveals that the t_{2g} states of Ir split into lower and upper Hubbard bands near the Fermi level, rendering the compound insulating at specific U values with SOC.

References:

- [1] B.J. Kim et. al., 2008. Novel $J_{\text{eff}}=1/2$ Mott State Induced by Relativistic Spin-Orbit Coupling in Sr₂IrO₄. Phys. Rev. Lett., **101**, p.076402.
- [2] M. Bremholm, S.E. Dutton, P.W. Stephens, and R.J. Cava, 2011. NaIrO₃—A pentavalent post-perovskite. J Solid State Chem., **184**, p.601–607.
- [3] L. Du, X. Sheng, H. Weng, and X. Dai, 2013. The electronic structure of NaIrO₃, Mott insulator or band insulator? Europhys. Lett., **101**, p.27003.

Cost-effective ZnO/GeO_x/Ge Heterostructure for Broadband Photodetection Applications

Nila Pal¹, Alope Kanjilal¹

¹Department of Physics, Shiv Nadar Institution of Eminence, Delhi-NCR,
Uttar Pradesh, 201314, India

Abstract: Broadband photodetectors with spectrum responsivity ranging from the ultraviolet to infrared (IR) have garnered significant attention due to their potential uses in optical communications, imaging, sensing, and spectroscopy [1]. The ultra-low photo sensitivity in the ultraviolet (<400 nm) and infrared (>1100 nm) bands, however, makes it difficult to realize these broadband photodiodes based on silicon (Si) itself as a light-sensitive layer. Since zinc oxide (ZnO) has a high excitation binding energy (60 meV at ambient temperature), is chemically and thermally stable, and is easily soluble, it is one of many wide band gap semiconductors that may be used as a UV detector. Because of its low bandgap (0.67 eV), fastest hole mobility, and CMOS compatibility, germanium (Ge) is a possible substitute to improve the detection performance of ZnO NWs/Si PDs in the infrared range (850–1800 nm). Here, ZnO thin film has been developed by cost effective solution processed spin coating technique with a small thermal budget (one-step annealing at temperature 400°C) on a Ge layer, for photodetection applications. The advantage of the use of intermediate Ge layer is thought to prevent the chemical reaction between ZnO and bottom SiO₂/Si, and to utilize both the contribution of ZnO and Ge layer in photodetection, which is a quite unique idea compared to earlier studies. Besides, the native GeO_x layer in between ZnO and Ge, merely formed during annealing, plays a decisive role in achieving broadband light absorbance. The ZnO/GeO_x/Ge heterostructure photodetectors show prominent photo response under UV (265 ± 10 nm), white (400-700 nm) light illumination. Reliable photodetection performance has been achieved in terms of the figure of merits with responsivity of 1.72 A/W at -1V (0.86 A/W at 1V), low response time 72 ms (rise) and 84 ms (fall). This work shows a new avenue to utilize low cost solution processable ZnO thin film grown on Ge layer for broadband photodetection.

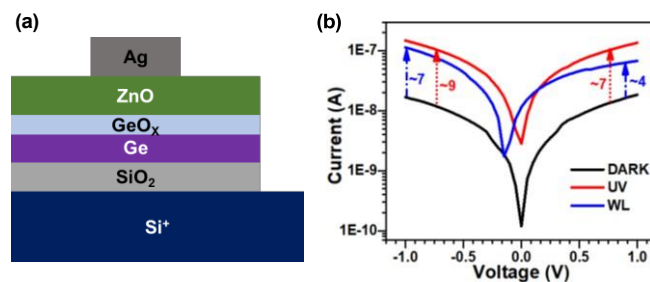


Figure 1 (a) Schematic presentation of device configuration, (b) current vs. voltage (*I-V*) characteristics under dark and illumination condition.

References:

[1] S. Chen, C. Teng, M. Zhang, Y. Li, D. Xie, and G. Shi, 2016. "A Flexible UV-Vis-NIR Photodetector based on a Perovskite/Conjugated-Polymer Composite," *Adv. Mater.*, vol. 28, no. 28, pp. 5969–5974.

Pressure studies on Os-based double perovskite oxides

Vineeta Yadav¹, Sromona Nandi¹, Bommareddy Poojitha¹, Kateryna Foyevtsova², Rudra Sekhar Manna¹

¹Department of Physics, IIT Tirupati, AP 517619, India

²Department of Physics and Astronomy, University of Notre Dame, Notre Dame, IN 46556, USA

¹Presenting author, e-mail: ph23d009@iittp.ac.in

Double perovskites (DPs), with the general formula $A_2BB'O_6$, exhibit unique properties due to their structural flexibility and compositional diversity. Due to their tunable electronic, magnetic, and optical properties, they are emerging as versatile materials for applications ranging from photovoltaics and spintronics to sensors and radiation detectors [1]. Especially, DPs with $5d$ elements such as Os, Ir, etc., introduce significant complexity such as spin-orbit coupling competes with crystal field splitting and Coulomb interactions, leading to intricate phase diagrams such as exotic quantum magnetism, spin liquids, etc. [2]. One can use chemical or hydrostatic pressure to alter the system properties which can give rise to insulator-metal transition, one of the highlighted topics in condensed matter physics [3]. We studied Ba_2XOsO_6 ($X = Ca, Mg$) both at ambient and hydrostatic pressure conditions using density functional theory. The electronic and magnetic properties of both compounds are first studied under GGA, GGA+ U , and GGA+ U +SOC at ambient pressure. In the case of Ba_2CaOsO_6 , GGA+ U gives antiferromagnetic metallic ground state for $U = 3$ eV with a magnetic moment of $1.63 \mu_B/Os^{6+}$ whereas for Ba_2MgOsO_6 , the ferromagnetic ground state is observed with a half-metallic nature showing a band gap of 1.51 eV in the spin-down channel with magnetic moment $1.6 \mu_B/Os^{6+}$ for $U = 2$ eV. In the case of Ba_2CaOsO_6 , a gap of 0.26 eV is perceived by introducing the spin-orbit coupling in the crystallographic direction [100]. For the Ba_2MgOsO_6 system, a hydrostatic pressure is applied on the ground state and a half-metal to a fully metallic state is observed at $P = 98.7$ GPa with a magnetic moment of $1.46 \mu_B/Os^{6+}$. On further increasing pressure, a non-magnetic phase is observed around $P = 312$ GPa showing nearly zero magnetic moment [4].

[1] S. Vasala *et al.*, Prog. Solid State Chem. **43**, 1 (2015).

[2] T. Saha-Dasgupta, Mater. Res. Express **7**, 014003 (2020).

[3] Yan-ling Tang *et al.*, Mater. Today Commun. **35**, 106137 (2023).

[3] V. Yadav, S. Nandi, B. Poojitha, K. Foyevtsova, and R. S. Manna (*private communications*).

Reversible Hydrogen Storage in NLi₄-Decorated Boron Phosphide Biphenylene

Divya Dange¹ and T.J. Dhillip Kumar¹

¹Department of Chemistry, IIT Ropar, Punjab, 140001, India

¹divya.23cyz0031@iitrpr.ac.in, 8288997871

Abstract: Hydrogen is considered one of the prominent choice for sustainable green energy applications. However, there is significant problem with its storage [1]. Taking this into consideration and utilizing first principles density functional theory, we conducted an extensive study to explore the reversible hydrogen storage of Boron Phosphide (BP) Biphenylene (see Figure 1(a)) decorated with superalkali NLi₄ clusters as shown in Figure 1(b). The PBE functional within the GGA was employed to approximate the exchange-correlation energy. The NLi₄ cluster exhibits binding energy of -5.34 eV/NLi₄, when positioned on both sides of BP Biphenylene monolayer. Partial density of states and Bader charge analysis are utilized to recognize the interaction which reveals that NLi₄ cluster binds to monolayer through electronic charge transfer mechanism which facilitates the polarized adsorption of H₂ molecules [2].

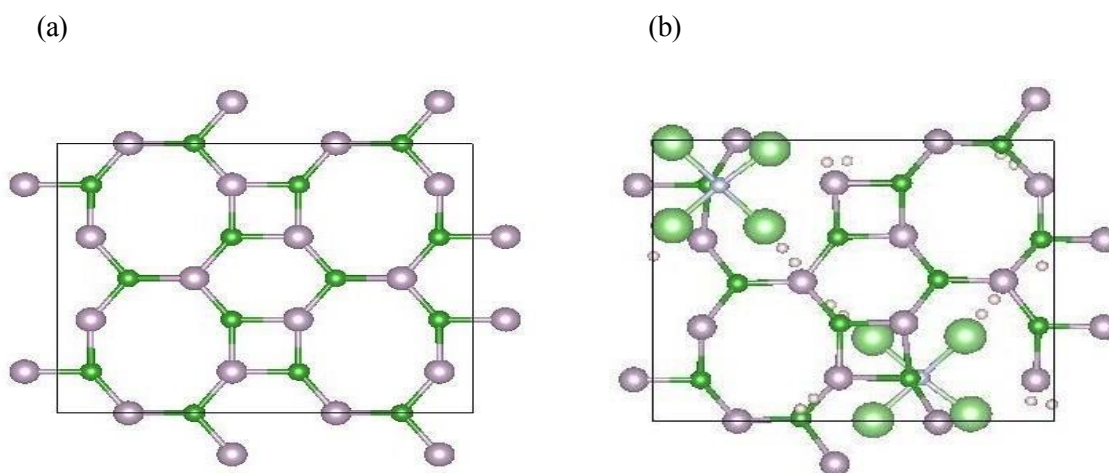


Figure 1. (a) Relaxed structure of BP Biphenylene and (b) Relaxed structure of H₂ loaded complex 2NLi₄@BP Biphenylene + 8H₂.

References:

- [1] Jena, P., 2024. Materials for Hydrogen Storage: Past, Present, and Future, *J. Phys. Chem. Lett.*, 2, 206-211.
- [2] P. Beniwal, P. Gautam, N. Duhan, and T. J. Dhillip Kumar, 2024. Reversible Hydrogen Storage in a Superalkali NLi₄-Decorated Biphenylene Monolayer: Insights from a First-Principles Study, *ACS Appl. Energy Mater.*, 7, 3263-3273.

Designing high performance doped Ni(OH)₂ electrocatalyst for Oxygen Evolution Reaction(OER) through water splitting

Electrocatalysis plays a critical role in advancing sustainable energy technologies, particularly in the development of efficient catalysts for hydrogen evolution (HER) and oxygen evolution (OER) reactions during water splitting. The design of electrocatalysts for these reactions is fundamental to improving the energy efficiency of water splitting processes, which are essential for producing hydrogen fuel in a clean and renewable manner. Recent advancements have focused on enhancing the performance of electrocatalysts through the development of earth abundant materials, nanostructures, and composite systems that exhibit high catalytic activity, stability, and conductivity. Ni(OH)₂ has been the subject of much recent interest due to its efficiency as an oxygen evolution catalyst. On the basis of findings from DFT calculations, we provide catalyst design strategies to improve the catalytic activity. Doping can enhance the efficiency of electrocatalytic performance of Ni(OH)₂. This work also demonstrates that Tungsten(W6+) doping can promote the electrocatalytic water oxidation activity of Ni(OH)₂ with the highest performance.

Enhancing the Electrochemical Properties of LiFePO_4 by Fe-Site Doping: An *ab initio* Study

Manorama Pandey and Hemant Kumar*

Department of Physics, School of Basic Sciences, IIT Bhubaneswar, Odisha, India, 752050

*hemant@iitbbs.ac.in

Abstract

Lithium-ion batteries are promising candidates for large-scale energy storage applications, with LiFePO_4 (LFP) being a widely studied cathode material due to its cost-effectiveness, safety, and structural stability. However, its electrochemical performance is hindered by low ionic conductivity, limiting fast ion transport. Fe-site doping with elements such as Mg, Zr, Ni, and Nb has emerged as an effective strategy to address these limitations [1, 2]. This study employs density functional theory (DFT) calculations to investigate the impact of doping concentrations ($x = 0.02, 0.125, 0.25$) on the electrochemical properties of $\text{LiM}_x\text{Fe}_{1-x}(\text{PO}_4)_3$ ($M = \text{Mg, Zr, Ni, Nb}$). Key parameters, including formation energy, volume change, Li intercalation/deintercalation voltage, band gap, and diffusion coefficient, are evaluated to identify the optimal dopant. Among the studied dopants, Mg demonstrates the most significant enhancement, increasing the Li diffusion coefficient from 10^{-14} to 10^{-11} cm^2/s . These findings underscore the potential of Mg doping to significantly improve the ionic conductivity and overall performance of LFP cathodes for advanced energy storage applications.

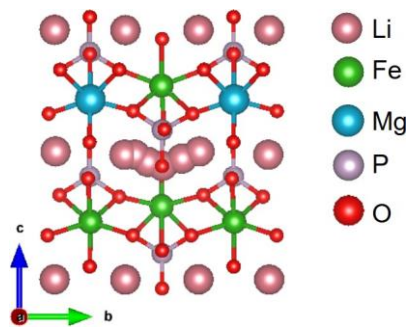


Figure 1: Li ion diffusion pathway.

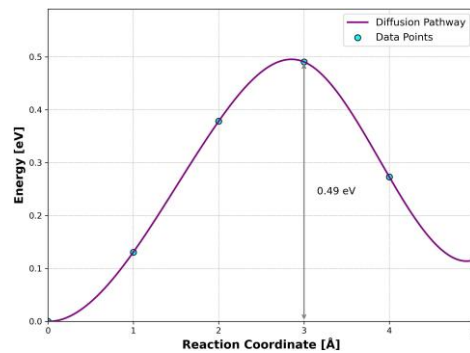


Figure 2: Activation energy in $\text{LiFe}_{0.75}\text{Mg}_{0.25}\text{PO}_4$.

References

- [1] Xingzhong Liu, Yue Zhang, Yanshuang Meng, Tai Kang, Hongfu Gao, Liangbiao Huang, and Fuliang Zhu. Influence mechanism of mg^{2+} doping on electrochemical properties of lifepo_4 cathode materials. *ACS Applied Energy Materials*, 5(7):8452–8459, 2022.
- [2] Bo Zhang, Yufang He, Hongqiang Gao, Xiaodan Wang, Jinli Liu, Hong Xu, Li Wang, and Xiangming He. Unraveling the doping mechanisms in lithium iron phosphate. *Energy Materials*, 2(2), 2022.

Tuning the Selective Sensing Properties of Molybdenum Carbide MXenes, (Mo_2CT_2 : $\text{T}_2 = \text{-O, -S and -F}$) Towards Volatile Organic Compounds (VOCs): An Ab-initio Approach

Abhishek¹ and Appala Naidu Gandhi¹

¹Department of Metallurgical and Materials Engineering, IIT Jodhpur, Jodhpur, 342030, India, abhishek.3@iitj.ac.in

Abstract: Detecting volatile organic compounds (VOCs) is essential due to their impact on environmental pollution and medical diagnostics. VOCs are present in industrial emissions and biological processes, negatively affect air quality and pose health risks [1]. This highlights the urgent need for highly sensitive and selective sensors. MXenes are a class of two-dimensional materials that were discovered in 2011 [2]. They have demonstrated significant potential across various fields, including energy storage, catalysis, and gas sensing. These materials, composed of transition metal carbides, nitrides, and carbonitrides, exhibit exceptional electrical conductivity, large surface area, and tunable surface chemistry, making them highly suitable for VOC detection. MXenes surfaces are pre-functionalized with various groups such as oxygen (-O), fluorine (-F), and sulfur (-S) during synthesis, which has proven effective in enhancing their adsorption capabilities and enabling selective VOC detection by modifying their electronic properties. Motivated by these characteristics, we employed density functional theory (DFT) simulations [3] to investigate the potential of Molybdenum carbide MXene (Mo_2CT_2 : $\text{T} = \text{-O, -F and -S}$) as a volatile organic compound (VOC) sensor. Using van der Waals calculations, we investigated the ground-state geometries, binding energies, electronic structures, and charge transfer mechanisms of functionalized Mo_2CT_2 for detecting VOCs such as isoprene, toluene, benzene, acetone, methanol, and formaldehyde. Our results show that Mo_2CF_2 has stronger interactions with VOCs, exhibiting binding energies between -0.82 and -1.30 eV. In comparison, Mo_2CS_2 shows binding energies from -0.20 to -0.77 eV, while Mo_2CO_2 ranges from -0.36 to -1.00 eV. Significant charge transfer and measurable changes in electrostatic potential further confirm the high sensitivity of Mo_2CT_2 -based sensors. Furthermore, a Boltzmann thermodynamic analysis assessed the sensing mechanisms under different temperature and pressure conditions, ensuring practical use. These findings highlight the potential of Mo_2CT_2 functionalized with specific surface groups as an efficient material for the detection of VOCs, presenting promising applications in environmental monitoring and medical diagnostics.

References:

- [1] Kumar, A.; Singh, D.; Kumar, K.; Singh, B. B.; Jain, V. K., 2018. Distribution of VOCs in Urban and Rural Atmospheres of Subtropical India: Temporal Variation, Source Attribution, Ratios, OFP and Risk Assessment. *Science of the Total Environment*, 613–614.
- [2] Naguib, M., Kurtoglu, M., Presser, V., Lu, J., Niu, J., Heon, M., Hultman, L., Gogotsi, Y. and Barsoum, M.W., 2011, Two-Dimensional Nanocrystals Produced by Exfoliation of Ti_3AlC_2 . *Adv. Mater.*, 23, 4248–4253.
- [3] Kresse, G.; Furthmüller, J., 1996, Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. *Phys Rev B Condens Matter Mater Phys*, 54, 16.

Thermoelectric behavior of directionally solidified $\text{Bi}_2\text{Te}_3\text{-Ga}_2\text{Te}_3$ eutectic alloy

Varinder Pal¹, Manas Paliwal¹ and Chandra Sekhar Tiwary¹

¹Metallurgical and Materials Engineering Department, IIT Kharagpur, Kharagpur, India

Abstract: Thermoelectricity, a waste heat recovery method uses a solid-state device to provide a reversible conversion between thermal and electrical energy. A thermoelectric material is characterised by higher figure of merit value which is determined by Seebeck coefficient, electrical and thermal conductivity of the material. Bi_2Te_3 a well-known thermoelectric is highly anisotropic with a rhombohedral crystal structure. On the other hand, Ga_2Te_3 a cubic phase is known to have very low thermal conductivity due to the ordered vacancies in the lattice[1]. In the $\text{Bi}_2\text{Te}_3\text{-Ga}_2\text{Te}_3$ pseudo-binary phase diagram (determined by CALPHAD approach), there is the eutectic point at around 25at.% Ga_2Te_3 [2]. In the present work, $\text{Bi}_2\text{Te}_3\text{-25at. \%Ga}_2\text{Te}_3$ alloy was synthesized using the flame melting of individual elements in an argon atmosphere. These melted alloys were then directionally solidified using the Bridgman Technique. Different solidification velocities (1mm/s to 10 $\mu\text{m/s}$) were provided to tune the microstructural features and the anisotropy of the solidifying phases. The changes in the directionality of two phases (Bi_2Te_3 and Ga_2Te_3) lead to changes in the electronic and thermal conductivity have been investigated. In addition, the growth of the Ga_2Te_3 can be seen in the transverse direction while the Bi_2Te_3 grows parallel to the solid/liquid interface movement, in all the investigated alloys. The role of interface between the Ga_2Te_3 and Bi_2Te_3 has been understood and its effect on the scattering of the electron and the phonons while conducting the electric and heat currents respectively has been discussed. In the investigated alloys, we observed the n-type as well as p-type conduction. In addition, there is a significant change in the electrical properties of the alloys observed on changing the solidification velocity.

References:

- [1] Kurosaki K, Matsumoto H, Charoenphakdee A, Yamanaka S, Ishimaru M, Hirotsu Y. Unexpectedly low thermal conductivity in natural nanostructured bulk Ga_2Te_3 . *Appl Phys Lett* 2008;93:012101. <https://doi.org/10.1063/1.2940591>.
- [2] Kumar B, Tiwary CS, Paek M-K, Paliwal M. Thermodynamic modelling of the ternary Bi-Ga-Te system for potential application in thermoelectric materials. *Calphad* 2021;74:102326. <https://doi.org/10.1016/j.calphad.2021.102326>.

Water Assisted Photoinduced Tautomerization in a Potential Bioactive Semicarbazone Schiff Base

Subham Chattopadhyay, Piyush Singh, Sujit Kumar Ghosh¹

¹Department of Chemistry, VNIT Nagpur, Maharashtra, 440010, India

subham.c2k@gmail.com

Abstract: Semicarbazone Schiff bases are bio-active heterocyclic compounds that have a wide range of applications in medicine, pharmacy, as probes, sensors and many more. In this article we have strategically designed and synthesized a Semicarbazone Schiff base (E)-2-(4-(diethylamino)-2-hydroxybenzylidene)hydrazine-1-carboxamide (DHHC). The photophysics of synthesized compound was investigated in various solvents employing electronic absorption, steady-state and time-resolved fluorescence spectroscopy. The experimental results were corroborated with DFT/TD-DFT based quantum chemical calculations. DHHC is feebly emissive in non-polar solvents and the fluorescence emission intensifies, at 406nm, in alcohols due to the effect of hydrogen bonding. However, in protic polar water the scenario is markedly different. In water the fluorescence emission intensity decreases a bit but the emission maxima shifted from 406nm to 430nm, due to solvent (water) assisted excited state proton transfer reaction (ESPT). In contrast to reported excited state intramolecular proton transfer reaction (ESIPT) in various compounds, the molecule DHHC on photoexcitation loses a proton from its phenolic -OH group to the water molecule which insists subsequent proton transfer from hydronium ion to imine nitrogen of DHHC. Feebly emissive nature of DHHC in non-polar solvents as well as the lower value of Stokes shift discard the ESIPT phenomenon and essentially supports ESPT reactions. The mechanism of ESPT was theoretically explored through the reaction kinetic of DHHC-water complex (in ratio 1:3) in explicit CPCM solvent model and the geometry of the transition state was optimized using STQN method (QST3). Furthermore, water-assisted ESPT reaction is justified from the temperature dependent emission spectra. The photoacid nature of DHHC is found to be pH sensitive in both acidic as well as basic medium. The illustration of the findings open-up enormous possibilities of the Semicarbazone Schiff base (DHHC) to be used as a probe for water sensing inside biomacromolecules like proteins for future medicinal chemistry research.^[1]

Reference:

- [1] P. Singh, T. Teena, K. Ganorkar, S. Kumar Ghosh, *ChemistrySelect* 2023, 8, DOI 10.1002/slct.202302869.

Unveiling the Dynamics of Triplet Exciton in Chalcone-based Donor-Acceptor System

Shrestha Banerjee, Piyush Singh, and Sujit Kumar Ghosh¹

¹ Department of Chemistry, VNIT Nagpur, Maharashtra, 440010, India

shresthabanerjee9@gmail.com

Abstract: Thermally activated delayed fluorescence (TADF) as an excited-state process has shown great potential in commercializing organic light-emitting diodes (OLEDs) for display applications. However, the comprehension of the reverse intersystem crossing (rISC) mechanism within the TADF process remains limited and is currently under development. In this study, our Theoretical and experimental findings uncover a novel mechanism for the reverse intersystem crossing (rISC) process within a chalcone-based donor- π -acceptor system. This mechanism involves the conversion of higher-energy triplet excitons into the lowest emissive singlet state. In contrast to conventional TADF-based systems, our newly designed molecule exhibits an increase in delayed fluorescence (DF) emission intensity at lower temperatures, a phenomenon unattainable in the up-converted TADF process. These comprehensive research outcomes have the potential to chart new directions in donor-acceptor systems, providing an alternative means of harvesting triplet excitons through rISC and thereby enabling DF.^[1]

Reference:

- [1] P. Singh, P. Pattanayak, P. Purkayastha, S. Kumar Ghosh, *Chemistry – A European Journal* 2023, 29, DOI 10.1002/chem.202302587.

High-temperature magnetism and strong spin-lattice coupling in two-dimensional CrTe₂

Anupama S¹, Deepak K Roy¹, Mukul Kabir¹

¹Department of Physics, Indian Institute of Science Education and Research, Pune 411 008

E-mail: anupama.s@students.iiserpune.ac.in

Abstract: Recent experimental studies on ultrathin films of CrTe₂ have shown potential for achieving room-temperature ferromagnetism. However, the results in single-layer CrTe₂ are widely debated in the literature, with conflicting findings ranging from intrinsic ferromagnetism^[1,2] to a ground state characterized by zigzag antiferromagnetism^[3]. We correlate these contrasting results to a very strong spin-lattice coupling, which is atypical for two-dimensional van der Waals materials. We examine the underlying phase diagram to understand these phenomena better and explore exchange interactions and magnetic anisotropies. Moreover, we employ long-range anisotropic Heisenberg Monte Carlo simulations to calculate ordering temperatures and investigate methods for manipulating the magnetic properties, focusing on compatibility with potential device applications.

References:

- [1] Meng, L., Zhou, Z., Xu, M. *et al.* Anomalous thickness dependence of Curie temperature in air-stable two-dimensional ferromagnetic 1T-CrTe₂ grown by chemical vapor deposition. *Nat Commun* **12**, 809 (2021)
- [2] Zhang, X., Lu, Q., Liu, W. *et al.* Room-temperature intrinsic ferromagnetism in epitaxial CrTe₂ ultrathin films. *Nat Commun* **12**, 2492 (2021)
- [3] Xian, JJ., Wang, C., Nie, JH. *et al.* Spin mapping of intralayer antiferromagnetism and field-induced spin reorientation in monolayer CrTe₂. *Nat Commun* **13**, 257 (2022)

First-Principle Study on Structural and Charge Conduction Parameters of CsPbX₃ (X= Cl, Br, I) for Memristor Applications

Rose Jose^{1,2}, Gayathri A Nair³, Rahul E^{1,3}, Sneha Krishnan³, Suseel Rahul K^{1,3}*

¹PG and Research Department of Physics, Sree Krishna College, Thrissur, (India)

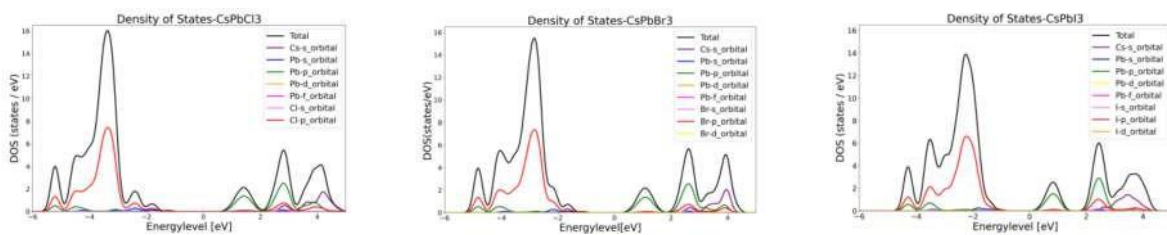
²Department of Physics, Mar Dionysius College, Thrissur, (India)

³Department of Physics, Sri Vyasa NSS College, Thrissur, (India)

*E-mail of the corresponding author: srk@srivyasanss.ac.in

Abstract: The discovery of memristors capable of mimicking biological synapses has paved a new path for high-speed and energy-efficient neuromorphic computations. Memristors are two-terminal devices which operates via mixed ionic-electronic conduction and its resistance can be tuned over a wide range[1]. Metal halide perovskites (MHP) possess the required resistive switching (RS) feature to combine the functions of computation and memory in memristors[2]. In this work first principle study using GGA-PBE exchange-correlation functional was performed to investigate the structural parameters and the charge conduction parameters like electronic band structure, density of states and effective mass of lead halide perovskite CsPbX₃ (X= Cl, Br, I). All calculations were based on plane-wave approach in GPAW and ASE package. Optimised structure is obtained using Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm with cut-off energy 650 eV with 4x4x4 k-mesh and convergence force of 0.01 eV/Å.

Our calculations revealed semiconducting nature of the composites under study and found descending trend in band gap (E_g) as E_g (CsPbCl₃) > E_g (CsPbBr₃) > E_g (CsPbI₃). The effective masses of holes and electrons were determined for all composites and observed a similar pattern of variation at various high-symmetry points. The lowest effective mass for holes were seen in MR path and for electrons were seen in GX path for all composites under study.



The presence of highly dense localised states indicated dominant contribution of Pb-s and Pb-p orbitals in conduction band and X-p orbitals in valence band. The density of states (DOS) outcomes suggests higher possibility of electron-hole migration in CsPbCl₃ and ion migration in CsPbI₃. The collective result of the study proposes CsPbX₃ composites as an excellent choice for memristors and associated applications.

References:

- [1] Funck, Carsten, and Stephan Menzel. "Comprehensive model of electron conduction in oxide-based memristive devices." *ACS Applied electronic materials* 3.9 (2021): 3674-3692.
- [2] Lee, Sumin, Jeonghyeon Son, and Beomjin Jeong. "Ion dynamics in metal halide perovskites for resistive-switching memory and neuromorphic memristors." *Materials Today Electronics* (2024): 100114.

A Density Functional Theory Based Study of the Optical properties of Oxygen-deficient SrVO₃

Purushothaman M and Debolina Misra

Presenting author email: bruse.higgs2cosmos@gmail.com

Materials Modeling and Simulation Laboratory, Department of Physics, Indian Institute of Information Technology, Design and Manufacturing, Kancheepuram, Chennai 600127, India

Abstract: The strongly correlated oxide SrVO₃ has recently been identified as a potential transparent conductor with its real part of dielectric function (plasma frequency) vanishing just below the red end of the visible spectrum [1]. Nevertheless, the optical absorption at the violet end restricts its use as an efficient transparent conductor [2]. In this work, the effect of oxygen vacancy on the optical properties of SrVO₃ has been investigated within the framework of density functional theory, with GGA+U functional, to treat the correlated ground state of the system. The frequency dependent dielectric functions for both pristine and oxygen deficient SrVO_{3-x} (x=0.5, 1) structures have been calculated and the other optical properties such as absorption coefficient and reflectivity are then computed from the complex dielectric functions. In order to make SrVO₃ transparent in the entire visible spectrum, effect of oxygen vacancy in pristine SrVO₃ has been studied in detail, and our results reveal that, in SrVO_{2.5}, the reflection edge remains below the visible region while the onset of optical absorption is after the violet end of the spectrum, making it suitable to be used as a potential transparent conductor. In SrVO₂ structure, on the other hand, the enhanced absorption is observed near the red end of the spectrum, limiting its application as transparent conductor. Further to understand the change in optical characteristics of SrVO₃ with oxygen concentration, electronic structure of pristine and oxygen deficient structures are analyzed and compared. Our results indicate that, oxygen vacancy plays an important role in tuning the optical properties of SrVO₃ for its intended use as an efficient transparent conductor.

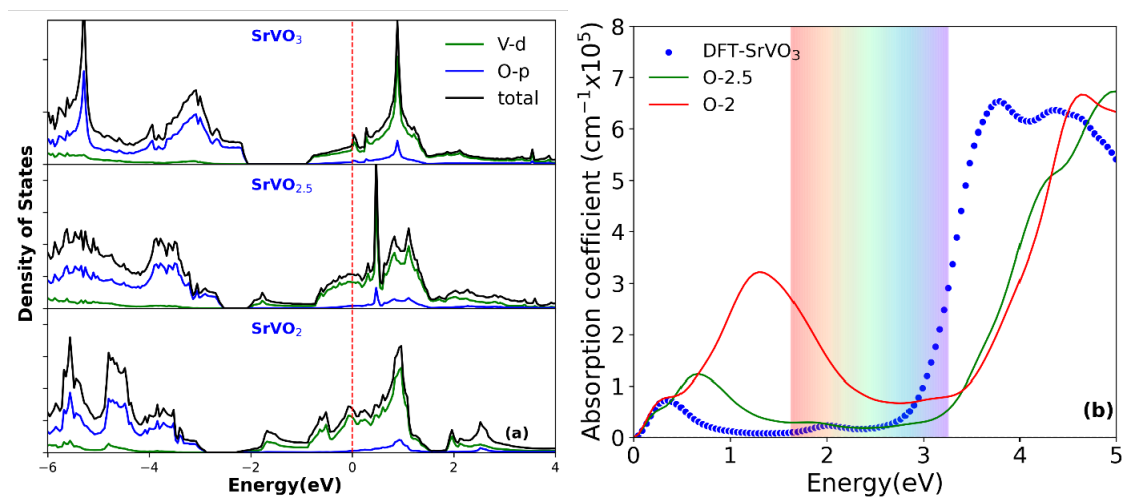


Figure 1: (a) Density of states plot of pristine SrVO₃ and SrVO_{3-x} (x=0.5, 1) (b) Absorption Coefficient of pristine SrVO₃ (blue bubbles) and SrVO_{3-x} (x=0.5, 1).

References

- [1] L. Zhang et al., Correlated metals as transparent conductors, *Nature Mater* **15**, 204 (2016).
- [2] L. Si, J. Kaufmann, Z. Zhong, J. M. Tomczak, and K. Held, Pitfalls and solutions for perovskite transparent conductors, *Phys. Rev. B* **104**, L041112 (2021).

Molecular Insights into Alkali Metal Interaction with Redox Active Covalent Organic Framework as Cathode in Batteries

Rashi Jain¹ and Sudhir K. Sahoo¹

¹Department of Chemistry, IIT Dharwad, Karnataka, 580007,
India Email: cy23dp003@iitdh.ac.in

Covalent organic frameworks containing carbonyl like redox active groups, crystalline and porous, two dimensional materials are promising candidates for organic electrodes in alkali ion batteries. However, the volume change, distortion of crystalline structures due to redox reaction are the main challenges, which are yet to be addressed. In this context, we studied an experimentally synthesized nitrogen rich redox active COF namely TQBQ (triquinoxaline benzoquinone) using density functional theory [1]. We investigated the periodic structure of TQBQ-COF, found to be in a hexagonal lattice with an inter-layer distance of 3.53 Å (See Figure 1). We studied the interaction of alkali metal atoms (Li, Na and K) with TQBQ using DFT and calculated various electrochemical parameters. The adsorption energies for Li, Na and K were in the range of - 4.12 to -3.19 eV, -4.45 to -3.23 eV and -5.32 to -3.81 eV, respectively. In total, a maximum of 72 AM atoms were adsorbed on the four-layered periodic TQBQ-COF. Our point charge analysis suggests that the charge transfers from AM atoms to TQBQ. The average voltages observed are in the range of 4.12 - 3.19 V, 4.45 - 3.23 V and 5.32 - 3.81 V for Li, Na and K, respectively. We observed that volume decreases on addition of AM atoms because of increased inter-layer interaction due to charge transfer. However, the decrease is less than 10% in all three cases. Our results indicate that TQBQ-COF will be best suited for a potassium ion battery with higher voltage and minimal volume change [2].

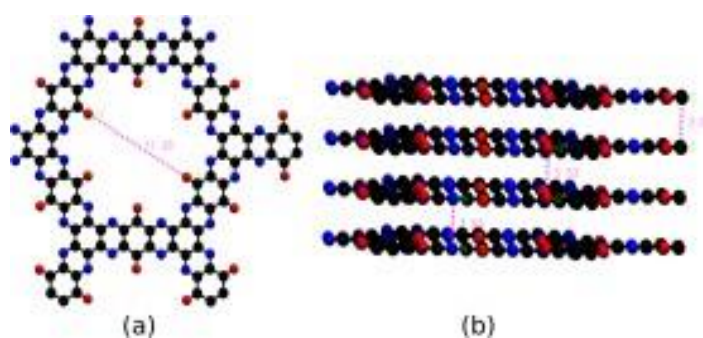


Figure 1. The DFT-optimized bulk structure of TQBQ-COF (a-top view and b-side view) in a hexagonal lattice. Atoms color: C-black, N-blue and O-red.

References:

1. Shi et al. Nature Communications 11, 178 (2020).
2. Rashi Jain, Sudhir K. Sahoo, Manuscript under preparation.

Tailored Surface Functionalization of $Ti_3C_2T_x$ MXenes through Transition Metal Doping : A DFT Study

S. Surya¹, C. Preferencial Kala^{1*}, John D Thiruvadigal¹

¹Computation Material Science and Nanodevice Simulation Laboratory

Department of Physics and Nanotechnology,

SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India, 603203.

*Corresponding author: preferec@srmist.edu.in

Abstract

$Ti_3C_2T_x$ MXenes have gained significant attention as advanced materials for biosensing applications due to their outstanding surface reactivity, electrical properties, and structural versatility. In this work, the Quantum ATK toolkit was employed with density functional theory (DFT) to investigate the surface functionalization of $Ti_3C_2T_x$ MXenes. The various surface terminations, including O, S, and N, were examined to enhance adsorption and sensing efficiency. To further improve the performance, transition metal dopants were strategically introduced, optimizing the adsorption energies and ensuring efficient recovery processes. The study reveals the synergistic effects of dopants and terminations in achieving high sensitivity and selectivity for specific medical biomarkers. These findings provide a pathway for developing next-generation $Ti_3C_2T_x$ -based biosensors with tailored properties, offering a robust platform for early disease diagnostics and personalized healthcare.

Keywords: Atomistic Tool Kit, Density Functional Theory, MXenes, Biomarkers.

References:

1. Alfalasi, Wadha, Tanveer Hussain, and Nacir Tit, Ab initio investigation of functionalization of titanium carbide Ti_3C_2 MXenes to tune the selective detection of lung cancer biomarkers, *Scientific reports* 14.1 (2024): 1403.
2. Panigrahi, Puspamitra, et al, Identification of Lung Cancer Biomarkers by Nanosensors Based on Titanium Carbide ($Ti_3C_2T_x$) MXenes, *ACS Applied Nano Materials* 6.23 (2023): 22117-22127.
3. Kumar, Narender, et al, Efficient Detection of Pancreatic-Cancer Biomarkers using Functionalized Titanium Carbide ($Ti_3C_2T_x$) MXenes, (2024).

Exploring Elastic Properties of ZnO Single-Walled Nanotubes: Insights from Zigzag, Chiral, and Armchair Configurations Using the Universal Force Field

Santanu Kumar Nayak, Padmaja Patnaik*, Dipan Kumar Das, Mandakini Baral

Centurion University of Technology and Management, Odisha, India

Corresponding author* -padmaja.patnaik@gmail.com

ABSTRACT

Mechanical properties calculation of a material reveals information about strain, stress, elasticity, flexibility etc. To understand the mechanical characteristics of ZnO Zigzag (8,0), armchair ZnO (8,8) and chiral ZnO (8,7) single wall nanotubes density functional theory (DFT) approach in conjunction with universal force field technique utilized. Mechanical and elastic characteristics including their Young's modulus (Y), Poisson's ratio (σ), bulk modulus (B), shear modulus (G), and compressibility (K) are computed and examined in preparation for potential applications in the future. The nature and behaviour of ZnO nanotubes including whether it is brittle or ductile, isotropic or anisotropic were verified. The three-dimensional structure of Young's modulus, bulk modulus, Poisson's ratio, linear compressibility, and shear modulus were plotted and analyzed.

Effects of Surface functionalization on electronic properties of Ti₂C MXene.

Kavyasree N^{1a}, Dr.Srurthi T^{1b}, Dr.Vincent Mathew^{1c}

¹Central university of Kerala, Periy

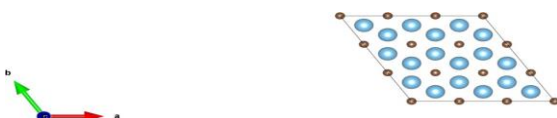
^a kavyasree.2300607003@cukerala.ac.in ^b drsrurthi2023@gmail.com

^c Vincent@cukerala.ac.in

Abstract

Surface functionalization of Ti₂C MXene significantly alters its properties, paving the way for enhanced performance in various application, including energy storage, sensing, and catalysis. The electronic properties of Ti₂C Mxene are highly sensitive to surface functionalization, offering opportunities for tunable material behavior. In this computational study we explore the effect of surface termination(-OH, -O, -F, -Cl) on the band structure and density of states of Ti₂C MXene using Density Functional Theory(DFT). The stability of each structure verified using phonopy calculation. The analysis reveals that functional groups significantly modify the bandgap and electronic states near the Fermi level, with oxygen terminations enhancing metallicity while hydroxyl and fluorine induce semiconductor - like features. These results provide a deeper understanding of how surface functionalization governs the electronic behavior of Ti₂C MXene, enabling optimization for electronic and energy applications.

Keywords: MXene, DFT, Band structure, DOS.



Ti₂C Monolayer.

References

[1] Siby Thomas, Sruthi Thulaseedasan, Mohsen Asle Zaeem, Surface functionalization effect on physical properties and quantum capacitance of Ca₂C MXenes, FlatChem, Volume 35, 2022, 100414, ISSN 2452-2627,

[2] Zafer, Kandemir., Engin, Torun., Fulvio, Paleari., Celal, Yelgel., Cem, Sevik. (2022). Surface termination dependence of electronic and optical properties in Ti₂CO₂ MXene monolayers. Physical Review Materials, doi: 10.1103/PhysRevMaterials.6.026001

Lead-Free, Vacancy-Ordered Double Halide Perovskite based material for Thermoelectric Energy Utilization

Subarna Ray, Rahul Sharma¹

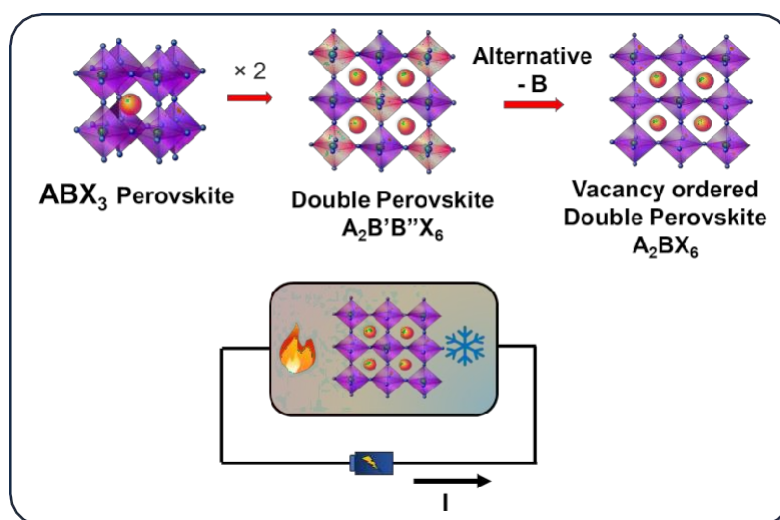
¹ Department of Physical Sciences, IISER Berhampur, Transit Campus, Govt. ITI Building Engg. School Junction, Berhampur, Odisha 760010, India.

Presenter E-mail: - subarnaray22@iiserbpr.ac.in

ABSTRACT

As non-renewable energy sources are finite and reducing rapidly, we need robust and sustainable energy sources to overcome the issue. Waste heat can be directly converted to electricity via the Seebeck effect by the thermoelectric materials. Halide perovskite materials are well-established and have multiple applications, including thermoelectric properties, but there are some difficulties, such as moisture degradation, ion migration, lead toxicity, etc. Therefore, it is important to think about different perovskite materials and related structures. The lead-free vacancy-ordered halide double perovskite has shown great promise for its stability, environmentally friendly nature, and unique optoelectronic properties. In this work, we have investigated the thermoelectric properties of Cs_2TeBr_6 as a possible thermoelectric material. We have calculated the octahedral factor and Goldschmidt tolerance factor to show that this vacancy-ordered double perovskite is stable. We have combined ab initio calculations with the Boltzmann transport theory to predict the thermoelectric properties. Our calculations reveal a good thermoelectric figure of merit (zT), indicating that this family of materials may have a promising future in renewable energy applications.

Keywords: Vacancy ordered Double Perovskite; Thermoelectric Effect; Boltzmann Transport Theory; Renewable Energy.



ASSESSING AI'S POTENTIAL IN GALLIUM NITRIDE MATERIAL DESIGN FOR SPINTRONIC APPLICATIONS

Dipan Kumar Das, Padmaja Patnaik*, Santanu Kumar Nayak, Mandakini Barala

School of Applied Sciences, Centurion University of Technology and Management, Odisha, India

*padmaja.patnaik@gmail.com

ABSTRACT:

The quest for designing intelligent and functional materials is a critical pursuit spanning diverse domains, from material science to electronics, biomedicine, and energy. This article delves into the transformative potential of artificial intelligence (AI), specifically ChatGPT, in the context of spintronics application for Gallium Nitride (GaN) material design. While researchers actively explore innovative models for material design, recent advancements in analytical tools and computer technology, along with the adoption of data-driven techniques like AI, have opened new avenues.

Our case studies employ Artificial intelligence to perform simple tasks across various subareas of computational material science, providing insights into its understanding of material science. Despite minor errors in general tasks, AI showcases adaptability through human interactions. The findings underscore the model's potential in aiding spintronics research, offering a unique perspective on the synergy between AI and GaN material design.

However, considerations such as output consistency, potential hidden errors, and ethical consequences are vital to address. This abstract highlights the promising aspects of leveraging AI, particularly ChatGPT, in the realm of spintronics, emphasizing the need for further exploration and refinement to unlock its full potential for GaN material design applications.

KEY WORDS: GaN, AI, GPT, Material design, Spintronics

Lithium and Sodium Superionic Conduction in Metal Borohydride Framework

Shweta Choudhary* and Swastika Banerjee

Department of Chemistry, Indian Institute of Technology Roorkee

Roorkee, Uttarakhand-247667, India

*E-mail: shweta_c@cy.iitr.ac.in

The development of all-solid-state batteries (ASSBs) utilizing non-flammable and safer solid superionic conductors (SICs: solid-electrolyte with Li/Na-ion conductivity ≥ 1 mS cm⁻¹) is critical in the societal shift to renewable energy.¹ Metal borohydrides represent a family of SICs that were recently discovered to have superionic conduction in disordered phase, making them promising candidates as electrolytes for solid-state batteries (SSBs).²⁻³ Nevertheless, achieving both high ionic conductivity and wide electrochemical stability window at room temperature remains a challenge. Moreover, the role of anion reorientation in facilitating rapid cation motion remains poorly understood and no design rules have yet been established to achieve liquid-like conduction within the borohydride framework. In this work, we describe our recent progress in identifying the suitable first-principles approach for analyzing the structures, stabilities, and dynamics of metal borohydrides, aiming at precise predictions of cation diffusion characteristics within the borohydride framework. This study offers a perspective that has the potential to pave the way for advanced Solid-State Ionic Conductors (SIC).⁴

Keywords: Solid-state batteries, superionic conductors, energy storage, metal borohydrides

References:

1. Y. Li, et al. *A Lithium Superionic Conductor for Millimeter-Thick Battery Electrode*, *Science*, 381(2023) 50–53.
2. C. Zhou et al. *Enhanced Electrochemical Performance of the Li₂B₁₂H₁₂-Li₂B₁₀H₁₀-LiBH₄ Electrolyte*, *ACS Appl. Energy Mater.*, 6(2023) 7346–7352.
3. P. Till et al. *On the Local Structure in Ordered and Disordered Closo-Hydroborate Solid Electrolytes*, *J. Phys. Chem. C*, 127(2023) 987–993.

A first principle characterisation on structural & electronic properties of 2D HfS₂ monolayer

Selvamani E¹, Preferencial Kala C^{1*} and John Thiruvadigal D¹

¹Computational Materials Science and Nanodevices Simulation Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur 603203, Tamil Nadu, India.

Abstract: Transition metal dichalcogenides (TMDCs) have gained much attention due to their high capability in nano energy. Semiconducting TMDC monolayers have been proven viable for numerous energy-related applications. In this current research, based on the first principle investigation, we have explored the structural and electronic properties of both T-phase and H-phase HfS₂ monolayers. For the structural property analysis, we have analysed systems symmetry, lattice parameters, bond lengths, and bond angles. To understand the electronic properties of the HfS₂ monolayer, band structure, density of states, projected density of states (PDOS), and electron difference density were assessed. The structure stability of the system was confirmed by using cohesive energy analysis. The pristine HfS₂ monolayer's both T-phase and H-phase exhibits an indirect bandgap semiconductor. Our findings suggest that T-phase and H-phase HfS₂ monolayers have interesting electronic characteristics for thermoelectric transport applications.

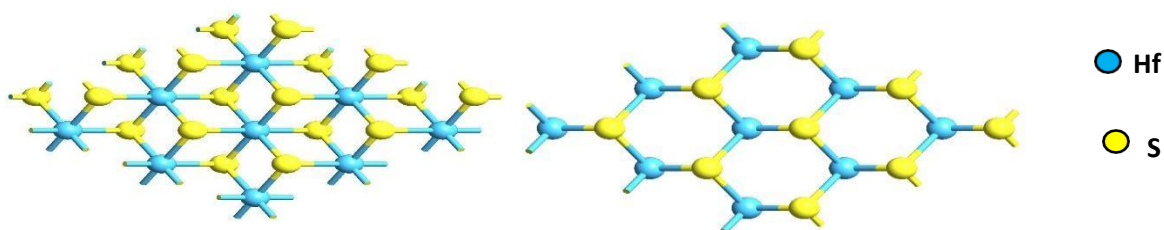


Fig1. Top view of T-Phase HfS₂

Fig2. Top view of H-Phase HfS₂

References:

- [1] Huynh, T.M.D., Nguyen, D.K., Nguyen, T.D.H., Dien, V.K., Pham, H.D. and Lin, M.F., 2021. Geometric and electronic properties of monolayer HfX₂ (X= S, Se, or Te): a first-principles calculation. *Frontiers in Materials*, 7, p.569756.
- [2] Nakamura, K., 2018. First-principles simulation on thermoelectric properties of transition metal dichalcogenide monolayers. *Japanese Journal of Applied Physics*, 57(6S1), p.06HE04.
- [3] Faghinasiri, M., Ahmadi, A., Alvankar Golpayegan, S., Garosi Sharifabadi, S. and Ramazani, A., 2020. A first-principles study of nonlinear elastic behavior and anisotropic electronic properties of two-dimensional HfS₂. *Nanomaterials*, 10(3), p.446.

Defect engineering and its impact on electrocaloric properties in non-stoichiometric BaTiO₃-based system

Eliya. Y and Murugavel. P

Perovskite Material Laboratory, Functional Oxides Research Group, Department of Physics,
Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu, India.
Email: elijah19d202@gmail.com

Abstract:

Recently, solid-state refrigeration systems for the electrocaloric effect (ECE) have become a popular research topic. The ECE occurs when an electric field is applied or withdrawn from a ferroelectric material, producing an adiabatic temperature change (ΔT) [1]. The site-engineered lead-free perovskite structure in the BaTiO₃ (BTO) system, with simultaneous substitution of the heterovalent ion at the Ba- site and the isovalent ion at the Ti-site, causes vacancies due to non-stoichiometry, which can lead to transition [2] other than structural transitions observed in BTO. In the context of well investigated EC research, temperature-dependent P-E hysteresis loops were retrieved rather than pyroelectric current measurements, where dynamic temperature effects were still lacking. In this context, the investigation of ECE was performed on synthesized Ba_{1-x}La_{2x/3}Ti_{1-y}Zr_yO₃ ($x = 0.05$; $y = 0.00, 0.01, 0.03, 0.05, 0.07$ and 0.09) samples via the solid-state method by temperature-dependent pyroelectric current measurements. The X-ray diffraction data, after Rietveld refinement, revealed the co-existence of both tetragonal and cubic phases in all samples. Raman spectroscopy investigations demonstrated the presence of locally generated vibrational modes caused by vacancies at the higher wavelength side, which arise to offset the total charge in the perovskite. Electron paramagnetic resonance (EPR) spectroscopy, in the X-band at 9 GHz using a JES-FFA200 Electron Spin Resonance Spectrometer revealed the existence of both Ti- vacancies and Ba-vacancies. Temperature-dependent dielectric measurements revealed a decrease in T_C and an increase in diffuseness (γ) parameters with increased incorporation of Zr. Using Maxwell's thermodynamic relations, the estimated EC parameter (ΔT) from the temperature-dependent pyroelectric current measurement showed three distinct EC responses (ΔT_{spike} , ΔT_s and ΔT_f) over three distinct transitions within the operational temperature window. The superior temperature stability of ΔT arising from three distinct transitions in these samples makes them potential for efficient cooling application.

References:

- [1] Y. Bai, X. Han, X. C. Zheng and L. J. Qiao, Sci. Rep. **3**, 02895 (2013).
- [2] M. Wu, Q. Zhu, J. Li, D. Song, H. Wu, M. Guo, J. Gao, et al., Appl. Phys. Lett. **114**, 142902 (2019).

Study of glassy phase transition in modified barium titanate system.

Utkarsh Jain, Pranab Kumar Roy, and P Murugavel

Perovskite Materials lab, Functional Oxides Research Group, Department of Physics, Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu

Email: utarshjain483@gmail.com

Relaxor ferroelectrics, similar to spin glasses in ferromagnetic systems, exhibit a disordered state characterized by polar nanoregions (PNRs) [1]. Compounds with phase transitions near the morphotropic phase boundary (MPB) show excellent properties like high piezoelectricity, dielectric permittivity, and electro-strain. However, in lead-free systems, MPB compositions exhibit large remanent polarization, limiting energy storage applications. Advanced energy storage devices require materials with high dielectric permittivity, maximum polarization, and low hysteresis over a wide temperature range. In literature, researchers have reported the aforementioned possibilities by combining the properties of both the ferroelectric (long-range order) and relaxor (PNRs) transitions. However, very few studies have reported the integration of two glass transitions (relaxor ferroelectrics) in ferroelectrics, especially in lead-free materials [2]. The approach to designing such a glass-glass transition remains unknown, as does the potential for this unique state to enhance dielectric energy-storage properties or exhibit other interesting characteristics. In this regard, the $\text{Ba}_{1-x}\text{Li}_x\text{Ti}_{1-x}\text{Nb}_x\text{O}_3$ ($x = 0, 0.01, 0.03, 0.04, 0.05, 0.07, \text{ and } 0.10$) samples are synthesized by the solid-state route. The XRD patterns exhibit that all samples are crystallized in pure perovskite form without impurity peaks. The Rietveld refinement reveals the systematic decrease in the orthorhombic phase with an increase in Li and Nb concentration. Compositions $x \geq 0.04$ do not show any (002) and (200) peak splitting indicating the system going into the cubic phase. Dielectric spectra indicate that, when the substitution $\geq 4\%$, the system shows broad peaks in the dielectric spectra. The highly diffusive peaks and not much dielectric dispersion across varying frequencies suggest that the system shows glassy behavior. The best fitting of T_g using Vogel-Fulcher law, confirms the existence of glass transitions. Ferroelectric properties at higher substitution also indicate the disordered nature present in the sample. These findings provide a new framework for the design of glass-glass transitions in ferroelectric systems, paving the way for the design of energy devices with high dielectric permittivity, maximum polarization along with lower hysteresis and remanent polarization over a wide range of temperatures.

References

1. A. A. Bokov and Z.G. Ye. 2006. Recent progress in relaxor ferroelectrics with perovskite structure. *J Mater Sci* 41, 31–52.
2. Le Zhang, *et al.* 2017. Glass-glass transitions by means of an acceptor-donor percolating electric-dipole network. *Phys. Rev. Appl.* 8.5 054018.

Berry curvature induced anomalous Hall effect in Pt₂MnGa

Bhargab Kakati^{1*} and Munima B. Sahariah¹

¹Institute of Advanced Study in Science and Technology, Guwahati-70135, India

*Corresponding author: bhargabkakoti@gmail.com

Abstract: The intrinsic anomalous Hall effect in ferromagnetic materials depends on the spin–orbit-coupling-induced effect in the electronic structure. The presence of anomalous Hall effect can be realized from the existence of the finite Berry curvature. Since the Heusler material Pt₂MnGa is ferromagnetic in its collinear state and no report on its transport properties has yet been made, the anomalous Hall effect in this system is investigated using a combined approach of the density functional theory and maximally localized Wannier function. Analysis of the Berry curvature reveals positive and negative peaks along the high symmetry k-points. These peaks together lead to a significant negative anomalous Hall conductivity, which makes the material a promising candidate for applications in spintronics.

Flexible Triboelectric Nanogenerator based on PVDF-BCZT Nanocomposite Films for piezo-tribo Hybrid Energy Harvesting

Ankita K¹ and P. Murugavel¹

¹Perovskite Materials Laboratory, Department of Physics, IIT Madras, Chennai, 600036,

India Email- ankita.ak04@gmail.com

Abstract: Triboelectric nanogenerators (TENGs) have gained significant attention in recent years as an effective technology to harvest ambient energy from day to day activities due to their high efficiency, simplicity and versatility[1-2]. The kinetic ambient energy e.g. walking, machine vibration can be harvested through triboelectric and piezoelectric energy harvesters. Ferroelectric materials having spontaneous, switchable, and remnant polarization shows potential to improve and control energy harvesters output [2-3]. In this work, 0.5(Ba_{0.7}Ca_{0.3})TiO₃- 0.5Ba(Ti_{0.8}Zr_{0.2})O₃ (BCZT) nanoparticles were synthesized using the sol-gel method and integrated into polyvinylidene fluoride (PVDF) matrix to create nanocomposite exhibiting enhanced triboelectric output. BCZT is a widely studied ferroelectric material, with its superior dielectric and piezoelectric properties, is expected to contribute to improve charge transfer and triboelectric charge density when incorporated into PVDF matrices. BCZT nanoparticles were synthesised using sol-gel synthesis. X-ray diffraction (XRD), scanning electron microscopy (SEM) results shows nanoparticles are of size < 70 nm and without any impurity. The PVDF- BCZT nanocomposite films were prepared using the spin coating technique, to form uniform and better ferroelectric film. The triboelectric performance of the composites was tested through TENG measurements in contact- separation mode, under application of periodic mechanical force (10 N, 6 Hz). Results showed that the addition of BCZT nanoparticles significantly increased the output voltage in composite films compared to pure PVDF films. To demonstrate application, a fabricated TENG was used to power light-emitting diodes (LEDs). These results highlight that PVDF- BCZT nanocomposite materials have the potential to be effective and scalable material for triboelectric energy harvesting applications.

References:

- [1] L. Zhou, D. Liu, J. Wang, and Z.L. Wang, (2020). Triboelectric nanogenerators: Fundamental physics and potential applications, *Friction* 8, 481.
- [2] Y.S. Choi, S.W. Kim, and S. Kar-Narayan, (2021). Materials-Related Strategies for Highly Efficient Triboelectric Energy Generators, *Adv Energy Mater* 11, 2003802.
- [3] J. Wang, C. Wu, Y. Dai, Z. Zhao, A. Wang, T. Zhang, and Z.L. Wang, (2017). Achieving ultrahigh triboelectric charge density for efficient energy harvesting, *Nat Commun* 8, 88.

Transport properties of AM_4X_8 Type Tetrahedral Cluster Compounds

Aravind V Raj¹ and C S Yadav¹

¹*School of Physical Science, Indian Institute of Technology Mandi, Kamand 175005*

The family of lacunar spinel compounds AM_4X_8 ($A = \text{Ga, Ge}$; $M = \text{V, Nb, Ta}$; $X = \text{S, Se}$) are well known for its different thermal and electronic transport properties. Here we had synthesized polycrystal GaV_4Se_8 using the solid state reaction method and confirmed single phase with powder XRD. It is skyrmion hosting, having a Mott insulating ground state with a structural phase transition from cubic to rhombohedral at a temperature of $T_S = 41\text{K}$ and magnetic ordering from paramagnetic to ferromagnetic at a temperature of $T_C = 17.5\text{K}$. The resistivity vs temperature plot of the compound reveals a Variable Range Hopping behavior while fitting with Mott's VRH. The Seebeck coefficient of the compound, measured up to 70K helps in obtaining the activation energy $E_a^S = 0.065\text{eV}$. This compound is getting more explored because of its topologically protected skyrmion hosting property, which is helpful in the field of memory devices, AI and quantum computing.

References

- [1] Rastogi *et al.*, J. Phys.: Condens. Matter **5** (1993) 5953-5962
- [2] Masatoshi Akazawa *et al.*, Phys Rev R **4**, 043085 (2022)
- [3] Y. Fujima *et al.*, Phy Rev B **95**, 180410(R) (2017)
- [4] L. Cario *et al.*, Advanced Materials **9**, 201002521 (2010)

First-principles study of the electronic structure, Z_2 invariant and Quantum oscillation in the kagome material CsV_3Sb_5

Shalika R. Bhandari¹, Md. Zeeshan², Vivek Gusain², Keshav Shrestha³, and D. P. Rai⁴

¹Department of Physics, Bhairahawa Multiple Campus,

Tribhuvan University, siddarthanagar-32900, Bhairahawa, Nepal

²Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi-110016, India

³Department of Chemistry and Physics, West Texas A and M University, Canyon, Texas 79016, USA

⁴Department of Physics, Mizoram University, Aizawl 796004, India

Contact: phz228539@iitd.ac.in

Keywords: Kagome materials, Z_2 invariant, Fermi surface, Charge density wave

This work presents the electronic structure, phonon dispersion, Z_2 invariant and the Fermi surface of the kagome type CsV_3Sb_5 compound by using the density functional theory calculations. The calculated phonon dispersion of CsV_3Sb_5 on pristine state at ambient pressure shows the negative phonon frequencies around M and L-points in the first Brillouin Zone, which is consistent with the literature [1, 2]. The L-point soft mode suggests the presence of a $2 \times 2 \times 2$ reconstruction of disordered phase and the M-point soft mode is associated with the breathing phonons of V atoms. We report the Fermi surface reconstruction which is responsible for the Charge Density Wave (CDW) formation. We have also studied the pressure effect on phonon dispersion for both the pristine and the distorted phases ranging from 1GPa to 6GPa pressure. The complete suppression of the CDW Phase takes place at and above the 4GPa pressure, which agrees well with the previous experimental data [3]. We have also calculated the Fermi Surface and Z_2 invariant for the above system. Our findings are key to understand the phenomenon like unconventional superconductivity, non-trivial topology and CDW formation in Kagome material CsV_3Sb_5 .

References:

1. Zhang, J. F., Liu, K., *et al.*, "First-principles study of the double-dome superconductivity in the kagome material CsV_3Sb_5 under pressure.", *Physical Review B*, 104, 195130 (2021).
2. Tan *et al.*, "Charge density waves and electronic properties of superconducting kagome metals.", *Physical Review Letters*, 127, 046401 (2021).
3. Z Zhang, *et al.*, "Pressure-induced reemergence of superconductivity in the topological kagome metal CsV_3Sb_5 .", *Physical Review B*, 103, 224513 (2021).

Role of Defect Migration in Wide-Bandgap Semiconductor for Memristor Application: An Ab-initio Analysis

Tejendra Dixit* and M. Julie Therese

Department of ECE, IITDM Kancheepuram, Chennai, 600127, India

*tdixit@iitdm.ac.in

Abstract: Memristors, as two-terminal passive devices, enable in-memory computing, addressing the bottlenecks inherent in traditional Von Neumann architecture. Their properties such as excellent scalability, low power consumption, and rapid switching speeds make them ideal for applications in artificial intelligence, Internet of Things (IoT), cloud services. Material defects in memristors introduce additional energy states that facilitate charge transport mechanisms. Oxide semiconductors like TiO_x , HfO_x , ZrO_x , and TaO_x are commonly utilized in memristive devices. In this work, ZnO is chosen as the active material due to its high carrier mobility, wide bandgap (~ 3.4 eV), CMOS compatibility, and large free exciton binding energy (~ 60 meV) at room temperature. The atomic structure of hexagonal wurtzite ZnO, with and without vacancies, was modelled using VESTA (version 3.5.8). In this structure, ZnO contains three-fold and four-fold oxygen atoms, with migration pathways occurring between three-fold- three-fold, three-fold-four-fold, and four-fold-four-fold configurations. Partial density of states (PDOS) plots were generated using first-principles calculations, allowing analysis of the band structures of both pristine and defect-induced ZnO. The defect formation energy (E_f) and activation energy (E_A) were computed using density functional theory (DFT) with the generalized gradient approximation (GGA). Literature indicates that defects such as zinc vacancy (Zn_v), zinc interstitial (Zn_i), zinc antisite (Zn_a), oxygen interstitial (O_i), and oxygen antisite (O_a) exhibit high formation energies. Our investigation reveals that oxygen vacancy (O_v) in ZnO has a comparatively low formation energy of -1.38 eV. In an Au/ZnO/Au device, among various migration pathways, the path with the lowest value of E_A is most conducive to conduction. Vacancies with charge states of $+1q$, $+2q$, and neutral were analyzed. The formation and dissolution of conductive filaments, responsible for resistive switching behavior, were studied using current-voltage (I-V) characteristics obtained from SCAPS-1D software.

References:

1. M. Therese, "First-principles calculations to establish the functionality of self-connected point-defect migrations in n-ZnO-and p-CuO-based memristive devices," *IEEE Transactions on Electron Devices*, 2023.
2. S. Nagendra, "Ab-initio Analysis of the Filamentary Behavior Assisted by Ionic Boron Frenkel-pair Defects in h- BN Planar-Atomristor," *IEEE Electron Device Letters*, 2024.

Modulating the sub-gap defects in titanium oxide using atomic layer deposition for the application in carrier selective Si solar cell

Namitha Dsouza¹ and Jatin K Rath¹

¹Department of Physics, IIT Madras, Chennai, 600036, India

Abstract: Atomic layer deposition (ALD) is a self-limiting chemisorption growth technique that offers advantages in developing c-Si based carrier selective contact solar cells (CSC). This study aims to develop titanium oxide for application in the electron transport layer (ETL) of CSC devices with different deposition recipes in ALD. By facilitating efficient electron extraction while minimizing recombination losses, TiO₂ enhances the overall photovoltaic performance of silicon-based cells[1]. The charge dynamics and defect states in ALD TiO₂ and carrier movement at the interface with Si is not well comprehended and utilized. TiO₂ film in this study is grown on Si using different configurations of precursor and co-reactants in ALD, and tetrakis- (dimethylamino)titanium (TDMAT) is used as the titanium precursor.

The defect states here are analyzed by means of sub-gap absorption happening in optical absorption spectroscopy. It is possible to significantly alter and tune the mid-gap defect concentration in TiO₂ to meet specific requisites. The TiO₂ film acts rather as a hole-blocking layer than an ETL, but the change in defect concentration tends to affect the carrier transport dynamics through the contact. The plasma ALD films exhibit lower mid-gap states in TiO₂ films compared to the thermal ALD films, and the inclusion of plasma treatment during and after the films' deposition helps manipulate the defects through the band gap. In addition, the band bending in Si at the interface changes with variations in deposition recipes and the defect state concentration. The optical absorption spectroscopy data is used to deduce the detailed band structure of these films. The results of the study highlight the use of ALD in modulating carrier transport in TiO₂ and the ease of engineering defects in oxides

References:

[1] Yang X, Weber K, Hameiri Z, De Wolf S. Industrially feasible, dopant-free, carrier-selective contacts for high- efficiency silicon solar cells. *Prog Photovolt Res Appl.* 2017;25(11):896-904. doi:10. 1002/pip.2901

Exploring Three-Dimensional Topological Weyl Semimetals Featuring Robust Fermi Arcs and Lifshitz Transition

Saurabh Kumar Sen,^{*} Shivendra Kumar Gupta and Poorva Singh[†]

*Department of Physics,
Visvesvaraya National Institute of Technology, Nagpur, 440010, India*

The Weyl semimetal is a novel state of quantum matter characterized by the presence of emergent quasi-particles known as Weyl fermions, which arise from the breaking of either inversion or time-reversal symmetry. Within a Weyl semimetal, chirality manifests as a topologically protected chiral charge. Weyl nodes with opposite chirality are spatially separated and connected through surface states known as Fermi arcs at the crystal's boundary. Our work introduces a ternary transition metal compound lacking inversion symmetry as a promising candidate for Weyl semimetal behavior, emphasizing its distinct characteristics. By incorporating spin-orbit coupling, the material exhibits a notable phenomenon: the emergence of Weyl fermions with linear dispersions and a chiral charge of ± 1 . Notably, the top and bottom surfaces of the (001) plane connect distinct Weyl points, leading to a topological Lifshitz transition, thereby enhancing our understanding of transport phenomena in three-dimensional topological semimetals and their potential practical applications.

References

- [1] Gao, H., Venderbos, J. W., Kim, Y., & Rappe, A. M. (2019). Topological semimetals from first principles. *Annual Review of Materials Research*, 49, 153-183.
- [2] Singh, B., Chang, G., Chang, TR. *et al.* Tunable double-Weyl Fermion semimetal state in the SrSi₂ materials class. *Sci Rep* 8, 10540 (2018).

^{*} saurabhgsen@gmail.com

[†] poorvasingh@phy.vnit.ac.in

Unraveling K-ion storage in MXenes films for flexible supercapacitor applications

Manuj Ahuja*, Priya Johari, and Binson Babu

Department of Physics, School of Natural Science,
Shiv Nadar Institution of Eminence (Deemed to be University),
Uttar Pradesh-201314, India

*Email: ma918@snu.edu.in

Abstract: MXene-based materials have garnered significant attention for their potential in energy storage applications due to their unique structure and surface chemistry. In this work, $Ti_3C_2T_x$ MXene freestanding films were synthesized through a mild wet-chemical process and explored its electrochemical performance in K-salt-based aqueous neutral electrolytes. The MXene films exhibit good potassium (K^+) ion intercalation with high volumetric capacitance and show a non-diffusion-controlled K- ion intercalation process of $\sim 94\%$ at a scan rate of 6 mVs^{-1} , indicating the suitability of use as an electrode for high-power applications. Moreover, density functional theory (DFT) calculations, conducted using VASP software, were employed to investigate the K-ion intercalation mechanism. The computational results corroborated experimental XRD observations, revealing a decrease in the d-spacing of MXenes during K-ion intercalation. This phenomenon is attributed to hydrogen bonding between the water molecules, inserted along with K-ions, and the oxygen or surface termination groups. Further, the symmetric supercapacitor fabricated with the $Ti_3C_2T_x$ films retained 98% of their initial capacitance after 10,000 cycles, highlighting their long-term stability. Furthermore, flexible symmetric supercapacitors fabricated with the films showed promising performance across a range of temperatures, further emphasizing their robustness and adaptability for practical applications. This combination of experimental and computational approaches highlights the potential of $Ti_3C_2T_x$ films as advanced electrode materials for high-performance energy storage devices.

References:

- A. Vahid Mohammadi, J. Rosen, Y. Gogotsi, Science 2021, 372, eabf1581
- B. A. Iqbal, N. M. Hamdan, Materials 2021, 14.
- C. B. Babu, P. Simon, A. Balducci; Adv. Energy Mater. (2020).

Unveiling the Coexistence of Giant Rashba Splitting and Topological properties in hexagonal crystal structure

Shivendra Kumar Gupta*, and Poorva Singh†

Department of Physics,

Visvesvaraya National Institute of Technology,

Nagpur, 440010, India

Composite Quantum Compounds (CQCs) have emerged as a powerful platform for investigating interactions between distinct quantum phenomena. Among these, topological superconductors, axion insulators, and materials exhibiting Rashba spin physics are particularly interesting. In this study, we focus on identifying materials that intrinsically combine giant Rashba splitting with topologically nontrivial states within a single crystalline framework.

Our investigation highlights three materials—RbSnBi, CsSnBi, and ZnBi—uniquely combining the above properties. RbSnBi and CsSnBi are strong topological insulators characterized by multiple band inversions and Dirac surface states. RbSnBi exhibits a Rashba splitting energy of 133 meV with a Rashba coefficient (α_R) of 4.26 eV Å, while CsSnBi exhibits a Rashba splitting energy of 228 meV with Rashba coefficient α_R of 6.4 eV Å—the largest reported among topological materials. Alongside this giant Rashba coefficient, CsSnBi and RbSnBi are strong topological insulators having multiple band inversion and multiple Dirac surface states in a single crystal. These extraordinary properties underline their potential for spintronics, where the coupling of spin and momentum is essential for developing high-efficiency devices.

In addition, ZnBi, with its hexagonal crystal structure, emerges as a topological type II Dirac semimetal with significant Rashba splitting. ZnBi exhibits a Rashba coefficient (α_R) of 2.1 eV Å and a splitting energy of 118 meV, This duality of properties positions ZnBi as a promising candidate for spintronic applications and quantum technologies.

The coexistence of Rashba spin physics and topological states in RbSnBi, CsSnBi, and ZnBi establishes a new paradigm for designing materials with multifunctional properties. This work paves the way for uncovering novel quantum phenomena and highlights the immense potential of intrinsic CQCs in advancing spintronics and next-generation quantum devices.

References

- [1] S. K. Gupta, A. Kore, S. K. Sen, and P. Singh, Coexistence of giant Rashba splitting, multiple band inversion, and multiple Dirac surface states in the three-dimensional topological insulator XSnBi (X= Rb, Cs), *Physical Review B* 107, 075143 (2023).
- [2] S. K. Gupta, N. Singh, S. K. Sen, and P. Singh, Pressure induced Topological Dirac semimetal in XcdP (X = na, K), *arXiv preprint arXiv:2312.05636*(2023).

* shivendrakumarg900@gmail.com

† poorvasingh@phy.vnit.ac.in

List of Total Participants - EESTER – 2025

Registration Number	Name of the participants	Organization
25001	Abinaya.V	SRMIST, KTR
25002	Sneha.J	SRMIST, KTR
25003	S.Susanna Ezhilarasi	QUEEN MARYS COLLEGE CHENNAI 600004
25004	Madhana Gopal G K	SRMIST, KTR
25005	S.M. Esther Rubavathy	SRMIST, KTR
25006	Astha. E	SRMIST, KTR
25007	Viveka N.	SRMIST, KTR
25008	Nivethitha Ganesan	SRMIST, KTR
25009	A Sakthi Balaji	SRMIST, KTR
25010	Jayendran S	SCANMAT Centre
25011	Abhishek K G	SCANMAT Centre
25012	Hemachandrika D	Central University of Tamil Nadu
25013	Lakshmi Naga Sai Laya Pagadala	SRM university - AP
25014	Jijila B	QUEEN MARYS COLLEGE CHENNAI 600004
25015	Rajib Sarkar	IISc
25016	C B Sarath Kumar	SRMIST, KTR
25017	Sreeram Jayan	SRMIST, KTR
25018	Aman Sardwal	IIT Madras
25019	S. Saral Sessal	SRMIST, KTR
25020	Shilpa Paul	IIT Bombay
25021	Rama Chandra Moharana	IIT Tirupati
25022	Smruti Mishra	SRMIST, KTR
25023	Sheik Sameem M	Vellore Institute of Technology, Vellore
25024	Mohsin Sayeed	Institute of Engineering and Technology , Lucknow (Dr. A.P.J. Abdul Kalam Technical University, Lucknow)
25025	Gowthami S	Jain (Deemed-To-Be University) Bangalore
25026	Thameemul Ansari A	SRMIST, KTR
25027	Dr. Pooja Vyas	IIT Bombay
25028	Hariharan Ramesh	SRMIST, KTR
25029	Hema G	SRMIST, KTR
25030	Gopalakrishnan C	SRMIST, KTR
25031	Giri Lakshman N	SRMIST, KTR
25032	Ghate Purohith Kumar	SRMIST, KTR
25033	Arka Bhowmick	IIT Hyderabad
25034	Namrata Das	IIT Hyderabad
25035	Sonali Srotaswini Pradhan	IIT Hyderabad
25036	Subhojit Roy	IIT Madras
25037	Sourin Chatterjee	IIT Madras
25038	Soumyasree Jena	IIT Madras

25039	K Dharmaraj	SRMIST, KTR
25040	Karthikraja E	CSIR - Central Leather Research Institute
25041	Thillaiarasi S	SRM university - AP
25042	Zayid Ahmed	Birla Institute of Technology and Science Pilani, K.K. Birla Goa Campus
25043	Rishab Sahoo	IIT Kharagpur
25044	Thatshinashree P	Vellore Institute of Technology
25045	Subhransu Kumar Negi	Centre for Nano Science and Engineering (CeNSE) ,Indian Institute of Science, Bangalore , Karnataka, India
25046	Muthupandi S	SRMIST, KTR
25047	Sathees Kumar R	SRMIST, KTR
25048	Deepak Upadhyay	The M. S. University of Baroda, Vadodara
25049	Kusum Kumari	IIT Hyderabad
25050	Priyanka Ghosh	IIT Indore
25051	Y.Dhakshayani	Anna University
25052	Monika S	Anna University
25053	Heli	The M. S. University of Baroda, Vadodara
25054	Ashish Priyam Goswami	IIT Bombay
25055	Heera T Nair	The M. S. University of Baroda, Vadodara
25056	Thingujam Yaiphalemba Meitei	SRMIST
25057	Dhori Bhautik Rameshbhai	The M. S. University of Baroda, Vadodara
25058	Ganavarshini S	IIT Madras
25059	Roshme	Anna University
25060	Zarna D. Ponkiya	The M. S. University of Baroda, Vadodara
25061	Rajdeep Banik	IIT Madras
25062	Maricherla Hemalatha	SRM university - AP
25063	Monikana Gope	IIT Roorkee
25064	Vijay Vel R	SRMIST, KTR
25065	Arkamitra Sen	Indian Association for the Cultivation of Science
25066	Anupam Mondal	Indian Association for the Cultivation of Science
25067	Ayan Chakravorty	SHIV NADAR INSTITUTION OF EMINENCE
25068	Sanjay Kumar	SRMIST
25069	Sanchi Monga	IIT Delhi
25070	Shantanu Pathak	IIT Delhi
25071	Mani Bharathi Manickavasagam	SRMIST, KTR
25072	Sumit Kumar	IIT Madras
25073	Ankita	IIT Madras
25074	K.Saikumar	SRMIST, KTR
25075	Mohd Rashid	IIT Indore
25076	Bubunu Biswal	IIT Madsras
25077	Samir Kumar Nayak	IIT Madsras
25078	Bommareddy Poojitha	IIT Tirupati

25079	Pritish Ranjan Joshi	Research Institute for Sustainable Energy, TCG CREST, Kolkata
25080	Sk.Soyeb Ali	Bennett University
25081	Shovan Gayen	Bennett University
25082	Dipanwita Bhattacharjee	IIT Bombay
25083	Ibtesham Tarannum	IIT Hyderabad
25084	Sarga P K	BITS PILANI KK BIRLA GOA CAMPUS
25085	Abhinava Goswami	NIT Manipur
25086	Kahkasha Parveen	IIT Indore
25087	R Kirthik	Regional Institute of Education, Mysuru
25088	Basantia Saswat Abhilash	IIT Hyderabad
25089	Suman	IIT Ropar
25090	Bindhya Krishna R	SRM university - AP
25091	Anjali Prajapati	SRM university - AP
25092	Sachin Kumar	Bhabha Atomic Research Centre, Mumbai
25093	Karthik HJ	BITS Pilani, Goa Campus
25094	Abhishek Hota	Institute Of Physics, Bhubaneswar
25095	Ramji V	IIT Madras
25096	Rooban P	N.M.S.SVN College
25097	R Jagadish	Indian Institute of Science
25098	Ardhendu Dey	SRMIST, KTR
25099	Syed Abubacker Siddique	SRMIST, KTR
25100	Singdha Sagarika Behera	KIIT University, Bhubaneswar, Odisha,751024
25101	Subhajit Sau	IIT Hyderabad
25102	Soumyadeep Bhattacharyya	IIT Goa
25103	Lokesh Yadav	IIT Indore
25104	Joyeta Saha	NISER
25105	Kousika	Indian Institute of Science
25106	Dr. Nila Pal	Shiv Nadar Institution of Eminence, Delhi-NCR.
25107	Anandu Muralidharan	IIT Madras
25108	Vineeta Yadav	IIT Tirupati
25109	Divya	IIT Ropar
25110	Manpreet Kaur	IIT Ropar
25111	Shikha	IIT Ropar
25112	Manorama Pandey	IIT Bhubaneswar
25113	Abhishek	IIT Jodhpur
25114	Pritesh Srivastava	Tata Institute of Fundamental Research, Mumbai
25115	Jithesh R K	N.M.S.S.V.N College
25116	Varinder Pal	IIT Kharagpur
25117	Subham Chattopadhyay	Visvesvaraya National Institute of Technology, Nagpur
25118	Chithresh T M	N.M.S.S.V.N. College
25119	Shrestha Banerjee	Visvesvaraya National Institute of Technology, Nagpur

25120	Anupama S	IISER Pune
25121	Jeet Sharma	National Institute of Science Education and Research
25122	Veerababu	IGCAR, HBNI
25123	Rose Jose	MAR DIONYSIUS COLLEGE, PAZHANJI
25124	Purushothaman M	IITDM Kancheepuram
25125	Rahul E	Sri Vyasa NSS College Wadakkanchery
25126	Rahul Ghosh	NISER
25127	Rashi Jain	IIT Dharwad
25128	Praveen N	IIT,Dharwad
25129	Surya S	SRMIST, KTR
25130	K Damodarreddy	SRMIST, KTR
25131	Bidyadhar Das	IISER Berhampur
25132	Harish Nanda A	SRMIST, KTR
25133	Vijayakumar B	SRMIST, KTR
25134	Babuji Dandigunta	IIT Madras
25135	Pratik Kumar Sahu	IIT Madras
25136	Muthukrishnan Sundaram	IIT Madras
25137	Ayusmin Panda	IIT Madras
25138	Shubhalakshmi Sahu	IIT Madras
25139	Pramod Kumar Verma	IIT Madras
25140	A. Amudhavalli	IIT Madras
25141	Arijit Mandal	IIT Madras
25142	Susmita Jana	IIT Madras
25143	Manas Biswal	IISER Berhampur
25144	Sidhi Vinayaka M Mallya	NIT SRINAGAR
25145	Santanu Kumar Nayak	Centurion University of Technology and Management, Odisha
25146	Kavyasree N	Central University of Kerala
25147	Khushboo	IIT Madras
25148	Akshara Ak	SRM University - AP
25149	Subarna Ray	IISER Berhampur
25150	Shanu Bandyopadhyay	Institute of Physics, Bhubaneswar
25151	Priyadarshini S	SRM IST
25152	Adabala Venkata Snehith	Tata Institute of Fundamental Research, Hyderabad
25153	Arindom Das	IIT Madras
25154	Dipan Kumar Das	Centurion University of Technology and Management
25155	Poonam Sharma	Indian Institute of Technology
25156	Shweta Choudhary	IIT Roorkee
25157	Yuvashri. R	Queen Mary's College (A)
25158	Selvamani E	SRMIST, KTR
25159	Hareram Swain	IIT Madras
25160	Deepak	NIT Kurukshetra

25161	Yammala Eliya	IIT Madras
25162	Utkarsh Jain	IIT Madras
25163	Bhargab Kakati	Institute of Advanced Study in Science and Technology (IASST), Guwahati
25164	Ankita K	IIT Madras
25165	Aravind V Raj	IIT Mandi
25166	Vivek Gusain	IIT Delhi
25167	M. Julie Therese	Indian Institute of Information Technology (IIITDM) Kancheepuram
25168	Md AZAD UL HAQ	IIT Madras
25169	Ajit Singh Jhala	Visvesvaraya National Institute of Technology, NAGPUR
25170	Nagarjuna Patra	Visvesvaraya National Institute of Technology Nagpur,Nagpur
25171	Namitha Dsouza	IIT M
25172	Saurabh Kumar Sen	VNIT, Nagpur, Maharashtra
25173	Soumyojit Chatterjee	IISER Berhampur
25174	Manuj Ahuja	Shiv Nadar Institution of Eminence
25175	Hariharan K S	Central University of Tamil Nadu
25176	Sujay Saha	IIT Madras
25177	G Raghanya	IIT Madras
25178	Arunava	Donostia International Physics Center in Spain
25179	Pratik Patra	NISER Bhubaneswar
25180	Anindit Das	NISER Bhubaneswar
25181	Shubhay Dikkar	NISER Bhubaneswar
25182	Gayatri Panda	NISER Bhubaneswar
25183	Shivendra Kumar Gupta	VNIT Nagpur
25184	Padmaja Patnaik	Department of Physics, Centurion University of Technology and Management, Bhubaneswar, Odisha
25185	Ashis Kumar Panigrahi	Institute of Physics, Bhubaneswar
25186	Alok Kumar	Institute of Physics, Bhubaneswar
25187	Gayathri P	SRMIST, KTR
25188	Gowsalya	SRMIST, KTR
25189	Prabhakaran	SRMIST, KTR
25190	Hansika	SRMIST, KTR
25191	Buveneswaran	SRMIST, KTR
25192	Sakshi	SRMIST, KTR
25193	Santhosh	SRMIST, KTR
25194	Priyanka B	SRMIST, KTR
25195	Perarasan	SRMIST, KTR
25196	Praveen	SRMIST, KTR
25197	Madhurja Buragohain	IIT Madras
25198	Vigneshwaran V	IIT Madras
25199	Subhadeep Banerjee	IIT Madras

25200	Pradeep Kumar Rana	IIT Madras
25201	Sandip Kumar Padhi	IIT Madras
25202	Rasmi Ranjan Mohapatra	IIT Madras
25203	Tiasha Roy	IIT Madras
25204	Priti Singh	CSIR - Central Leather Research Institute
25205	Soumyaranjan Sahoo	IIT Madras
25206	Abhijeet	IIT Madras
25207	Balaji Sriram	IIT Madras
25208	Javed Akhtar	IIT Madras
25209	Prasanna M	IIT Madras
25210	Mohanraj B	IIT Madras
25211	Praveen	IIT Madras
25212	Ramesh R	IIT Madras
25213	Madhesh P	Anna University
25214	P K Samay	
25215	Suresh	
25216	Sravani Bontha	
25217	Debankita Ghosh	
25218	Manpreet Kaur	NIT KKR

Funding and Support



GLOBAL ENGAGEMENT
Indian Institute of Technology Madras



Netweb[®]
TECHNOLOGIES

Tyrone[®]

Conveners

Dr. Ranjit Nanda

Department of Physics,
Indian Institute of Technology Madras, Chennai, India

nandab@iitm.ac.in



Dr. Saurabh Ghosh

Department of Physics and Nanotechnology,
SRM Institute of Science and Technology, Chennai, India

saurabhs@srmist.edu.in



Dr. Sudakar Chandran

Department of Physics,
Indian Institute of Technology Madras, Chennai, India

csudakar@iitm.ac.in



Dr. Jaivardhan Sinha

Department of Physics and Nanotechnology,
SRM Institute of Science and Technology, Chennai, India

jaivardr@srmist.edu.in

