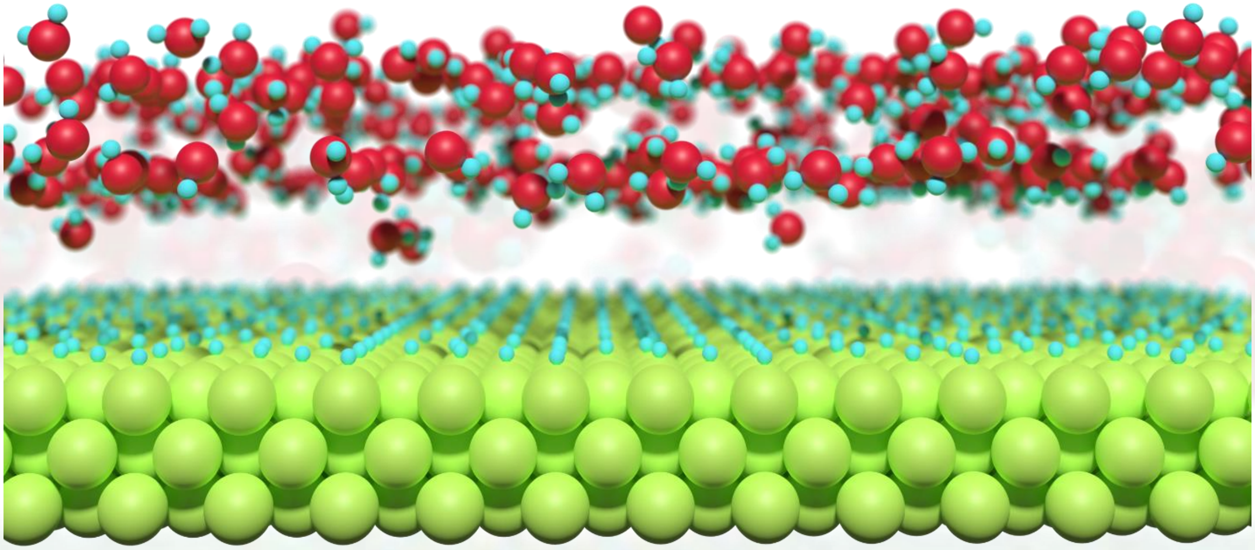
3rd International Conference on Materials Genome

ICMG – III

SRM University – AP, Andhra Pradesh

22nd - 24th February, 2024



Sponsored by :

President lays the foundation ………

Dr. P. Sathyanarayanan
Pro Chancellor

Message

It is with immense pleasure and pride that I extend a warm welcome to each and every one of you to the 3rd International Conference on Materials Genome, hosted by SRM University - AP, from February 22nd – 24th, 2024.

As we embark on this significant journey of exploration and collaboration in the realm of materials science, it is truly gratifying to witness the convergence of brilliant minds and innovative ideas from across the globe under one roof. This conference serves as a platform for the exchange of knowledge, experiences, and breakthroughs in the fascinating field of materials genome.

Our university takes great pride in being at the forefront of research and innovation, and hosting this esteemed conference underscores our commitment to fostering academic excellence and pushing the boundaries of scientific discovery. I would like to express my heartfelt gratitude to the organizing committee, speakers, and all participants for their invaluable contributions in making this conference a reality. A special word of thanks is due to our esteemed collaborators, the Asian Consortium on Computational Materials Science, for their unwavering support and partnership in organizing this event. I extend my sincere appreciation to:

Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore
National Chemical Laboratory, Pune
Virginia Commonwealth University, USA
Indian Institute of Technology, Madras
Indian Institute of Technology, Bombay
TCG Crest, Kolkata

Furthermore, I extend my heartfelt gratitude to the Science and Engineering Research Board and the Council of Scientific & Industrial Research, Govt. of India for their partial financial support. Once again, a warm welcome to SRM University - AP. Let us join hands in embracing the spirit of inquiry, discovery, and excellence as we embark on this enlightening journey together.

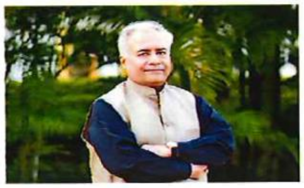
Wishing you all a fruitful and enriching conference experience.

Warm regards,

Pro Chancellor

From Vice-Chancellor desk ………

Prof. Manoj K Arora
Vice-Chancellor, SRM University-AP



Dear Esteemed Colleagues and Participants,

It is with immense pleasure and pride that I extend my warmest greetings to each of you on behalf of SRM University - AP.

We are honored to host the 3rd International Conference on Materials Genome (ICMG-III) and the parallel Symposium, Collective Phenomena in Disordered Systems, in collaboration with esteemed partners including the Asian Consortium on Computational Materials Science (ACCMS); Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru; CSIR-National Chemical Laboratory, Pune; Virginia Commonwealth University, USA; Indian Institute of Technology, Madras; Indian Institute of Technology, Bombay; TCG, Crest, Kolkata.

From February 22nd to 24th, 2024, our university will serve as a beacon of knowledge and collaboration, bringing together experts, scholars, and researchers from around the globe to delve into the forefront of computational materials science.

The significance of this gathering cannot be overstated, as we explore the remarkable advancements in computational methodologies and experimental techniques that have revolutionized our understanding of materials over the past three decades. With a primary focus on Quantum Mechanics-based calculations complemented by Machine Learning techniques (QM/ML), we aim to pave the way for the discovery of novel materials with diverse applications.

Moreover, Symposium: Collective Phenomena in Disordered Systems provides a unique platform to delve into the intricacies of mechanics in various materials, from porous media to bio-materials, through the lens of statistical physics.

I extend my heartfelt gratitude to the conveners and the bright minds whose dedication and hard work have made these conferences possible. Such collaborative endeavors not only showcase our commitment to academic excellence but also foster a vibrant ecosystem for knowledge exchange and innovation.

To all our esteemed participants, I offer a warm welcome. Your presence and contributions are invaluable as we embark on this journey of exploration and discovery. I am delighted to announce that select papers from this conference will be published in the esteemed journals "Computational Materials Science", "Catalysis Today,", "The Journal of Electronic Materials", and "Discover Chemical Engineering journal" further amplifying the impact of our collective research efforts.

As Vice Chancellor, I am confident that this joint endeavor will not only foster academic excellence but also nurture meaningful collaborations and inspire further breakthroughs in materials genome research.

Warm regards,

Preface by Prof. Kawazoe

This is the third meeting of the series of International Conference of Materials Genome, ICMG-III. Four years back the first meeting ICMG-I was conceived and arranged by Professor Ranjit Thapa at the SRM University-AP. It was just when COVID-19 problem started. Many oversea speakers could not join physically by this disease, but the meeting itself was successfully held and all participants enjoyed. After 2 years from the first meeting, ICMG-II was held, but COVID-19 situation was still becoming worse and worse and the second meeting was decided to be held completely online, and many participants wanted a physical meeting again. Now the disease is thought to be not much severe and the third meeting has been organized as a physical conference, and as usual by the big support of the SRM University-AP, Amaravati in association with Asian Consortium on Computational Materials Science ACCMS, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, National Chemical Laboratory, Pune, Virginia Commonwealth University, USA, Indian Institute of Technology, Madras, Indian Institute of Technology, Bombay, and TCG, Crest, Kolkata. Although two-day conferences have been organized up to the second one, this time three day schedule is fully made to accommodate a large number of high level lectures each has enough time to be delivered.

The subject of this series of meetings is very trendy based on the concept of materials genome, which aims to incorporate materials informatics (MI) based on constructing and utilizing a high level and large-scale materials database. We have been successful to invite a large number of international level good speakers; 6 keynote lectures, 50 invited lectures, and 8 oral talks, 2 young scientist talks, and 70 poster presentations. Please enjoy our warm conference environment in three days.

As the founder of ACCMS, I am very much thankful to all the participants to this meeting from India and oversea and the support by SRM University-AP. Professor Ranjit Thapa and his group have worked out to make this conference an excellent one. I very much appreciate their sincere contribution to this important meeting.

Yoshiyuki Kawazoe

Yoshiyuki Kawazoe
Founder of ACCMS
Senior Research Fellow and Professor Emeritus
New Industry Creation Hatchery Center, Tohoku University
Sendai. Japan

Program Schedule

3rd International Conference on Materials Genome (ICMG-III)

Organized by SRM University – AP, Amaravati

In association with

Asian Consortium on Computational Materials Science

Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

National Chemical Laboratory, Pune

Virginia Commonwealth University, USA

Indian Institute of Technology, Madras

Indian Institute of Technology, Bombay

TCG, Crest, Kolkata

22- 24 February 2024

22nd February, Thursday 2024

Venue: SR Block, Mini Auditorium, Hall 1 (S - 206), Hall 2 (S - 207) and Hall 3 (S - 201)

(All time are in IST)

8.30 a.m. to - 9.30 a.m.: Registration, Mini Auditorium, SR Block, SRM University-AP

9.30 a.m. - 10.00 a.m.: Inaugural Session, Mini Auditorium, SR Block, SRM University-AP

Lectures are in Mini Auditorium , Hall 1 and Hall 2 are on 2nd Floor of SR Block

Morning Session: 10.00 a.m. – 1.00 p.m. Keynote Session

Session I

Session Chair: Prof. Ranjit Thapa and Dr. Pankaj Bhalla

10.00 a.m. – 10. 50 a.m.	Mini Auditorium	Invited Key Note Lecture 1	Prof. Puru Jena	Title: Cluster-based Energy Materials – A Paradigm shift in Design and Synthesis
20 Mins Break				
11.10 a.m. – 12.00 p.m.	Mini Auditorium	Invited Key Note Lecture 2	Prof. Bikas Chakrabarti	Title: FRACTURE STORY: A Personal Summary
12:05 a.m. – 12:55 p.m.	Mini Auditorium	Invited Key Note Lecture 3	Prof. G. P. Das	Title: Designing solid electrolytes for cheaper, safer and greener batteries

45 mints lecture + 05 mints discussion

01. 00 p.m. – 2.00 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.00 p.m. – 5.45 p.m.: Three Parallel Sessions *and One Symposium*

Parallel Session I

Session Chair: Prof. Prasenjit Sen

2.00 p.m. – 2.30 p.m.	Mini Auditorium	Invited Lecture 4	Dr. Jun Zhou	Title: Emergent magnetic properties in electrenes
2.35 p.m. – 3:05 p.m.	Mini Auditorium	Invited Lecture 5	Dr. Kartik Rajendran	Title:
3.10 p.m. – 3.40 p.m.	Mini Auditorium	Invited Lecture 6	Dr. A. Lorenzo Mariano	Title: Spin-phonon interactions in single-molecule magnets: from theory to material design

Parallel Session I

Session Chair: Prof. Shen Lei and Dr. Debabarata Pramanik

4.00 p.m. – 4.30 p.m.	Mini Auditorium	Invited Lecture 7	Prof. Ranjit Thapa	Title: Electronic Descriptor then Predictive model using QM/ML Approach then Experimental Validation
4:35 p.m. – 5:05 p.m.	Mini Auditorium	Invited Lecture 8	Dr. Sharan Shetty	Title: Computational Study of CO_2 Capture and Conversion : An Industrial Perspective
5:10 p.m. – 5.40 p.m.	Mini Auditorium	Invited Lecture 9	Prof. Prasenjit Sen	Title: Machine Learning assisted materials screening and design: Attempts at designing rare earth free permanent magnets

25 mints lecture + 5 Questions > Invited Lecture

Parallel Session II

Session Chair: Dr. Tanmoy Paul and Mr. E. S. Erakulan

2.00 p.m. – 2.30 p.m.	Hall 1 *(S – 206)*	Invited Lecture 10	Dr. Debabrata Sarkar	Title: Ultra-thin Nanofibrous Membranes as high efficient and lightweight air filter
2.35 p.m. – 3:05 p.m.	Hall 1 *(S – 206)*	Invited Lecture 11	Dr. Mahesh Kumar Ravva	Title: Computational Design and Performance Prediction of Organic Near-infrared Thermally Activated Delayed Fluorescent Molecules
3.10 p.m. – 3.40 p.m.	Hall 1 *(S – 206)*	Invited Lecture 12	Dr. Uttam Kumar Ghorai	Title: Electrocatalytic Synthesis of Green Ammonia and Green Urea Using Metal Phthalocyanine Nanotubes: A Lab-to-Land Initiative

Parallel Session II

Session Chair: Dr. E Varathan

4.00 p.m. – 4.30 p.m.	Hall 1 *(S – 206)*	Invited Lecture 13	Dr. Chiranjib Majumder	Title: 'Atom-by-Atom' design of catalyst using Density Functional theory
4:35 p.m. – 5:05 p.m.	Hall 1 *(S – 206)*	Invited Lecture 14	Dr. Ujjwal Pal	Title: Prospective Ultrathin 2D-Materials for Large-Scale Solar to Hydrogen
5:10 p.m. – 5.40 p.m.	Hall 1 *(S – 206)*	Invited Lecture 15	Dr. Abir De Sarkar	Title: DFT perspectives on valleytronics, piezoelectricity and flexible piezo-

				spintronics in selected functional 2D materials

25 mints lecture + 5 Questions > Invited Lecture

20 mints lecture + 5 Questions > YSS Lecture

Parallel Session III

Session Chair: Prof. Dilip Kanhare

2.00 p.m. – 2.30 p.m.	Hall 2 *(S – 207)*	Invited Lecture 16	Dr. Jatis Kumar Dash	Title:TBA
2.35 p.m. – 3:05 p.m.	Hall 2 *(S – 207)*	Invited Lecture 17	Prof. Phan Bach Thang	Title: Electrocatalytic activity and thermal properties of Metal-organic frameworks for Lithium-ion batteries, Hydrogen evolution reaction, Oxygen evolution reaction and Thermoelectric conversion
3.10 p.m. – 3.40 p.m.	Hall 2 *(S – 207)*	Invited Lecture 18	Dr. D. H. Nagaraju	Title: Nanostructured Electrode Materials for High Energy Density Symmetric and Asymmetric Supercapacitors

Parallel Session III

Session Chair: ***Dr. Baswanth Oruganti***

4.00 p.m. – 4.30 p.m.	Hall 2 *(S – 207)*	Invited Lecture 19	Prof. Dilip Kanhare	Title: Machine-Learned Potential Energy Surfaces for clusters of Sodium and Aluminium Clusters with Density Functional Accuracy: Applications to Melting
4:35 p.m. – 5:05 p.m.	Hall 2 *(S – 207)*	Invited Lecture 20	Dr. Pankaj Bhalla	Title: Light-induced Nonlinear Spin Hall Current in Single-layer WTe$_2$

25 mints lecture + 5 Questions > Invited Lecture

SYMPOSIUM : Collective Phenomena in Disordered Systems

Afternoon Session: 2.00 p.m. – 5.45 p.m.

Session Chair: Prof. Purusattam Ray

2.00 p.m. – 2.50 p.m.	Hall 3 *(S – 201)*	Invited Lecture 21	Prof. Lucas Goehring	Title: Cohesive Granular Media
2.55 p.m. – 3.45 p.m.	Hall 3 *(S – 201)*	Invited Lecture 22	Dr. Tapati Dutta	Title: Real disordered dynamical systems locked in topological signatures

45 mints lecture + 5 mints discussion <u>10 Mints Break</u>

Session Chair: Dr. Tapati Dutta

4.00 p.m. – 4.50 p.m.	Hall 3 *(S – 201)*	Invited Lecture 23	Dr. Jordi Baro	Title: Avalanches at the arcade: understanding the statistics of avalanches and aftershock production in mean-field models.
4.55 p.m. – 5.45 p.m.	Hall 3 *(S – 201)*	Invited Lecture 24	Prof. Abhik Basu	Title: Mobility-induced order in active XY spins on a substrate

Evening Session: 6.00 p.m. – 7.30 p.m.: Cultural Program, Main Auditorium, X Lab

7.30 p.m. – 9.30 p.m.: Dinner, In front of SR Block

Bus will leave to Red Fox Hotel at 9:30 p.m

<u>23rd February, Friday 2024</u>

Venue: Mini Auditorium, Hall 1, Hall 2 and Hall 3

Morning Session: 9.20 a.m. – 1.05 p.m.

Session Chair: Prof. Kavita Joshi and Dr. Pranab Mandal

9.20 a.m. – 10:00 a.m.	Mini Auditorium	Invited Key Note Lecture 25	Prof. Yoshiyuki Kawazoe	Title: Parameter-free and Predictable Molecular Dynamics Simulation
10.05 a.m. – 10:45 a.m.	Mini Auditorium	Invited Key Note Lecture 26	Prof. Swapan Pati	Title: Computational Modeling of Thermoelectricity and Mobility in Semiconductors

Parallel Sessions and One Symposium

Parallel Session I

Session Chair: ***Dr. Debabrata Sarkar***

11:00 a.m. – 11:30	Mini Auditorium	Invited Lecture 27	Prof. Shen Lei	Title: High-Throughput Computational Discovery and Intelligent Design of Two-Dimensional Functional Materials for Various Applications
11.35 a.m. – 12.05 p.m.	Mini Auditorium	Invited Lecture 28	Dr. Anirban Mukerjee	Title: Quantum Computational chemistry protocols for porting Density functional approximation onto Quantum Processing units
12.05 a.m. – 12.35 p.m.	Mini Auditorium	Invited Lecture 29	Dr. Priya Johari	Title: Computational Search for Potential Anode Materials for Li-ion Batteries
12:40 a.m. – 1:05 p.m.	Mini Auditorium	YSS	Dr. Tanmoy Paul	Title: Novel Na-ion Battery Cathodes Prediction using Machine Learning and Density Functional Theory Approach

25 mints lecture + 5 Questions > Invited Lecture

20 mints lecture + 5 Questions > YSS Lecture

Parallel Session II

Session Chair: **Dr. Srinuvasu Kancharlapalli**

11:00 a.m. – 11:30	Hall 1 *(S – 206)*	Invited Lecture 30	Prof. Asim Bhaumik	Title: Porous Nanomaterials for CO2 Storage and Fixation Reactions
11.35 a.m. – 12.05 p.m.	Hall 1 *(S – 206)*	Invited Lecture 31	Dr. Abhijit Chattopadhyay	Title: SUSTAINABLE MATERIAL INNOVATION USINGGENRATIVE MATERIAL DESIGN – A DIGITAL TWIN
12.05 a.m. – 12.35 p.m.	Hall 1 *(S – 206)*	Invited Lecture 32	Dr. Annapureddy V.	Title: ARE LEAD-FREE PIEZOELECTRIC MATERIALS SUITABLE FOR ENERGY STORAGE AND ENERGY HARVESTING IN INTEGRATED WEARABLE SYSTEMS?

25 mints lecture + 5 Questions > Invited Lecture

20 mints lecture + 5 Questions > YSS Lecture

01. 05 p.m. – 2.15 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.15 p.m. – 5.45 p.m.:

Parallel Session I

Session Chair: **Dr. Ananth Govind Rajan**

2.15 p.m. – 2.45 p.m.	Mini Auditorium	Invited Lecture 33	Dr. Srinuvasu Kancharlapalli	Title: Computational High-Throughput Screening of Metal Organic Frameworks for Separation and Storage Gas Mixtures
2.50 p.m. – 3:20 p.m.	Mini Auditorium	Invited Lecture 34	Dr. Satadeep Bhattacharjee	Title: Computational Design of Hydrogen Storage Materials: Integrating Density Functional Theory and Data Analytics
3.25 p.m. – 3.40 p.m.	Mini Auditorium	Oral1	Li Yifan	Title: A machine learning framework based on Local environment descriptors for adsorption energy prediction.
3:40 p.m – 3:55 p.m	Mini Auditorium	Oral2	Ashwini Verma	Title: Machine Learning-Driven Design and Synthesis of Materials for Solid-State Hydrogen Storage

Parallel Session II

Session Chair: **Dr. Manjusha Shelke**

2.15 p.m. – 2.45 p.m.	Hall 1 *(S – 206)*	Invited Lecture 35	Dr. Ramendra Sundar Dey	Title: Understanding the Rules of Electrochemical Nitrogen Reduction to Ammonia
2.50 p.m. – 3:20 p.m.	Hall 1 *(S – 206)*	Invited Lecture 36	Dr. Brahmananda Chakraborty	Title: 2D Nanomaterials for Hydrogen Storage and Electro-chemical Energy Storage: Computational Design using DFT & MD Simulations
3:25 p.m – 3:40 p.m	Hall 1 *(S – 206)*	Oral3	Kshitij Srivastava	Title: Defect-mediated $NaBH_4$ as solid-state electrolytes

SYMPOSIUM: Collective Phenomena in Disordered Systems

Morning Session: 10.00 a.m. – 1.00 p.m.

Session Chair: **Prof. Geza Odor**

10.00 a.m. – 10.50 a.m.	Hall 3 *(S – 201)*	Invited Lecture 37	Prof. Neelima M. Gupte	Title: Synchronization on Simplicial complexes
11.00 a.m. – 11.50 a.m.	Hall 3 *(S – 201)*	Invited Lecture 38	Prof. Takahiro Hatano	Title: Triggering of unstable slip of granular matter by weak acoustic waves

45 mints lecture + 5 mints discussion **10 Mints Break**

12.00 p.m. – 12.50 p.m.	Hall 3 *(S – 201)*	Invited Lecture 39	Dr. Ferenc Jarai-Szabo	Title: Avalance statistics on different scales

01. 00 p.m. – 2.00 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.00 p.m. – 3.45 p.m.

Session Chair: **Prof. Takahiro Hatano**

2.00 p.m. – 2.50 p.m.	Hall 3 *(S – 201)*	Invited Lecture 40	Prof. Géza Ódor	Title: Improving power-grid systems via topological changes or how self-organized criticality can help stability
2.55 p.m. – 3.45 p.m.	Hall 3 *(S – 201)*	Invited Lecture 41	Dr. Subhadeep Roy	Title: Effective rheology of two-phase flow through porous media

45 mints lecture + 5 mints discussion

Evening Session: 3.45 p.m. – 5.45 p.m.: Poster session with Tea/Soft drinks in front of SR Block

7.30 p.m. – 9.30 p.m.: Banquet Dinner by Vice Chancellor, SRM University -AP

Bus will start at 6:00 P.M to venue for Banquet Dinner, please wear the conference ID card

24th February, Saturday 2024

Venue: Mini Auditorium and Hall 1 and Hall 3

Morning Session: 9.30 a.m. – 1.00 p.m.

Parallel Session I

Session Chair: **Dr. Priya Johari**

9.30 a.m. – 10.00 a.m.	Mini Auditorium	Invited Lecture 42	Dr. Kavita Joshi	Title: Understanding catalytic activity through electronic structure
10:05 am. – 10.35 a.m.	Mini Auditorium	Invited Lecture 43	Dr. Ananth Govind Rajan	Title: Predicting Defect Topologies in 2D Materials By Combining First-Principles Calculations and Machine Learning
10:40 p.m. – 11.10 p.m.	Mini Auditorium	Invited Lecture 44	Dr Uday Narayan Maiti	Title: Crystallization selective growth of metallic nanoclusters on graphitic layers for efficient water splitting
11:15 p.m. – 11:45 p.m.	Mini Auditorium	Invited Lecture 45	Dr. Debabrata Pramanik	Title: Understanding thermodynamic and kinetic properties of complex biomolecular systems employing molecular dynamics simulation
11:50 p.m. – 12:10 p.m.	Mini Auditorium	Oral 4	Mr. E. S. Erakulan	Title: Site Specific Descriptor for Metals to Predict Oxygen Evolution Reaction Activity on Single Atom Catalysts
12:25 p.m. – 12:35 p.m.	Mini Auditorium	Oral 5	Dr. Sheik Haseena	Title: Application of Newly Designed Y series Non fullerene Acceptors for High-Efficient Organic Solar Cells

25 mints lecture + 5 Questions > Invited Lecture

Parallel Session II

Session Chair: **Dr. Satadeep Bhattacharjee**

9.30 a.m. – 10.00 a.m.	Hall 1 *(S – 206)*	Invited Lecture 46	Dr. Awadhesh Narayan	Title: Berry curvature dipole and non-linear Hall effect in two-dimensional materials
10:05 am. – 10.35 a.m.	Hall 1 *(S – 206)*	Invited Lecture 47	Dr. Manjusha Shelke	Title: Regulating Lithium Metal Plating/Stripping via 3D Host Materials
10:40 p.m. – 11.10 p.m.	Hall 1 *(S – 206)*	Invited Lecture 48	Dr. Pralok Kumar Samanta	Title: Modelling Excited State Properties and Processes in Mult-Resonant OLED Emitters
11:15 p.m. – 11:45 p.m.	Hall 1 *(S – 206)*	Invited Lecture 49	Dr. E. Varathan	Title: Theoretical Actinide Molecular Science: Macrocycle Complexes

11:50 p.m. – 12:10 p.m.	Hall 1 *(S – 206)*	Oral 6	Mr. Mukaddar S K	Title: 16.35 % efficient Cs 2 GeSnCl 6 based heterojunction solar cell with hole-blocking SnO 2 layer: DFT and SCAPS-1D simulation
12:25 p.m. – 12:35 p.m.	Hall 1 *(S – 206)*	Oral 7	Khusnul Yakin	Title: Mechanism of Proton Transfer at Poly (acrylic acid)-Imidazole

SYMPOSIUM: Collective Phenomena in Disordered Systems

Morning Session: 10.00 a.m. – 1.00 p.m.

Session Chair: Prof. Bikas K. Chakrabarti

10.00 a.m. – 10.50 a.m.	Hall 3 *(S – 201)*	Invited Lecture 51	Prof. Purusattam Ray	Title: Nucleation and Growth of Damage in Disordered System
11.00 a.m. – 11.50 a.m.	Hall 3 *(S – 201)*	Invited Lecture 52	Prof. Parongama Sen	Title: Disorder and polarisation induced by extreme switches in kinetic exchange models of opinion dynamics.

45 mints lecture + 5 mints discussion** **10 Mints Break

12.00 p.m. – 12.50 p.m.	Hall 3 *(S – 201)*	Invited Lecture 53	Dr. Supravat Dey	Title: Role of cilia activity and surrounding viscous fluid on properties of emergent waves

Closing Session 12:45 to 1:15 P.M

Lunch 01:15 pm to 2:15 p.m.

Half Day Tour 2:00 to 6:00 p.m.

Invited Speakers

IL - 1

Cluster-based Energy Materials – A Paradigm shift in Design and Synthesis

Puru Jena[1]

[1] Virginia Commonwealth University, Richmond, Virginia

Abstract: Although the Periodic Table of elements is the mother of all materials, it has limitations; the number of elements is fixed, their chemistry is pre-determined and cannot be altered, and some of them are either rare and toxic. Atomic clusters, composed of a few to a few thousand atoms, provide a way to overcome these limitations, because their chemistry can be tailored by customizing their size, composition, symmetry, and charge state. This talk will deal with the rational design of these superatomic clusters [1] that not only mimic the chemistry of atoms but also can be assembled to form bulk materials with properties superior to those of conventional atom-assembled materials. The examples will include superatomic clusters that promote unusual reactions such as making noble gas atoms form chemical bonds at room temperature [2], activate gas molecules such as CO 2 [3], and form the building blocks of all solid-state Li-ion batteries with high ionic conductivity and interfacial stability [4-6]. These results based on multi-scale first-principles theory are validated by experiments.

[1] Jena, P. and Sun, Q.: "Super Atomic Clusters: Design Rules and Potential for Building Blocks of Materials", Chem. Rev. 118, 5755-5870 (2018)

[2] Zhong, M. M., Fang, H., and Jena, P.: "Super-electrophiles of Tri- and Tetra-Anions Stabilized by Selected Terminal Groups and Their Role in Binding Noble Gas atoms", Phys. Chem. Chem. Phys. 23, 21496 (2021)

[3] Kilic, M. E. and Jena, P.: "Catalytic Potential of [B 12 X 11] 2– (X = F, Cl, Br, I, CN) Dianions", J. Phys.Chem. Lett. 14, 8697−8701 (2023)

[4] Zhao, H., Zhou, J., and Jena, P.: "Stability of B 12 (CN) 12 2- : Implications for Lithium and Magnesium Ion Batteries", Angew. Chem. Int. Ed. 55, 3704 (2016)

[5] Fang, H. and Jena, P.: "Li-rich antiperovskite superionic conductors based on cluster ions", Proc. Nat. Acad. Sci. 14, 1047 (2017)

[6] Fang, H., Jena, P.: "Argyrodite-type advanced lithium conductors and transport mechanisms beyond paddle-wheel effect", Nature communications 13 (1), 1-11 (2022) 10.1038/s41467-022-29769-5

IL - 2

FRACTURE STORY: A Personal Summary

Bikas Chakrabarti*
Email: bikask.chakrabarti.retd@saha.ac.in

Abstract: Will present briefly the story of the intriguing statistical physics of extreme events through the understanding of the phenomenon of fracture in disordered materials. In this biased summary, I will start with more than five hundred years old observation by Leonardo da Vinci, Alan Arnold Griffith in 1920s, Pierre-Gilles de Gennes in early 1970s, Puruasattam Ray and collaborators in late 1970 through 1980s, Srutarshi Pradhan and collaborators in early 2020s, Soumyajyoti Biswas and collaborators starting early 2020s. Ray et al. first demonstrated how the percolation theory would lead to the extreme distributions of Weibull or Gumbel kind in different limits of disorder. Pradhan et al. gave the first exact recursion relation for failure dynamics in equal-load-sharing fiber bundle model. Biswas et al. showed how extending the statistical social inequality analysis for the local failure avalanches in such materials one could get the precursor indicators of global failures.

IL - 3

Designing solid electrolytes for cheaper, safer and greener batteries

G.P. Das[1], Tanmoy Paul[1], Abhik Banerjee[1], Biplab Sanya[l,2]

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

[2] Department of Physics and Astronomy, Uppsala University, Box-516, 75120 Uppsala, Sweden

Abstract: Lithium-ion batteries have proven to be the industry standard for efficient storage of energy in terms of their efficiency, reliability and cyclability. However, higher energy density, enhanced safety and fast charging are some of the key issues that are prompting world-wide effort for all solid-state batteries (ASSB) based on solid electrolytes [1]. In this talk, we shall focus on first- principles approach, based on DFT and NVT ensembled AIMD, to design some promising candidate materials for solid electrolytes in Li-ion ASSBs. Trigonal structured Li 3 YCl 6 with TM partially substituting Y turns out to be a candidate material from the point of view of high Li-ion diffusion. The specific properties that we have addressed are electrochemical stability, Li-diffusion mechanism and ionic conductivity in Li 3 Y 0.875 TM 0.125 Cl 6 [2]. And for TM = V, Co we have found the lowest activation energy (0.11 and 0.14eV respectively) and highest Li-ion mobility (σ= 0.31 and 0.39 mS cm -1 respectively) at room temperature, that are three orders of magnitude higher than in the pristine compound. Using Crystal Orbital amilton Population (COHP) method [4] that quantifies bond ionicity, we have explained the origin of the higher ionic conductivity of TM (V, Co) substituted Li 3 YCl 6 . Our results provide insights into the substitution effect in Li 3 YCl 6 superionic conductors, which could serve as a guide for the design and development of high-performance Li-ion batteries based on cheaper, safer, and greener solid electrolytes.

[1] A solid future for battery development, Jürgen Janek and Wolfgang Zeier, Nature Energy 1(9), 16141 (2016).

[2] Optimizing solid electrolytes with 3d transition metal doped Li 3 YCl 6 for Li-ion batteries, Tanmoy Paul, Abhik Banerjee, Gour P. Das and Biplab Sanyal, J. Phys D: Appl. Phys. 57, 145503 (2024).

[3] COHP method as a tool to visualize and analyse chemical bonding in intermetallic compounds, Simon Steinberg and Richard Dronskowski, Crystals 8, 225 (2018).

IL – 4

Emergent magnetic properties in electrenes

Jun Zhou

Abstract: Monolayer electrides, or electrenes, possess distinctive features due to the presence of anionic electrons, holding promise for various practical applications. In this talk, we will explore the unique magnetic properties of electrenes, specifically focusing on $LaBr_2$ as an exemplary case. Through first-principles calculations and a low-energy effective model, we unveil the atomic orbital-free anionic electrons in this material are fully spin polarized. The long tails of anionic electron states enable an extended ferromagnetic direct exchange to second-nearest neighbors (up to 7–8 Å), a notable departure from conventional short-ranged direct exchanges. Then, we will discuss how uniaxial strains stabilize long–range ferromagnetic ordering in $LaBr_2$, by effectively changing its magnetic anisotropy from the original easy plane to an easy axis. Finally, we will show a novel coexistence of charge density wave (CDW) and magnetism in T-phase $LaBr_2$, which undergoes a 2×1 CDW transition to a semiconducting T′ phase. This transition introduces a magnetic form of CDWs, with interstitial anionic electrons promoting a Mott insulating state and full spin-polarization. These results offer promising opportunities for exploring novel fundamental physics and advanced spintronics applications.

IL - 5

Yet to be announced

IL - 6

Spin-phonon interactions in single-molecule magnets: from theory to material design

A. Lorenzo Mariano[1], Vu Ha Anh Nguyen[1], Sourav Mondal[1], Alessandro Lunghi[1]

[1] School of Physics, Trinity College Dublin, Dublin, Ireland

Email: a.lorenzo.mariano@tcd.ie

Abstract: Single-molecule magnets (SMMs) are metal-organic complexes exhibiting long-lived electronic spin states due to their intrinsic magnetic anisotropy. The magnetic behavior of SMMs has attracted the attention of the scientific community in view of their potential application as building blocks for quantum technologies and memory devices. Nevertheless, the technological relevance of these systems is highly dependent on the magnetic relaxation time, i.e. the time scale beyond which a random change in the magnetic moment is expected.

Spin-lattice interactions represent a primary constraint on the lifespan of spin in SMMs, and the importance of developing a theoretical framework capable of describing spin-phonon relaxation mechanisms in open-shell compounds is twofold: i) to rationalize the origin of the slow relaxation observed in certain classes of materials; ii) to construct an efficient design strategy enabling exploration of a vast chemical space, aiming to identify novel compounds with improved properties.

In this contribution, I will show how the theory of open quantum systems, in conjunction with electronic structure methods, can quantitatively describe the dissipative effect of phonons on the spin degrees of freedom [1,2]. I will illustrate how such theoretical tools, along with machine-learning techniques, can be used for the in silico design of new SMMs.

The systematic generation of SMMs, involving the combination of ligands and magnetic centers, acts as our initial step in creating an extensive dataset of compounds. Patterns, correlations, and relationships between molecular structures and magnetic properties are then extracted to identify the design principles for generating novel molecular structures with optimized magnetic properties.

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Keywords: Single-magnet molecules; spin-phonon interaction; coordination compounds

IL - 7

Electronic Descriptor then Predictive model using QM/ML Approach then Experimental Validation

Ranjit Thapa

Department of Physics and Centre for Computational and Integrative Sciences, SRM University -AP, Amaravati - 522240, Andhra Pradesh, India

Email: ranjit.t@srmap.edu.in

In our recent work, we have shown that with this approach only one DFT calculation of the host surface can estimate the overpotential and energy parameter of all active sites belonging to the host surface using a predictive model developed using ML technique. In this way, by doing DFT calculation for 100 host surfaces we can estimate the overpotentials of more than 3000 active sites. In this project initially, we will generate the data using our predictive model equation. Then we need to extend our approach by developing a general descriptor (structural + electronic descriptor) and in the second work, we plan to find a descriptor and ML-assisted predictive model for molecular materials towards OER. The work is done with collaborators.

The need is the development of a Materials Database (Make in India) with 5 Lakhs Materials in the database. Database for the catalyst is developed by our group: http://energymaterials.org:3000/

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IL – 8

Computational Study of CO_2 Capture and Conversion: An Industrial Perspective

Sharan Shetty[1]

[1] *Shell Technology Centre, Bangalore*

Abstract: Carbon dioxide capture and its conversion to useful chemicals is an attractive route to decarbonize the petrochemical industry and to achieve the sustainable targets. In recent years, there has been an incredible growth in research activities towards the design of novel materials to improve the efficiency of the electrocatalysts for the CO_2 reduction process. Synthesis of low-cost and scalable materials is needed for large scale deployment in the industry for CO_2 capture and conversion. However, the discovery of novel materials is constrained by the underlying chemical complexity of the structure-property relationship.

Computational materials science has become a guiding principle to provide fundamental insight for CO_2 capture and conversion of CO_2. These methods in conjunction with experimental inputs has accelerated the discovery of new materials at low cost and time. In this presentation, we will discuss the combination of DFT and Machine learning approaches for the CO_2 capture and reduction to CO and its industrial feasibility and challenges.

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IL - 9

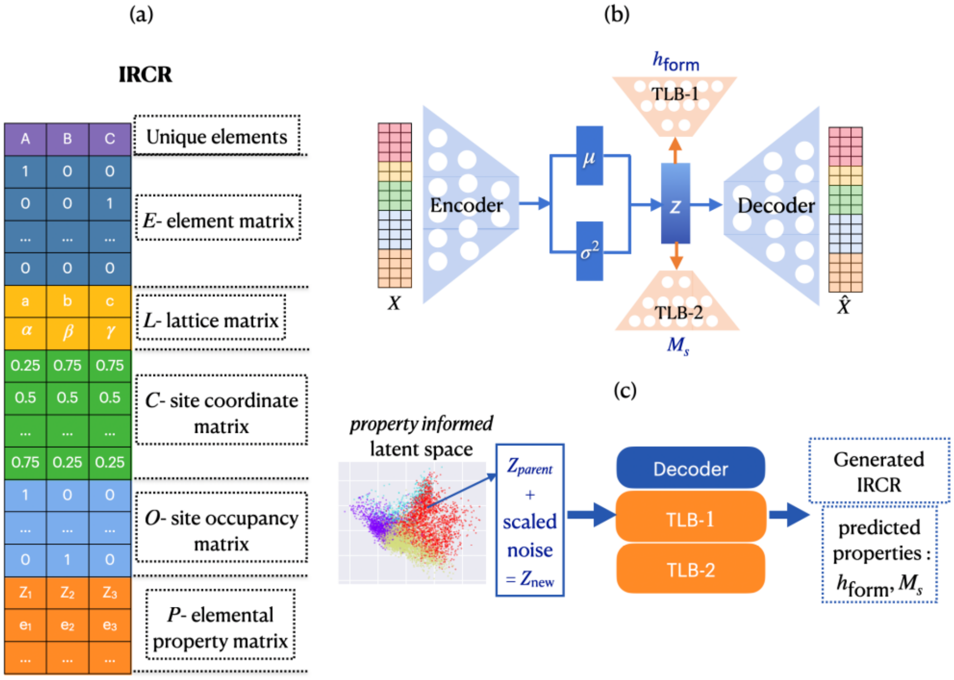
Machine Learning assisted materials screening and design: Attempts at designing rare earth free permanent magnets

Sourav Mal[1] and Prasenjit Sen[1,2]

[1] Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj UP 211019

[2] IISER Tirupati, Karkambadi Road, Mangalam, Tirupati 517507 AP.

Abstract: Permanent magnets (PMs) are essential for modern technology with their applications ranging from laptops computers, smart phones to electric vehicles, wind turbines etc. Today's PMs are mostly based on expensive rare-earth (RE) elements. Therefore, designing new PMs without RE elements is of utmost importance. Designing and discovering new materials traditionally proceed through trial and error experimental approach, which is extremely time consuming. For the last couple of decades density functional theory (DFT) has greatly accelerated the search process by making calculation of material properties possible. Though less expensive than experiments, DFT still requires significant computational resources when the search space is large. Machine learning (ML), being computationally less expensive than DFT, has the potential to revolutionize the whole field. We take two different approaches to identify new RE free PM materials. In the first, ML models are trained on available thermodynamic and magnetic properties of materials. The trained ML models are subsequently used to screen a large number of candidate materials for target properties. Materials which are predicted to satisfy all target properties are finally validated by DFT calculations. Employing this strategy, we have discovered more than a dozen of new RE-free candidate PM materials in much less time compared to a complete DFT screening.



IL - 10

Ultra-thin Nanofibrous Membranes as high efficient and lightweight air filter

Debabrata Sarkar[1]

[1] Applied Nano Physics Laboratory, Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, 603203, India

Abstract: Environmental and energy issues are the two major concerns that are assigned among researchers all over the world. According to the International Energy Agency's (IGA), energy consumption is expected to increase by 40% between 2009 and 2035, and fossil fuels—coal, natural gas, and petroleum—will continue to be the major sources utilized to fulfill humanity's energy demands. However, the present situation indicates a troublesome environmental scenario mainly due to the improper way of utilizing fossil fuels, and overconsumption leads to the emission of hazardous CO2 gases to the Earth's atmosphere with the contamination of air and water. To achieve these demands researchers are focusing more on enhanced functional nanosized materials.

Presently, air pollutants are serious havoc which is very difficult to minimize as the ongoing processes taking place in the atmosphere are far beyond control. With the outbreak of the infectious SARS-CoV2 disease, even a small increase in air pollution has a great impact on a large increase in bacteria, virus infectivity and mortality. Fine particulate matter (PM), one of the major air pollutants, particularly in many developing countries. When the PM is sized under 2.5 μm (PM2.5), it can reach the end of the respiratory tract with airflow and penetrates into the alveolus and blood vessel through air exchange in the lungs. It came to know that annually 4.2 million deaths occur worldwide in cities and rural areas because of the more PM2.5 presence in the air. To tackle this problem, we are developing a class nanofiber air filter media with strong antibacterial activity, hydrophobic nature, high filtration efficiency with low pressure drop. It is found that polar polymeric nanofiber network system present high filtration efficiency. The air filter is designed to collect PM through dipole-dipole or induced dipole force.

IL – 11

Computational Design and Performance Prediction of Organic Near-infrared Thermally Activated Delayed Fluorescent Molecules

Mahesh Kumar Ravva[1,*]

1 Department of Chemistry, SRM University-AP, Andhra Pradesh, India 522240

Email: mahesh.r@srmap.edu.in

Abstract: Due to the inherent energy gap law, developing near-infrared (NIR) TADF emitters still needs to catch up to RGB-TADF emitters. In this presentation, I will first discuss different strategies we used to design organic TADF emitters. I will then discuss some of our recent computational results, highlighting the progress made in understanding TADF emitters for organic light-emitting diodes applications.

Keywords: OLEDs, TADF, Hot-excitons, multiple channels, NIR emission, energy-gap law

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IL – 12

Electrocatalytic Synthesis of Green Ammonia and Green Urea Using Metal Phthalocyanine Nanotubes: A Lab-to-Land Initiative

Uttam Kumar Ghorai[1]

[1] Department of Industrial Chemistry & Applied Chemistry, Swami Vivekananda Research Centre, Ramakrishna Mission Vidyamandira, Belur Math, Howrah, 711202, India

Email: uttam.indchem@vidyamandira.ac.in

Abstract: There are numerous varieties of fertilizers that primarily consist of macronutrients such as phosphorus, potassium, and nitrogen. As fixed nitrogen is typically the rate-limiting macronutrient for plant growth, the production of nitrogen-based fertilizers (ammonia, nitrate, and urea) has always posed a significant global challenge. To combat global starvation over the next three decades, nitrogen-based fertilizer usage will continue to rise. This will have a significant effect on energy and the environment, as nearly all nitrogen-based fertilizers are manufactured from ammonia and nitric acid, which have high energy and carbon footprints. In order to produce ammonia, urea, and nitric acid without the use of fossil fuels, therefore, new technological solutions must be invented.

In our laboratory, we have designed and developed electrocatalytic methods to produce green ammonia, green urea, and nitric acid under ambient conditions using electrocatalysts. All these processes are protected with appropriate IPR. We have completed the field trial of the green ammonia synthesis and initiated the technology transfer and process of licensing for pilot scale production of green ammonia with a multinational company.

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IL – 13

‘Atom-by-Atom’ design of catalyst using Density Functional theory

Chiranjib Majumder[1]

[1] Chemistry Division, Bhabha Atomic Research centre, Trombay, Mumbai 400085

Email: chimaju@barc.gov.in

Abstract: Molecular interactions with small atomic clusters are very interesting as they show non-linear chemical reactivity with size specific selectivity. Taking this clue, a large number of studies have been carried out to investigate the catalytic activity of sub nanometer metal clusters deposited on a surface. This gives fundamental understanding about a chemical reaction at the atomic scale. Moreover, due to the advent of modern computational resources, it is possible to mimic the realistic experimental conditions where reactions happen on small clusters deposited on the surface.

In recent years, the research on catalysis has undergone a paradigm shift since the idea of single atom catalyst emerged [1]. This presentation is divided into two parts; (i) In the first part we shall demonstrate the mechanism of O2 and CO2 reduction and (ii) in the second part we shall demonstrate the decomposition of NH3 and SO3 on various substrates. Design of each substrate was made based on the criteria that suits for higher catalytic efficiency.

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IL - 14

Prospective Ultrathin 2D-Materials for Large-Scale Solar to Hydrogen

Saddam Sk,[1,2] Ujjwal Pal[1,2]*

[1] Department of Energy & Environmental Engineering, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007, India

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

*Corresponding author: upal03@gmail.com, ujjwalpal@iict.res.in, (U. Pal)

Abstract: Topologically, ultrathin 2-D layered double hydroxide (LDH) film can be integrated into the predetermined ordered structures of Metal-organic frameworks (MOFs) through the judicious assembly of tailor-made synthesis approach. In earlier study, we showed that the 2-methyl imidazole-induced ultrathin 2D NiCo-LDH nanosheet arrays in NiCo-LDH@NH_2-UiO-66 worked as an effective bifunctional electrocatalytic system for exceptionally high performance of overall H_2O splitting and stability. The application of templated strategy using 2-Methylimidazole as complexing agent, involves a substitution reaction through the −OH functional moiety. In this report, the modulated MOF@LDH was further employed hydrogen evolution reaction (HER). Both the pristine and Zr^{3+} defect-rich MOFs exhibit a strong preference for electrostatic self-assembly, promoting the formation of nano-composites that enhance charge transfer and heterostructure separation during the photoreduction of water for hydrogen evolution (Fig. 1). The defect-rich MOFs@LDH, a noble metal-free concept and a resilient photocatalyst, displays substantial charge transfer and separation, holding great promise for large-scale hydrogen generation.

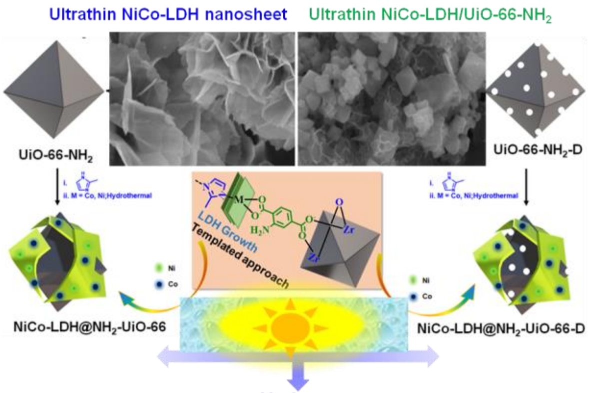

Fig. 1: Schematic non-defect and defected MOF@LDH heterostructure for the enhanced H_2 evolution under visible light irradiation.

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IL - 15

DFT perspectives on valleytronics, piezoelectricity and flexible piezo-spintronics in selected functional 2D materials

Abir De Sarkar[1]

[1] Institute of Nano Science and Technology, Knowledge City, Sector 81, Manauli, Mohali,

Punjab – 140306, India

E-mail: *abir@inst.ac.in*

Abstract: Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the materials. HfN_2 monolayers [1] exhibit valleytronic properties complementary to that in single-layer MoS_2, while the merger of spintronic with valleytronic properties is observed in h-NbN and h-TaN monolayers[2]. 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 together with the enhanced electrical conductivity arising from nearly free electron gas (NFEF) states [3]. Origin of strain tunability in flat valence band and ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb) will also be covered. The conflux of tunable Rashba effect and piezoelectricity observed in flexible MgTe, CdTe, and ZnTe monolayers signify its super high prospects for self-powered flexible-piezo-spintronics [5]. The nature of metal-semiconductor contacts plays a crucial role in determining device performance. Non-resistive/Ohmic contact is found to occur in graphene/MgS vdWH, rendering it ideal for charge injection [6].

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IL - 16

Yet to Announced

IL - 17

Electrocatalytic activity and thermal properties of Metal-organic frameworks for Lithium-ion batteries, Hydrogen evolution reaction, Oxygen evolution reaction and Thermoelectric conversion

Phan Bach Thang[1,2]

[1] Center for Innovative Materials and Architectures, Ho Chi Minh City 700000, Viet Nam

[2] Vietnam National University, Ho Chi Minh City 700000, Viet Nam

Abstract: The development of a CO_2-neutral energy supply is one of the most significant social and scientific challenges facing humanity today. Electrocatalysis based on electrochemical reduction is a driving force in renewable energy conversion, such as Lithium-ion batteries (LIBs), an oxygen evolution reaction (OER), and a hydrogen evolution reaction (HER). Transition metal oxide-derived MOFs catalysts have emerged as alternatives to noble metal catalysts due to their affordability and high catalyst activities. Herein, I report the electrocatalytic activity of oxide-derived MOFs materials for both LIBs and HER/OER applications. In addition, the thermal transport of MOFS also is introduced.

IL - 18

Nanostructured Electrode Materials for High Energy Density Symmetric and Asymmetric Supercapacitors

Nagaraju D. H.[1]

[1] Professor, School of Applied Sciences, REVA University, Bengaluru-560064

Mobile: 9900634435; Email: dhnagu@gmail.com

Abstract: Herein, we provide a concise examination of conductive electrode materials for achieving high energy density. Focused on enhancing the electrochemical performance of asymmetric supercapacitors (ASC) the discussion arrives on various materials, including transition metal oxides, chalcogenides, and advanced activated carbon structures. Key aspects such as specific capacitance, energy, and power density, and cycling stability are highlighted to underscore the significance of electrode material selection. We prepared MoO 3 nanorods as negatrode and V 2 O 5 nanowires as positrode for the construction of ASC device with high energy density. Also, fabricated an ASC with CoNi 2 S 4 flowers derived from layered double hydroxide as cathode material in combination with hydrothermally synthesized oxygen-rich tapioca-derived activated carbon (AC) as anode material that fetched a very high energy density of 57 Wh/kg. Apart from these, we have prepared high surface area and porous AC from Rhizophora mucronata and Arecanut husk, self-heteroatom doped carbon from Allium sativum, and O-rich Manihot esculenta AC with high power densities with excellent stability without compromising energy density in symmetric supercapacitor configuration.

Keywords: Nanostructured Electrode Materials, MoO 3 nanorods, V 2 O 5

nanowires, LDH-derived CoNi 2 S 4 , Asymmetric and symmetric supercapacitors.

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IL - 19

Machine-Learned Potential Energy Surfaces for clusters of Sodium and Aluminium Clusters with Density Functional Accuracy: Applications to Melting

D G Kanhere[1]

[1] Savitribai Phule Pune University, Ganeshkhind Rd, Ganeshkhind, Pune, Maharashtra 411007, India

Abstract: Gaussian Process Regression-based Gaussian Approximation and MACE have been used to develop machine-learned interatomic potentials having density-functional accuracy for free sodium and Aluminium clusters. The training data was generated from a large sample of over 100,000 data points computed for clusters in the size range of $N=40-200 (For Na) using the density-functional method. The model is intended for computing thermodynamic properties using molecular dynamics. Hence, particular attention has been paid to improve the fitting of the forces. Interestingly, it turns out that the best fit can be obtained by carefully selecting a smaller numberof data points , about 1,900 . Although it was possible to obtain a good fit using the data of Na55 only, additional data points from larger clusters were needed to get better accuracies in energies and forces for larger sizes. There is an excellent agreement between the computed and experimentally measured melting temperatures. The geometries of these isomers when further optimized by DFT, the mean absolute error in the energies between DFT results and those of our models is about 7 meV/atom or less. The errors in the interatomic bond lengths are estimated to be below 2% in almost all the cases. Similar results have been obtained for clusters of Al using Mace and GAP. We also used recently developed DEEPMD potential for Al clusters to obtain heat capacity and melting temperature for clusters in the range of 40 to 128 atoms for which experimental data is available. The results are in excellent agreement with the experiment for all clusters.

IL – 20

Light-induced Nonlinear Spin Hall Current in Single-layer WTe$_2$

Pankaj Bhalla[1]

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

Abstract: We study the nonlinear spin Hall current driven by an intense laser pulse in a gated single-layer 1T$'$-WTe$_2$ with strong spin-orbit coupling. We obtain a large third-order two-color rectified spin current generated by the interference of two co-linear polarised light beams. To shed further light, we also compute the second-order rectified spin-current by a single-color light beam and compare the two-color spin current with the second-order single-color effect. We focus on the Hall spin response flowing transverse to the incident laser polarisation direction. In this talk, we will explore the avenues of both the second-order and third-order spin transverse currents.

IL - 21

Cohesive Granular Media

Lucas Goehring

Abstract: A wide range of solid, porous materials, such as sandstone, concrete, bird nests and snow, can be described as cohesive granular media. These materials are made of rigid particles with sticky, sintered or cohesive contacts. Here, we consider the general behaviour of cohesive granular media, and how they fail. The work looks at a simple experimental realization of a cohesive granular material, consisting of glass beads bound together by narrow polymer (PDMS) bridges, which has tunable properties including its elasticity, fracture toughness, and permeability. I will describe and characterize this material and show how its macroscopic properties follow from the microscopic constitutive laws linking adjacent particles. Surprisingly, almost all of the material's response to strain is determined by the bonds between particles, which can be as little as one percent of the volume of the solid structure. I will detail a minimal model of these materials, which is fully constrained by experimental measurements. Under simple compression, this model shows a smooth transition from shear banding, to plastic deformation, to compaction banding (“anti-cracks”), as porosity decreases. More recently, we have monitored the acoustic emissions of these materials as they fail, and used them as a means of exploring porous media flow and salt-induced damage in heritage buildings.

IL - 22

Real disordered dynamical systems locked in topological signatures

Tapati Dutta[1]

[1] Physics Department, St. Xavier's College, Kolkata 700016, India

Abstract: We demonstrate that information of real multiphase time evolving systems can be efficiently summarized using topological tools that can act as low dimensional signatures of their dynamics. To develop these tools, we take the example of flow patterns observed in a drying water droplet impregnated with micron sized particles. In order to do an analysis of the extracted image at different resolutions, we introduce the concept of Euler Characteristic at a specific scale $r > 0$. The time development of the drying process is described by defining the 'Euler Characteristic Surface' which provides a multi -scale topological map of the dynamical system. A novel method is adopted to analyse the images extracted from experimental video sequences. Experimental image data is converted to binary data through appropriate filters and optimal thresholding, and analyzed using the Euler Characteristic determined on a lattice grid. The multi-scale time evolution of the connectivity information of aggregates in water is summarized in an Euler Characteristic Surface. Plotting lines of equal Euler Characteristic result in an Euler Characteristic Level Curve Plot that can help distinguish between topological transitions in the dynamical system. The Euler Metric is introduced as a measure between different Euler Characteristic Surfaces to quantify similarity between two dynamical situations. The Euler Metric so proposed, gives it a Hilbert space structure which allows the use of modern statistical techniques for a more extensive experimental program. The constructions proposed by us can be used to characterise dynamical patterns and their stability against small perturbations.

IL - 23

Avalanches at the arcade: understanding the statistics of avalanches and aftershock production in mean-field models.

Jordi Baró-Urbea[1]

[1]UBICS & Dept. of Condensed Matter Physics, Universitat de Barcelona, Martí i Franquès,

108028 Barcelona, Spain

Email: jbaro@ub.edu

Abstract: Avalanches in mean-field models define a universality class with characteristic profiles and statistics. Most remarkably, the distributions of avalanche sizes and durations exhibit universal power-laws with exponent 3/2 and 2, respectively. The simple conceptual model presented here, which can be mnemotechnically explained as a 'Pac-Man' arcade, maps the independent avalanche profiles emerging from the interplay between all-to all interactions and random disordered fields to a memory-less branching process with Poisson reproduction numbers. Durations are linked to extinction rates and the universal exponent 3/2 appears as the large-number approximation of the Borel distribution. We provide the exact mapping at the thermodynamic limit for the subcritical and critical regimes of the athermal random field Ising model [1] and the democratic fiber bundle model [2], and as an approach to the self-organized critical slip mean-field theory [3]. The evolution of the branching parameter alone determines the dynamics of the system in the different models and serves as a single indicator for statistically based hazard assessment and the forecasting of non-linear regime transitions. The model serves as a steppingstone to address more complex phenomena, such as the statistics of event-event triggering emerging from retardation mechanics [4]. As a novel result, we provide an analytical solution for the so-called productivity law of aftershocks and the origin of foreshocks close to critical transitions [4].

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Keywords: avalanche statistics; mean field theory; triggering; branching proces.

IL – 24

Mobility-induced order in active XY spins on a substrate

Abhik Basu

Abstract: We elucidate that the nearly phase-ordered active XY spins in contact with a conserved, diffusing species on a substrate can be stable. For wide-ranging model parameters, it has stable uniform phases robust against noises. These are distinguished by generalized quasi-long-range (QLRO) orientational order logarithmically stronger or weaker than the well-known QLRO in equilibrium, together with miniscule (i.e., hyperuniform) or giant number fluctuations, respectively. This illustrates a direct correspondence between the two. The scaling of both phase and density fluctuations in the stable phase-ordered states is nonuniversal: they depend on the nonlinear dynamical couplings. For other parameters, it has no stable uniformly ordered phase. Our model, a theory for active spinners, provides a minimal framework for wide-ranging systems, e.g., active superfluids on substrates, synchronization of oscillators, active carpets of cilia and bacterial flagella, and active membranes.

IL – 25

Parameter-free and Predictable Molecular Dynamics Simulation

Yoshiyuki Kawazoe[1,2,3,4,*]

[1] New Industry Creation Hatchery Center (NICHe), Tohoku University, Aobaku, Sendai 980-8579, Japan,

[2] Schoolof Physics, Institute of Science and Center of Excellence in Advanced Functional Materials, Suranaree

[3] University of Technology, Nakhon Ratchasima, Thailand 30000, and Department of Physics and

[4] Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu-603203, India.

Abstract: With rapid development of high-speed computer technology, molecular dynamics (MD) simulation methods have become increasingly sophisticated, allowing for a substantial increase in the number of atoms (particles) that can be effectively treated. Over the course of more than 60 years since the first phase transition process simulation work by Alder, classical MD, assuming atomic force potentials, has been a primary tool. Researchers have endeavored to construct a "transferable potential" capable of tracing atomic movements based on ab initio calculations, which are too expensive to trace time course. Unfortunately, this method faces challenges in its applicability to a broad range of atomic motion beyond initially assumed configurations. The subsequent model employed is quantum MD (ab initio MD), primarily utilizing density functional theory (DFT). In this approach, electronic states are computed step by step, converging to the electronic ground state, and the forces between atoms are computed using these electronic wavefunctions, representing the present-day standard in quantum MD simulations. A more advanced theory, surpassing this level, is Time-Dependent DFT (TDDFT), which maintains electronic states in an excited state throughout the time evolution, which is more similar to real experimental condition. However, these methods, while employing DFT, a ground-state theory, face limitations as the exchange-correlation functional Exc cannot be determined within the theory, leading to the use of phenomenological adjustments such as LDA+U or hybrid functional, violating the necessary conditions of the virial theorem.(1)

In our research, we are developing a fundamentally new quantum MD theory devoid of phenomenological parameters to fit experimental observations. This Time-Dependent GW MD method, implemented in TOMBO code,(2) ensures a well-defined and sustained representation of electronic states over time. This theory demonstrates predictive power for experimental chemical reactions over time, as quasi-particle wavefunctions estimated by the GW method adhere to the extended Koopmans' theorem,(3) certifying accurate determination of excited electronic states. As TOMBO is an all-electron computer code, it enables the estimation of absolute energy levels from electronic core levels. This capability is crucial for providing Ionic Potential (IP) and Electronic Affinity (EA) values to experimentalists.

We present examples showcasing the efficacy of TOMBO TD GW MD, including the dissociation of a hydrogen atom from a methane molecule under a transition metal catalyst, and a rearrangement of hydrogens between nucleobases in DNA.

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IL – 26

Computational Modeling of Thermoelectricity and Mobility in Semiconductors

Swapan K Pati[1]

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

Jawaharlal Nehru Centre for Advanced Scientific Research,

Jakkur Campus, Bangalore 560064, India.

Abstract: The Boltzmann transport equations for charge carriers and phonons have been developed along with first principles calculations to model and understand the transport processes in materials, for their applications in advanced devices. Using this method, we have computed the thermoelectric efficiency in n-type Gd doped PbTe systems, which was synthesised and studied by an experimental group [1]. We also have computed thermoelectric efficiency of a few interesting and unique materials, namely, p-type SnO-PbO superlattice and n type S and Te doped Ag2Se systems [2]. In the second part of my talk, I shall discuss the computational modelling for obtaining thermal conductivity in TlAgSe, which also have been synthesized and investigated experimentally [3]. Our computational efforts on comparing the role of 3d and 4d orbitals in phonon-phonon scattering in determining the thermal conductivity values in two half-Heusler alloys, TiRhBi and TiCoBi will be discussed [4]. To estimate the charge carrier mobility for designing photovoltaics, we have modelled the mobility in □-TeO2 with application of strain along various directions [5a]. I shall also discuss one of our recent attempts in finding the reasons behind the contradictory results from the theoretical calculations which predicted orders of magnitudes higher carrier mobility than what was observed experimentally in the transition metal di-chalcogenides (TMDC), HfSe2 [5b].

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IL – 27

High-Throughput Computational Discovery and Intelligent Design of Two-Dimensional Functional Materials for Various Applications

Lei Shen[1], Jun Zhou[2], Tong Yang[3], Ming Yang[4], Yuan Ping Feng[3]

[1]Department of Mechanical Engineering, NUS, Singapore 117575, Singapore

[2]Institute of Materials Research and Engineering, Agency for Science, Technology and Research (A*STAR), 138634, Singapore

[3]Department of Physics, NUS, Singapore 117551, Singapore

[4]Department of Applied Physics, The Hong Kong Polytechnic University, Hong Kong, SAR, China

Email: Shenlei@nus.edu.sg

Abstract: Novel technologies and new materials are in high demand for future various applications to overcome the fundamental limitations of current techniques. Two-dimensional (2D) materials show promising applications in various applications because they can be tailored to the specific property on which a technology is based and may be compatible with other technologies. Although the number of experimentally discovered 2D materials is growing, the speed is very slow and only a few dozen 2D materials have been synthesized. Recently, high-throughput computational materials design has become a burgeoning area of materials science, which is a combination of quantum mechanical theory, materials information, and database construction. This new and powerful tool can greatly accelerate the discovery, design, and application of 2D materials by creating a database containing many 2D materials with calculated fundamental properties and then intelligently mining the database in the search for 2D materials with the desired properties for particular applications, such as energy conversion/storage, catalysis, and optoelectronics.

In this talk, I will summarize our recent progress in the emerging area of 2D materials discovery, database construction, 2D functional materials design, and device development by quantum-mechanical modeling, high-throughput calculations, and machine learning. We developed an open 2D materials database: 2D materials encyclopedia (2DMatPedia) http://www.2dmatpedia.org, which includes a variety of structural, thermodynamic, mechanical, electronic, and magnetic properties of more than 10,000 two-dimensional materials. Using high-throughput computational screening and machine learning techniques, we identified exotic 2D materials and heterojunctions with desired properties for several applications.

Keywords: 2D materials database; high-throughput calculations; machine learning; 2DMatPedia

IL – 28

Title-Quantum Computational chemistry protocols for porting Density functional approximation onto Quantum Processing units

Anirban Mukherjee[1], Ananthakrishna Gopal[1], Ritam Banerjee[1]

[1] TCS

Abstract: Density functional theory is the most widely used quantum chemistry approach in Pharma and Material science R&D. They also provide a starting point for post-Hartree Fock ab-initio approaches, albeit the computational cost of implementing these approaches for large number of basis functions is large owing to cubic scaling bottlenecks at each self-consistency steps. We have developed a Quantum algorithm to first: encode the building blocks of density functional theory

1. Basis functions,
2. the electronic repulsion integrals
3. density matrix.

These are encoded onto quantum processing units using qubit count + circuit depth optimized quantum circuits. Secondly from there we build the Fock Matrix by carrying out Tensor contractions, numerical integrations and partial differentiation on the quantum circuit. Thirdly the Kohn-Sham eigenvalue equation is solved on the quantum circuit. These steps are repeated on the quantum circuit as a part of the self-consistency scheme.

For a class of Quantum circuits, we show that a superquadratic advantage is obtained for the number of elementary quantum circuit operations with respect to classical floating-point operations for the different mathematical operations involved the Density functional theory workflow.

IL – 29

Computational Search for Potential Anode Materials for Li-ion Batteries

Priya Johari[1]

[1] Department of Physics, School of Natural Sciences, Shiv Nadar University, Dadri, Greater Noida, U.P.-201314, India.

Email: priya.johari@snu.edu.in

Abstract: In current times the advanced computational methods and resources are capable to reliably predict potential electrode materials for the rechargeable batteries in a cost and time effective manner. This may provide an efficient route to guide experimentalists in improving the battery performance and realizing the next-generation energy efficient batteries for grid storage and electrical vehicles in terms of capacity and energy density. In view of that, using various approaches like the first-principles density functional theory and evolutionary algorithms, we comprehensively study a variety of materials to develop an understanding at the atomistic level and predict efficient anode materials for the Li-ion batteries.

IL – 30

Computational High-Throughput Screening of Metal Organic Frameworks for Separation and Storage Gas Mixtures

Srinivasu Kancharlapalli[1]

[1] Theoretical Chemistry Section, Chemistry Division, Bhabha Atomic Research Centre,
Mumbai-400085, India

Email: ksvasu@barc.gov.in

Abstract: Computational high-throughput screening (HTS) is a powerful tool to screen a large database of materials and identify the top performing candidates for specific application.[1-2] Metal organic frameworks (MOFs) are a new class of inorganic-organic hybrid ordered materials with potential applications for separation and storage of different important gases like H_2, CO_2, CH_4 etc.[3-4] We carried out a systematic computational HTS of computational ready experimental (CoRE)-MOF 2019 database using a multi-scale modeling strategy that includes, machine learning model, density functional theory (DFT) calculations, force field optimization and grand canonical Monte Carlo (GCMC) simulations to identify the top performing MOFs for selective adsorption of CO_2 under wet flue gas conditions. For fast and accurate calculation of atomic charges, we trained and tested a Random Forest machine learning model involving a list of features that represent both the elemental properties and the local bonding environment to predict the partial atomic charges in MOFs accurately.[5] Atomic charges calculated using the machine learning model are used to screen the MOF database using the force field simulations. CO_2 selective MOFs from force field simulations are further screened using the more accurate adsorption energies from DFT calculations. MOFs showing strong affinity towards CO_2 compared to H_2O and N_2 are further studied for their loading capacities and adsorption selectivity by simulating the adsorption isotherms under wet flue gas conditions using GCMC simulations. Our HTS results could find good number of CO_2 selective MOFs and the selectivity is mainly driven by the confinement effects.[6] Entrapment of radioactive noble gases is a challenging issue in nuclear waste management. To address this, we screened a database of around 20,000 MOFs for separation and storage of xenon/krypton mixture. Initial screening using the structural properties was followed by adsorption studied using the GCMC simulations to identify the top 10 MOFs for effective separation of Xe/Kr with high loading capacities and selectivity factors. Shortlisted MOFs are under experimental validation and the preliminary results are consistent with the computational predictions.

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IL – 31

Computational Design of Hydrogen Storage Materials: Integrating Density Functional Theory and Data Analytics

Pritam Das[1], Krishnamohan Thekkepat[2], Young-Su Lee[3], Seung-Cheol Lee[1,2]
and Satadeep Bhattacharjee1*
[1] Indo-Korea Science and Technology Center (IKST), Jakkur, Bengaluru 560065, India.
[2] Electronic Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea
[3] Energy Materials Research Center, Korea Institute of Science and Technology, Seoul 02792, Seoul, Republic of Korea
*Email: s.bhattacharjee@ikst.res.in

Abstract: This presentation discusses the use of density functional theory (DFT) and data analysis to identify efficient hydrogen storage materials at ambient temperatures and the computational design of new hydrogen storage materials. The presentation highlights the improvement of the Pd(110) surface through the incorporation of Au and Rh, which achieves optimal hydrogen adsorption energy and a suitable release temperature for hydrogen fuel cell applications. The modified Pd(110) surface also shows improved catalytic activity in oxygen evolution reactions. In addition, the presentation explores Ti2AC (A = Al, Ti, Cr, Mn, Fe, Co, Ni, Cu, and Zn) MAX phase alloys using both DFT and cluster expansion methods. The presentation focuses on the Ti2CuC phase with high hydrogen adsorption energy and the remarkable hydrogen storage capacity of the Ti2AlxCu1−xC alloy under ambient conditions. Finally, the presentation introduces an efficient semi-supervised deep neural network framework for predicting hydrogen storage capacities in metal hydrides. This framework demonstrates the successful integration of advanced computational methods and data analytics in the search for next-generation hydrogen storage materials.

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IL – 32

Porous Nanomaterials for CO_2 Storage and Fixation Reactions

Asim Bhaumik[1,*]

[1] *School of Materials Sciences, Indian Association for the Cultivation of Science, Jadavpur,*
Kolkata – 700 032, India,

*Corresponding address. *E-mail:* msab@iacs.res.in

Abstract: CO_2 is a major greenhouse gas and excessive burning of fossil fuels caused steady increase in CO_2 concentration in air over the years leading to global warming, ocean acidification and related environmental disasters. To mitigate this problem designing of suitable adsorbents for CO_2 Capture and Utilization (CCU) is highly demanding.[1] Porous nanomaterials by virtue of in-built pores of nanoscale dimensions and high specific surface areas can capture huge amount of CO_2 in their void spaces.[2] Further, CO_2 can be utilized as C1 feedstock for the synthesis of value added chemicals. Porous nanomaterials can be used as heterogeneous catalyst for these CO_2 fixation reactions, which are highly desirable in the context of economy and the sustainability of the processes.[3-6] Moderate to high pressure conditions are needed to make CO_2 chemically reactive over the surface of these porous materials.

We have designed supported metallic nanoparticles (NPs, viz. Ni, Pd or Ag) on the surface functionalized micro/mesoporous materials or metal-free porous organic polymers (POPs) and used them as catalysts for carrying out the CO_2 fixation reactions under relatively low CO_2 pressure autoclave conditions.[2-7] Low band gap Fe-MIL-101-NH_2 has been employed as photocatalyst for the thiocarboxylation of olefins with CO_2 and thiols in the presence of visible light.[8] Phosphonate based MOF is used as catalyst for the synthesis of polyurethanes,[9] whereas N-heterocyclic carbene moiety in POPs act as organocatalyst for the synthesis of benzimidazole derivatives using CO_2 as a reactant.[10] High surface area and N-rich basic sites are responsible for high CO_2 capture and excellent catalytic activity of these materials.

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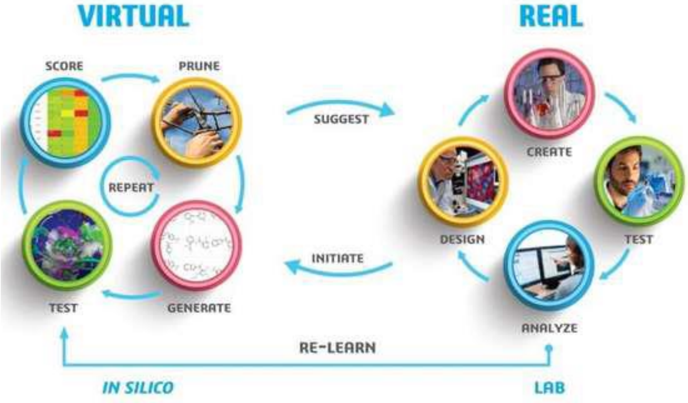
IL – 33

SUSTAINABLE MATERIAL INNOVATION USINGGENRATIVE MATERIAL DESIGN – A DIGITAL TWIN

Abhijit Chatterjee[1]
[1] DASSAULT SYSTEMES BIOVIA, 2-1-1 Osaki, Shinagawa-ku, Tokyo-to, ThinkPark Tower 20F/21F | 141-6020 Tokyo | Japan

Abstract: Despite its potential to transform society, materials research suffers from a major drawback: its long research timeline. Recently, machine-learning techniques have emerged as a viable solution to this drawback. As we know that the digital twin is a digital model of an intended or actual real-world physical product, system, or process (a physical twin) that serves as the effectively indistinguishable digital counterpart of it for practical purposes, such as simulation, integration, testing, monitoring, and maintenance. Using that concept we have adopted a Generative Material Design is a cloud-based integrated solution that optimizes materials design and discovery combining the virtual and real world — potentially saving millions of research dollars. This process includes: a) Combine advanced data science, machine learning, cheminformatics and structure-based modeling to explore chemical space, b) Automate the virtual creation, testing and selection of novel small molecules, c) Reduce the cost of physical testing and then revalidate with laboratory including formulation/reformulation. Generative Design 1 therefore combines Virtual and Real (V+R) lead optimization to support the "active learning" innovation cycle:



Virtual cycles: Explore chemical space by "learning" from real experiments. The system virtually screens and optimizes candidate compounds using a combination of Machine Learning models and structure-based modeling and simulation methods.
Real cycles: Synthesize and test the most promising virtual compounds in the lab. Use the new data to improve predictive models and refine the exploration of chemical space. These V+R active learning cycles continue until you identify compounds that meet the TPP (target principal property).

This talk will show real life examples of utilization of this digital twin for designing materials from drugs to battery materials with a goal to fit the regulation needs of the world to provide sustainable materials.

Reference:1. L. Bleicher et al Enhanced utility of AI/ML methods during lead optimization by inclusion of 3D ligand information Drug Discovery Volume 2 – 2022 https://doi.org/10.3389/fddsv.2022.1074797

IL – 34

ARE LEAD-FREE PIEZOELECTRIC MATERIALS SUITABLE FOR ENERGY STORAGE AND ENERGY HARVESTING IN INTEGRATED WEARABLE SYSTEMS?

Annapureddy Venkateswarlu[1,*]

[1] Flexible & Multi-Functional Materials Device Lab, Department of Physics, National Institute of Technology Tiruchirappalli, Tiruchirappalli 620015 Tamil Nadu, India

**Mobile No.:* *+91-9177977948* & *E-mail:* *annp@nit.edu*

Abstract: The increasing demands of the Internet of Things (IoTs) and the emergence of low-power consumption electronic modules are driving energy harvesting systems, commonly referred to as 'self-powered electronic devices' from niche applications to widespread practicality. These devices are anticipated to play a crucial role in advancing next-generation wireless sensor networks, as the reliance on traditional batteries may prove limiting for IoT electronics in terms of lifespan.

Additionally, the omnipresent but imperceptible magnetic noise fields generated by electric power transmission lines and electronic devices represent a source of essentially wasted energy. The question arises: how can we harness this energy for practical applications? A recently introduced Magneto-Mechano-Electric generator, leveraging magnetoelectric coupling of piezoelectric and magnetostriction, along with the magnetic interaction of magnet mass, shows promise in addressing this challenge. However, traditional ME composites have struggled to fully exploit the potential of weak and low-frequency stray magnetic noise, primarily due to the limited magnitude of ME coupling.

Over the past decades, lead-based ceramics have found extensive use in various devices owing to their outstanding piezoelectric properties. Nevertheless, the environmental concerns associated with the lead content have led researchers to explore eco-friendly alternatives for various applications. In this presentation, I will delve into the current trends, challenges, applications, and future developments in the realm of emerging energy storage and energy harvesting using environmentally friendly ceramics.

Keywords: Lead-free, energy scavenging; IoT electronics, energy harvester, and energy storage.

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IL – 35

Understanding the Rules of Electrochemical Nitrogen Reduction to Ammonia

Ramendra Sundar Dey[1]

[1] Institute of Nano Science and Technology, Sector-81, Mohali-140306, Punjab, India.

Email: rsdey@inst.ac.in

Abstract: The over-consumption of the non-renewable energy sources tends the worldwide research to incline towards development of sustainable approaches to withstand the global energy demand. In this scenario, the vital question of the hour is; ammonia was a saviour once to meet the global food scarcity, so can it save the world again? Although to meet the practical demands of ammonia, the century-old Haber Bosch process is the sole option, but it deviates from the goal to a carbon neutral society. The electrochemical ammonia synthesis from dinII- itrogen reduction reaction (NRR) thus has been an emerging hotspot in the academia as well as industries owing to the ever-growing demands of green ammonia. With a pledge of the "Net-Zero", different nations have been setting up ammonia plants with a target of few million tons of ammonia production in the coming two-three years. This calls for the electrochemical approach and we have thus keenly focused to work on different cell component including suitable electrocatalyst materials to achieve a significant ammonia production by nitrogen reduction reaction (NRR) in aqueous electrolytes.

Acknowledgement: R.S.D. acknowledges DST SERB (CRG/2020/005683) funding agencies for financial support.

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IL – 36

2D Nanomaterials for Hydrogen Storage and Electro-chemical Energy Storage: Computational Design using DFT & MD Simulations

Brahmananda Chakraborty[1,*]

[1] High Pressure & Synchrotron Radiation Physics Division, Bhabha Atomic Research Centre, Mumbai-400085, Homi Bhabha National Institute, Mumbai

Email: brahma@barc.gov.in

Abstract: Various 2D nanomaterials have drawn immense attention as energy storage devices (hydrogen energy & electro-chemical energy) due to their high surface area, high conductivity and high mechanical strength. For pristine carbon nanostructures H 2 adsorption is due to weak Van der Waals interactions and it can't hold H2 at room temperature. The adsorption energy can be increased by: (i) attachment of metals, (ii) Applying strain, (iii) By substituting B and N in place of C. Carbon nanostructures functionalized by transition metals are most promising candidates as adsorption energy can be increased through Kubas interactions. This presentation will describe Density Functional Theory (DFT) results on interaction, charge transfer mechanism and hydrogen storage capability of various 3d and 4d transition metals attached on various carbon nanostructures (graphene, graphyne, holey graphene, biphenylene etc.). The effect of strain on 2D materials for enhancing the hydrogen storage capability will also be addressed.

This talk will also highlight electro-chemical energy storage performance of various hybrid 2D structures based on graphene, transition metal dichalcogenides and MXene, e.g., MoO3/RGO, VSe2/RGO, VSe2/MXene etc. as electrodes for supercapacitors. Recent synthesized 2D materials MXene and their hybrid structures are more promising for energy storage applications. Some of our recent work on MXene based materials will also be described.

Keywords: Graphene, Hydrogen Storage, Carbon Nanomaterials, Supercapacitors , Transition metal dichalcogenides

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IL – 37

Synchronization on Simplicial complexes

Neelima Gupte, Samir Sahoo and Bosiljka Tadic

Abstract: The synchronization of oscillators based on nodes of simplicial complexes --structures made by aggregation of generalized triangles (simplexes of different sizes) exhibits some exciting features. In our analysis, considering 4-dimensional simplicial complexes, the transition to a synchronized state can be abrupt or smooth depending on the geometry and spectral dimension of the underlying simplicial complex, the internal frequency distribution of the oscillators, and the initial conditions, i.e., the distribution of phase angles. The level of synchrony is described by an order parameter that suitably quantifies both partial and complete synchronization. Adding interactions of higher order, e.g., three-point interactions based on triangle faces of the simplexes, modifies these features further with new phenomena, especially where the interactions tend to be of opposite signs. Mainly, the hysteresis loop appears with an abrupt desynchronization transition and cluster synchronization, leading to partial order with multifractal oscillations of the order parameter [3]. Similar dynamical behaviours can be expected in realistic systems such as nanomaterials and the brain connectome.

IL – 38

Triggering of unstable slip of granular matter by weak acoustic waves

Ryunosuke Sakamoto[1], Takahiro Hatano[1,*]

[1] Department of Earth and Space Science, Osaka University, Toyonaka 5600043, Osaka, Japan

Email: hatano.sci@osaka-u.ac.jp

Abstract: The phenomenon of transient strain from seismic waves triggering earthquakes is a robust observation. However, our understanding as to why seismic waves can trigger earthquakes remains incomplete. In this study, we use particle simulations to investigate the response of sheared granular matter to dynamic strain perturbations in order to better understand the dynamic triggering of earthquakes. In our simulation, an unstable slip is triggered when the dynamic strain above a threshold (critical strain) is applied to the system. We show that the critical strain is of the same order ($O(10^{-6})$) as those in some experimental and observational studies. This enhanced response is observed in two wavelength bands. One is the wavelength corresponding to the characteristic frequency of the systems. In this case, the shear strength of the system decreases due to the amplified oscillation of particles due to resonance. The other is the wavelength band at which modulus softening occurs. In this case, the shear strength of the system is reduced due to the reduced shear modulus, leading to unstable slip. This modulus softening is due to the persistence of many slipping contacts between particles. These two wavelength bands are on the same order of the system thickness. Our results suggest that the decrease in the shear strength is caused by seismic waves with wavelengths on the same order of the damage zone thickness of earthquake faults.

Keywords: granular matter; dynamic triggering of earthquakes

IL – 39

Avalance statistics on different scales

Ferenc Járai-Szabó[1], Dávid Antal[1], Attila Gergely[1], Zoltán Néda[1]

[1] Faculty of Physics, Babeș-Bolyai University, M.Kogălniceanu street 1, Cluj, Romania

Email: ferenc.jarai@ubbcluj.ro

Abstract: Universalities in the statistics of avalanches are present in physical systems of different scales like earthquakes resulting from tectonic dynamics, micro-quakes resulting from slipping crystallographic planes in metals and the one-dimensional spring-block type Burridge-Knopoff (BK) model realized at room scale. The earthquakes are studied by reprocessing the available earthquake catalogs for three distinct tectonic zones (Romania, Southern-California, and Japan). The data is standardized by converting all magnitudes to energy scale, that allows us to reveal additional universalities in the statistics. Similar statistical analyses are applied for the micro quakes observed in compressed micropillars. In case of the room-scale realization of the BK model blocks interconnected by bidirectional springs are placed on a treadmill. Additionally, the blocks are connected to a horizontal bar fixed to the ground using extending springs. The velocity of the treadmill is kept at a constant low value. To assess the system dynamics and to perform statistical analyses the position of each block is digitized via calibrated 50 fps HD video recordings. The Gutenberg-Richter's law validity for the probability density of energy dissipated in avalanches is verified for all three systems through a proposed theoretical probability density function. Furthermore, similarities in the recurrence times of earthquakes, micro-quakes and room-sized quakes are also considered.

Keywords: earthquakes, micro-plasticity, avalanches, universalities, Burridge-Knopoff model

IL – 40

Improving power-grid systems via topological changes or how self-organized criticality can help stability

Geza Odor, Istvan Papp, Kristof Benedek, Balint Hartmann

Abstract: Cascade failures in power grids occur when the failure of one component or subsystem causes a chain reaction of failures in other components or subsystems, ultimately leading to a widespread blackout or outage. Controlling cascade failures on power grids is important for many reasons like economic impact, national security, public safety and even rippled effects like troubling transportation systems. Monitoring the networks on node level has been suggested by many, either controlling all nodes of a network or by subsets.

We identify sensitive graph elements of the weighted European power-grids (from 2016, 2022) by two different methods. We determine bridges between communities and point out "weak" nodes by the lowest local synchronization of the swing equation. In the latter case we add bypasses of the same number as the bridges at weak nodes and we compare the synchronization, cascade failure behavior by the dynamical improvement with the purely topological changes. We also compare the results on bridge removed networks, similar to islanding, and with the addition of links at randomly selected places. The synchronization improves the best by the bypassing, while the average cascade sizes are the lowest with bridge additions.

However, for very large or small global couplings these network changes do not help, they seem to be useful near the synchronization transition region, where self-organization drives the power-grid. Thus, we provide a demonstration for the Braess' Paradox on continental sized power grid simulations and uncover the limitations of this phenomenon. We also determine the cascade size distributions and justify the power-law tails near the transition point on these grids.

IL – 41

Effective rheology of two-phase flow through porous media

Subhadeep Roy[1*], Alex Hansen[2], Santanu Sinha[2], Hakon Pedersen[2], Hursanay Fyhn[2].
[1] Dept. of Physics, Birla Institute of Technology and Sciences Pilani,
Hyderabad Campus, Secunderabad, Telangana, India.
[2] Porous Media Laboratory, Norwegian University of Science and
Technology, Trondheim, Norway.
*Email: *subhadeep.r @hyderabad.bits-pilani.ac.in*

Abstract: The study of multi-phase flow involves understanding the behavior of largescale processes (oil recovery, CO2 sequestration, groundwater collection, etc.) by breaking down the dynamics of fluid in the pore-scale [J. Bear, Dynamics of Fluids in Porous Media], a process widely known as the upscaling. In the pore scale, when two immiscible fluids flow in a porous media the flow does not obey linear Darcy law [Transp. Porous Med. 1, 3 (1986)] in the regime where the capillary forces are comparable to the viscous forces. The transient behavior of the model shows viscous fingering, capillary fingering, and stable displacement depending on driving parameters such as capillary number or the viscosity ratio. In the steadystate, the flow rate was observed both numerically [Europhys. Lett. 99, 44004 (2012)] and experimentally [Phys. Rev. Lett. 102, 074502 (2009)] to scale in a quadratic manner with the pressure gradient. The disorder in capillary barriers at pores effectively creates a yield threshold in the porous medium, introducing an overall threshold pressure in the system making the fluids reminiscent of a Bingham viscoplastic fluid [Europhys. Lett. 4, 1227 (1987)]. In this talk, I will discuss a dynamic pore network model (in 1d, 2d, and 3d) [Front. Phys. 8, 548497 (2021)] to explore above rheology where the time evolution of the interfaces is observed by solving three coupled equations. Well-understood rheology can be obtained from the scaling of the pressure gradient and flow rate (or the capillary number) it generates. A transition from nonlinear rheology to a linear Darcy flow is observed here with an increasing external drive (pressure gradient or flow rate) where the nonlinear region is observed to be highly influenced by parameters like (i) pore structure [Front. Water 3, 709833 (2021)], (ii) flow distribution [Front. Phys. 7, 92 (2019)], and (iii) wetting condition [Transport in Porous Media 139, 491 (2021)].

Keywords: multi-phase flow, porous media, rheology, dynamic pore network model, Darcy flow.

IL – 42

Understanding catalytic activity through electronic structure

Kavita Joshi[1,2]

[1] Physical and Materials Chemistry Division, CSIR – National Chemical Laboratory, Pune, 411008 India.

[2] Academy of Scientific and Innovative Research (AcSIR), Sector 19, Kamla Nehru Nagar, Ghaziabad, Uttar Pradesh- 201002, India.

Email: k.joshi@ncl.res.in

Abstract: In the present talk, I will discuss some success stories and unresolved puzzles we encountered while designing catalysts in silico. We investigate reactions at surfaces, and the questions one would ask are: What is the role of a facet? Can we distill out factors responsible for a specific end-product? Do we understand the interaction between a molecule and a surface in terms of the underlying electronic structure of the material? Why does a specific catalyst demonstrate better reactivity? We try to answer these questions while investigating the interaction of CO 2 /CH 4 /MeOH with various catalysts, including SACs, binary alloys, metal oxides and mixed metal oxide. The present talk will be an account of our journey searching for electronic structure descriptors to understand reactivity at surfaces.

IL – 43

Predicting Defect Topologies in 2D Materials By Combining First-Principles Calculations and Machine Learning

Ananth Govind Rajan[1]
[1] Department of Chemical Engineering, Indian Institute of Science, Bengaluru

Abstract: Defects, whether intentionally created or inadvertently formed, are ubiquitous in all materials, including two-dimensional (2D) materials. Nevertheless, not much is known as to how these defects form, what topologies of defects are more likely to form, and how the defect topology affects the performance of 2D materials in various applications. Our group has been working to combine quantum-mechanical density functional theory (DFT) calculations with classical molecular dynamics (MD) and kinetic Monte Carlo (KMC) simulations to understand the formation of nanopores in 2D materials and their effects on molecular and ion transport on and through these materials. In this talk, I will discuss the combined use of DFT, KMC, and chemical graph theory to predict nanopore shapes in graphene in excellent agreement with transmission electron microscopy images. I will introduce the use of gradient-boosted machine learning strategies, coupled with structural features of nanopores, to predict the probabilities and formation times of arbitrary nanopore shapes in graphene. I will also outline the use of combinatorial mathematics and DFT calculations to create a large database of stable nanopores in graphene, which can be used in high-throughput screening of nanopore topologies. Finally, I will outline the development of a novel string representation of nanopores in 2D materials. Overall, the multi-scale simulations and the machine learning approaches presented in this talk will help understand and advance the controlled synthesis of nanoporous 2D materials.

IL – 44

Crystallization selective growth of metallic nanoclusters on graphitic layers for efficient water splitting

Uday Narayan Maiti[1]
[1] Associate Professor, Department of Physics, IIT Guwahati, Guwahati-781039

Abstract: I my talk, I shall be discussing on how the level of graphitization of carbon support (GN) can control the crystallization status of metal nanoclusters to selectively generate single-atom, amorphous to crystalline nanoclusters. Particularly, focus will be paid on ultrafine (~ 0.7 nm) amorphous-ruthenium nanoclusters linked with GN (a-Ru@GN) which demonstrates a state-of-the-art performance in hydrogen evolution reaction (HER) that requires very low overpotentials of only 23.0 mV and 285.0 mV to achieve current densities of 10 mA cm-2 and 500 mA cm-2, respectively. Further, a-Ru@GN exhibits exceptional operational stability for 100 hours under the high HER currents of 100 mA cm-2, 200 mA cm-2, and 400 mA cm-2. A discussion will be made based on density functional theory to understand the origin of high catalytic activity.

IL – 45

Understanding thermodynamic and kinetic properties of complex biomolecular systems employing molecular dynamics simulation

Debabrata Pramanik[1,2]

[1] Department of Physics, SRM University – AP, Amaravati, Andhra Pradesh - 522502, India

[2] Centre for Computational and Integrative Sciences, SRM University – AP, Amaravati, Andhra Pradesh - 522502, India

Abstract: Understanding functionalities and mechanistic behavior of biomolecular systems such as protein – ligand and protein – DNA are highly desirable due to implication in basic biology as well as various diseases. Often, experimental techniques can be useful in measuring various thermodynamic quantities, but they cannot, at least directly, provide microscopic details and kinetics, pathways etc. Employing state of the art, classical all-atom molecular dynamics (MD) simulation and integrating with biased sampling techniques, we explore thermodynamics and kinetics of such complex systems. In this talk I will discuss a few of these methods and our efforts in understanding the stability, thermodynamics, and kinetics for different protein – ligand systems.

IL – 46

Berry curvature dipole and non-linear Hall effect in two dimensional materials

Awadhesh Narayan[1]*

[1] Indian Institute of Science, Bangalore, India.

**Email:* awadhesh@iisc.ac.in

Abstract: In recent years, it has been discovered that inversion symmetry broken quantum systems can exhibit non-linear Hall effect even under time-reversal symmetric conditions [1]. The underlying quantum object leading to this effect is the first order moment of the Berry curvature, termed the Berry curvature dipole. Such non-linear Hall effects open up different possibilities for direct applications, such as non-linear photocurrents and terahertz radiation detection [2]. However, despite such promise for exciting physics and applications, the Berry curvature dipole 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 dipole.

In this talk, I will give examples from our work where such a controllable Berry curvature dipole has been predicted. First, we propose Janus monolayers of transition metal dichalcogenides as a promising materials platform to explore the non-linear Hall effect and Berry curvature dipole physics [3]. Here the topology and the Berry curvature dipole are tunable by chemical composition. Second, we discover a giant non-linear Hall effect in the elemental buckled honeycomb lattices -- silicene, germanene, and stanene [4]. In this case, 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.

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IL - 47

Regulating Lithium Metal Plating/Stripping via 3D Host Materials

Manjusha V. Shelke[1,*]

[1] CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411008, India

Abstract: The development of high-capacity and stable lithium metal anodes is pivotal for advancing the performance of next-generation lithium-ion batteries. However, several critical challenges, such as dendrite formation, capacity decay, and safety concerns, have hindered its practical application. All the strategies to prevent Li dendrites are based on the space-charge model for Li dendrite nucleation and growth which predicts that cationic and anionic concentrations exhibit unusual behaviour at Sand's time resulting in the development of excess positive charge and uneven electric fields at negative electrode which ultimately leads to dendrite nucleation and subsequent growth. Thus, Sand's time is the period of actual dendrite-free deposition after the onset of electrodeposition. Though the dendrite growth issue could be mitigated to a large extent, huge volume changes and poor coulombic efficiency (CE) persist at higher current density and high Li intake deposition in host less Li metal which can further deteriorate the overall battery performance. In this talk I will deliberate on the critical role of host materials in stabilizing lithium metal anodes by providing a protective environment that mitigates the formation of dendrites, a major cause of short circuits and safety concerns. The discussion will cover various aspects of host engineering, including material selection, design principles, and the influence of host structure on lithium metal deposition and stripping processes.

Ref:

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IL – 48

Modelling Excited State Properties and Processes in Mult-Resonant OLED Emitters

Dr. Pralok Kumar Samanta[1]

[1] Department of Chemistry, Birla Institute of Science and Technology (BITS) - Pilani,
Hyderabad Campus, Hyderabad 500078, India

Abstract: In my talk, I will present our works on excited state radiative and non-radiative processes in organic emitters and discuss the dependence of their rate constants on the nature of singlet and triplet excitations. I will describe, in detail, the methodology that we have developed to calculate the up-conversion (also known as "reverse") intersystem crossing rate constant, which increases the population of the lowest excited singlet state from the lowest excited triplet (T_1) state for multi-resonant thermally activated delayed fluorescence (MR-TADF) light emitters. In addition, I will discuss the role of intersystem crossing in increasing the population in the T_1 state, which is required for room-temperature phosphorescence and photodynamic therapy.

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IL – 49

Theoretical Actinide Molecular Science: Macrocycle Complexes

Dr. E. Varathan[1,*]

[1] Department of Chemistry, SRM Institute of Science and Technology, Kattankulathur, Chennai 603203, Tamil Nadu, India.

*Corresponding author: Email: varathae@srmist.edu.in

Abstract: Actinide macrocycle complexation is an area of research within the field of coordination chemistry, focusing on the interaction of actinide elements with macrocyclic ligands. The prominence of actinides in nuclear waste draws attention to its separation and transmutation for a safe disposal of these radioactive species. Computational methods, including Density Functional Theory (DFT) have become an invaluable tool in understanding and predicting the structural and electronic properties of these complexes. DFT calculations play a pivotal role in elucidating the thermodynamics and energetics of actinide macrocycle complexation. By employing quantum mechanical principles, DFT allows researchers to model the electronic structure, energetics, and geometries of actinide macrocycle complexes accurately. This aids in predicting stability constants, electronic transitions, and other key properties. Organic macrocycles with a central cavity that can encapsulate metal ions are modelled and their chelation property and selectivity. Our studies delve into comprehensive studies on the complexation properties of high-valent actinyl moieties, namely U, Np, Pu, Am, and Cm, with various ligands through the application of density functional theory (DFT) calculations. Our investigations include three distinct ligands: dipyriamethyrin, pyrrophen, and DOTA (1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid), studied for their complexation property with actinyl. In the context of the dipyriamethyrin ligand, we evaluated the complexation characteristics of actinyls in their pentavalent, hexavalent and heptavalent oxidation states.

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IL – 50

Nucleation and Growth of Damage in Disordered Systems

Purusattam Ray[1]

Abstract: Nucleation and subsequent growth have received lots of attention in the context of statistical physics of nonequilibrium systems. We discuss the physics behind the phenomena in disordered systems in the backdrop of damage formation and fracture in complex materials.

IL – 51

Disorder and polarisation induced by extreme switches in kinetic exchange models of opinion dynamics

Parongama Sen

Abstract: In a kinetic exchange model of opinion formation, popularly known as the BChS model, an order disorder transition can be induced when the fraction of negative interaction between the agents exceeds a certain value. In this case, the negative interaction plays the role of noise. In the discrete version, when the opinion can take values -1, 0 and 1, the dynamical rules used in the model allow no transition between the two extreme states. However, increasing the magnitude of the interaction strength, it is possible to have extreme switches of opinion values. We consider such stronger interaction that occurs with a probability, which acts as a second source of noise. We present here how this noise enhances the disorder using several different approcahes and topologies.

IL – 52

Role of cilia activity and surrounding viscous fluid on properties of emergent waves

Supravat Dey[1,*]

[1] Department of Physics, SRM University – AP, Amaravati 522502, Andhra Pradesh, India

Email : supravat.d@srmap.edu.in

Abstract: Large groups of active cilia collectively beat in a fluid medium as metachronal waves, essential for some micro-organisms motility and for flow generation in mucociliary clearance. Several models can predict the emergence of metachronal waves, but what controls the properties of metachronal waves is still unclear. We investigate numerically a simple model for cilia in the presence of noise on regular lattices in one- and two-dimensions. We characterize the wave using spatial correlation and the frequency of collective beating. Our results clearly show that the viscosity of the fluid medium does not affect the wavelength; the activity of the cilia does. These numerical results are supported by a dimensional analysis, which is expected to be robust against the model for active force generation, unless surrounding fluid influences the cilia activity. This result might have significance in understanding paramecium locomotion and mucociliary clearance diseases.

Young Scientists

Novel Na-ion Battery Cathodes Prediction using Machine Learning and Density Functional Theory Approach

Tanmoy Paul[1]

[1] Research Institute for Sustainable Energy, TCG-CREST, Kolkata, West Bengal, India

Email: *tanmoy.paul@tcgcrest.org*

Abstract: Sodium-ion batteries (SIB) have gained significant attention as the next generation of rechargeable batteries based on natural abundance and low cost. Transition metal oxides with layered structures have been successfully commercialised in the Li-ion batteries (LIB) systems and have been reported to be one of the promising electrode materials for SIBs. [1] Among layered oxides, polyanions, and other types of electrode materials, P2 type Na_xTMO_2 (TM = different 3d transition metals) shows a simple crystal structure and high capacity [2]. Despite these advantages, P2-type phases exhibit poor cyclability and inferior high-rate performance compared to O3-type Na-ion battery cathodes. Recently, it has been found that the P2-$Na_xFe_{0.5}Mn_{0.5}O_2$ cathode exhibits a high discharge capacity of 190 mAh/g at a rate of 0.07 C. However, there is no systematic study exists considering different combinations of TMs in this chemical formula. In this report, we have enumerated a series of promising cathode compositions using the parent P2-$Na_xFe_{0.5}Mn_{0.5}O_2$ compound as a starting point. The structural parameters (cell parameters, angle and cell volume) are obtained from density functional theory (DFT) calculations and various physical parameters (viz., ionisation energies of constituting atoms) and several physics-based descriptors have been used as input descriptors to predict the average voltage and gravimetric capacity for those compounds. As obtained from the Materials Project database, various Na-ion cathode materials and their properties have been used to construct an ML model. The Mean Absolute error and R^2 score were obtained as 0.80 V and 0.62, respectively, during the training. Overall, we have obtained some candidate compositions which show AV ~ 4 V from our target pool of elements. The AV as predicted by our ML model is verified by the enthalpy calculations using DFT.

Oral

O-01

A machine learning framework based on Local environment descriptors for adsorption energy prediction

Li Yifan[1], Wu Yihan[2], Han Yuhang[3], Lyu Qiujie[4], Wu Hao[5], Zhang Xiuying[6], Shen Lei[7,*]

[1] Department of Mechanical Engineering, NUS, 9 Engineering Drive 1, Singapore 117575

[2] Engineering Science Programme, NUS, 9 Engineering Drive 1, Singapore 117575

[3] Department of Mechanical Engineering, NUS, 9 Engineering Drive 1, Singapore 117575

[4] Department of Mechanical Engineering, NUS, 9 Engineering Drive 1, Singapore 117575

[5] Department of Mechanical Engineering, NUS, 9 Engineering Drive 1, Singapore 117575

[6] Department of Mechanical Engineering, NUS, 9 Engineering Drive 1, Singapore 117575

[7*] Department of Mechanical Engineering, NUS, 9 Engineering Drive 1, Singapore 117575

* *Email: liyifan@nus.edu.sg*

Abstract: Machine learning models in Materials Science predominantly focus on global properties such as formation energy, band gap, and elastic modulus, often falling short in describing localized characteristics, like adsorption energy. In this study, we introduce a local environment framework that extracts geometric features from 3D crystal structures to portray the environment surrounding specific adsorption sites. Utilizing various well-established machine learning models, including convolutional neural networks, this framework was trained to achieve a significant enhancement in accuracy. Furthermore, the employment of this approach reduces data requirements and augments computational speed specifically for deep learning algorithms. The precise characterization of local environments realized through our proposed method demonstrates remarkable prediction accuracy and versatility. Such precision translates into high applicability across a broad spectrum of molecular studies, including applications in catalysis and sensor technologies, signifying a novel and promising avenue in the field of computational materials science.

Keywords: Local Environment Framework, Geometric Features, Adsorption Energy, Machine Learning Models, Computational Materials Science

O-02

Machine Learning-Driven Design and Synthesis of Materials for Solid-State Hydrogen Storage

Ashwini Verma[1,2], Kavita Joshi[1,2]

[1] Physical and Materials Chemistry Division, CSIR-Nati onal Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune-411008, India

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

Email: ad.verma@ncl.res.in

Abstract: Solid-state hydrogen storage in metal alloys holds the potential to outperform conventional (liquid/compressed) methods on a accounts of volumetric capacity, safety, and durability.[1] Despite significant performance improvements in metal hydrides over the past two decades, their practical application is hindered by the unattainable thermodynamic and kinetic properties at ambient conditions for economical viability.[2] The Pressure-Composition Temperature (PCT) analysis is an experimental procedure employed to assess the suitability of an alloy for hydrogen storage. PCT isotherms provide crucial information, like reversible storage capacity, hydrogen pressure for phase transition, and the plateau pressure.[3] Unfortunately, PCT analysis of the materials is resource-intensive and time-consuming as it involves series of measurements to represents the relationship between hydrogen pressure, concentration and temperature of a sample at equilibrium. Hence, limiting the number of compositions that can be investigated. In light of this, we have built a machine learning model, PCT isotherm predictior (PCTpro) for multicomponent metal alloys. The model is trained on diverse family of metal alloy's PCTs data and the feature set includes easily calculable elements' periodic table properties, hydriding properties, and experimental parameters. The comprehensive feature set equips PCTpro to predict the PCT isotherms for any metal alloy based on its composition, hydrogen pressure, and temperature. The model is validated across diverse alloy families, agreeing with experimental results. The model also predicts temperature-dependent variations in plateau pressure, enabling the mapping of predicted PCTs onto Van't Hoff plots to determine enthalpy and entropy of hydride formation.

Keywords: Hydrogen Storage; Metal Hydrides; Machine Learning; PCT isotherm prediction

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O-03

Defect-mediated NaBH 4 as solid-state electrolytes

Kshitij Srivastava[1,*], César Menéndez Muñiz[2], Tapasendra Adhikary[3], Gour P. Das[4], Nicholas Bedford[1] and Kondo-Francois Aguey-Zinsou[2]

[1] School of Chemical Engineering, The University of New South Wales, Sydney, Australia

[2] School of Chemistry, The University of Sydney, Sydney NSW 2006, Australia

[3] Department of Metallurgy, Indian Institute of Technology, Kharagpur 721302, India

[4] Research Institute for Sustainable Energy (RISE), TCG-CREST, Kolkata 700091, India

** Email: k.srivastava@unsw.edu.au*

Abstract: In view of economic and safety concerns surrounding conventional Li-ion batteries based on liquid/polymer electrolytes, researchers are focusing attention on Na-ion based solid-state electrolytes. Recently, borohydrides such as LiBH 4 and NaBH 4 have been reported to be candidate materials for solid-state batteries. 1, 2 Although NaBH 4 has high deformability and electrochemical stability against Na-anodes, it still has the limitation of low ionic conductivity ~10 -10 S cm -1 . 3 In the present work, we have investigated the possible ways to improve the ionic conductivity using the first-principles calculations. We first present the importance of the type of crystal structure and defects that could significantly improve the ionic conductivity of NaBH 4 by ionic substitution. In this computational work, we present some novel results and clarifications on the material Na 2 (BH 4)(NH 2). First, we identified two stable structures and potential high conductive phases that we labeled α and β. These two phases present natural vacant sites that should enable high ionic conductivity. The activation energies calculated with the Nudged Elastic Band (NEB) method are found to be 0.8 and 0.2 eV, respectively. While we relate the α phase of our study with the previously reported 4 high conductive phase of Na 2 (BH 4)(NH 2), the β-phase we present here has never been reported before. Given its structural properties and energy lower than the α phase, this β phase has been shown to become conductive at conditions closer to room temperature. In addition to the structural characterization, one of the most important outcomes of our study is the understanding of the double paddle wheel mechanism for Na-ion diffusion, assisted by in both phases and the role of neighboring NH 2 - and BH 4 - units..

Keyword: Na 2 (BH 4)(NH 2), Defects, Nudged Elastic Band, Activation Energy, Paddle-wheel mechanism

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O-04

Site Specific Descriptor for Metals to Predict Oxygen Evolution Reaction Activity on Single Atom Catalysts

Erakulan E. Siddharthan[1], Sourav Ghosh[1], Ranjit Thapa[1,2,*]

[1] Department of Physics, SRM University–AP, Amaravati, Andhra Pradesh 522 240, India

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

Email: erakulan_es@srmap.edu.in

Abstract: Computational studies have proven to be a vital tool to predict new materials and also assess the behaviour towards various catalytic reactions. They also identify the innate properties of the material which drives the catalytic activity. It helps in designing the material with desired property to improve the catalytic activity. Descriptors are such computationally obtained properties/parameters of a material that has a meaningful relation with any catalytic property of a chemical reaction. d-band center, given by Hammer and Norskov in 1995, explained the binding strength of oxygen atom on pure transition metals. The adsorbate state after interaction with delocalized s-states of the metal atom is almost constant while that resulting from d-states interaction split into bonding and antibonding states. Hence the s-states were not considered. It is well known that, when the dimensions of a system is lowered the states become narrow and localized. In such systems, the d-band center does not explain the catalytic activity well and it is an open research problem. Following the criteria of localized states, single atom catalysts (SAC) are the materials, where the metal atom states are localized. The easily tunable electronic structure of the graphene nanoribbons (GNRs) with just width variation. SAC on GNRs could be used to obtain several parameters that that can be utilized in machine learning to do a deeper search for a better descriptor that could explain as well as predict the catalytic activity.

Keywords: DFT, Machine learning, descriptor, d-band, SAC.

O-05

Application of Newly Designed Y-series Non fullerene Acceptors for High-Efficient Organic Solar Cells

Sheik Haseena[1], Mahesh Kumar Ravva[1,*]

[1] Department of Chemistry, SRM University-AP, Andhra Pradesh, India 522240

Email: sheik_haseena@srmap.edu.in

Abstract: The electron acceptor materials in organic solar cells (OSCs) play an essential role in enhancing power conversion efficiency (PCE). Here, we have designed symmetric and asymmetric non- fullerene acceptors (NFAs), in which a donor is flanked between two end-group units. The NFAs are constructed by considering the Y6-based core and various types of end-group units. The impact of end- group units on geometric, electronic, and excited state properties of NFAs is studied using state-of-the- art density functional theory (DFT) methods. A systematic selection criterion is applied to screen potential NFAs among newly designed 18 NFAs. The interfacial electronic properties between conjugated polymer and NFAs are fully evaluated in the excited state. Overall, these evaluations give helpful guidance for developing a new NFA to enhance OSCs' PCE.

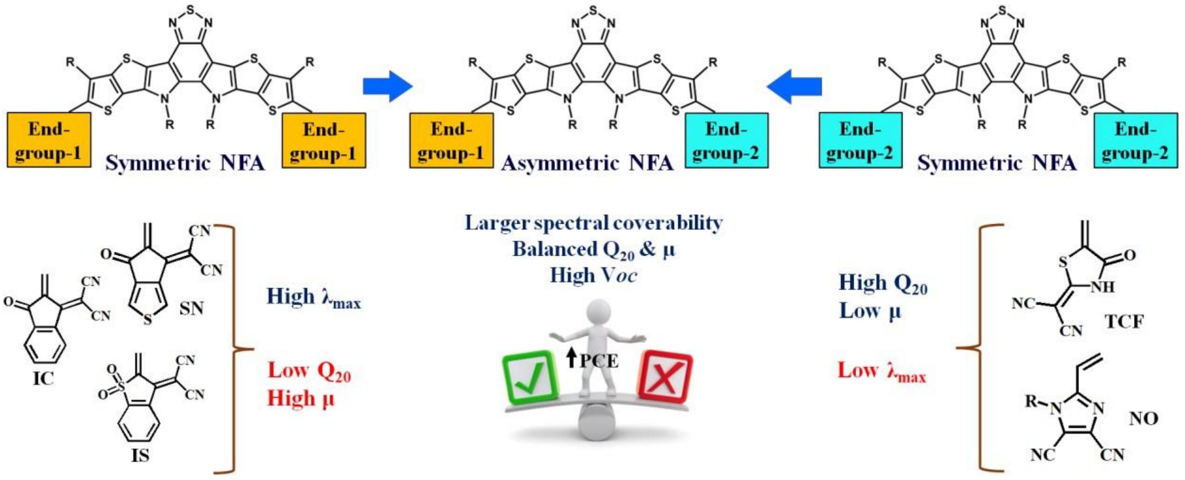

Figure 1. Schematic representation of design of symmetric and asymmetric NFAs.

Keywords: Organic solar, non-fullerene acceptors; charge transfer; density functional theory

O-06

16.35 % efficient Cs2GeSnCl6 based heterojunction solar cell with hole-blocking SnO2 layer: DFT and SCAPS-1D simulation

Mukaddar Sk[1,2]

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

[2] Department of Physics and Centre for Computational and Integrative Sciences, SRM
University – AP, Amaravati, Andhra Pradesh, 522240, India

Abstract: In this article, we have systematically investigated its structural, electronic, optical and photovoltaic properties of Cs 2 GeSnCl 6 by using first-principles and SCAPS-1D simulations. The negative formation energy along with absence of imaginary phonon frequency demonstrated the thermodynamic stability of this compound. The electronic band structure calculation revealed the direct band gap nature of Cs 2 GeSnCl 6 with values of 0.52 eV (with GGA-PBE) and 0.93 eV (with GGA-PBE + mBJ + SOC). This dispersed direct band gap of Cs 2 GeSnCl 6 provides the outshining optical properties of this compound such the large dielectric constant, excellent absorption coefficient (10 5 cm -1), appreciable optical conductivity and low reflectivity. Furthermore, motivated by good optical properties, we have modelled ITO/SnO 2 / Cs2GeSnCl 6 /Au heterojunction solar cell which shows optimum PCE (%) of 16.35 % higher than the previously reported value from lead-free halide double perovskites halide. Thus, we believe our studies will provide guidelines for the construction of lead-free double perovskite based high efficiency solar cell.

O-07

Mechanism of Proton Transfer at Poly (acrylic acid)-Imidazole

Khusnul Yakin[1]

[1] Department of Physics, Maulana Malik Ibrahim State Islamic University, Gajayana No.50,
Malang, 65144, East Java, Indonesia.

Email: khusnulyakin@uin-malang.ac.id

Abstract: The composition of polymeric acids and proton carrier molecules as proton conduction materials determines the efficiency of fuel cells through proton transfer [1]. According to previous experimental studies, the mixture of poly (acrylic acid) (PAA)-imidazole (Im) has the highest conductivity of [2] when compared to the proton conductivity of poly(vinylphosphonic acid)-imidazole, that is [3], and alginic acid-imidazole, that is [4]. The proton transfer process that occurs between polymeric acid and the proton carrier is experimentally difficult to explain. This study focuses on the analysis of proton transfer from PAA-Im materials using density functional theory. We performed first-principles density functional calculations using the PBE exchange-correlation and def2-TZVP basis set function. We created three proton transfer models: Im pair (i.e., imidazole and protonated imidazole (Im+)), PAA-Im pair, and PAA-Im pair- PAA. We discovered that the proton transfer barrier (barrier energy) of the Im pair is dependent on the proton donor-acceptor distance (PDAD). The lower the PDAD in the Im pair, the lower the barrier energy, making proton transfer easier. The hydrogen bond between PAA and Im+ or PAA and Im reduces the PDAD of the Im pair for the PAA-Im pair and PAA-Im par- PAA.

Keywords: imidazole; poly(vinylphosphonic acid); proton transfer; barrier energy

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Poster

P-01

What leads to direct epoxidation?

An exhaustive DFT investigation of electrophilic oxygen mediated epoxidation of ethylene on Ag (100)

Aathira Nair[1,2] and Kavita Joshi[1,2]

[1] Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India.

[2] Academy of Scientific and Innovative Research (AcSIR), Sector 19, Kamla Nehru Nagar, Ghaziabad, Uttar Pradesh- 201002, India

Email: a.nair@ncl.res.in

Abstract: Extensive research has contributed to a better understanding of the commercially important epoxidation reaction. Selectivity, a crucial aspect of this reaction, has received significant attention in both experimental and theoretical investigations. However, a consensus regarding the role of electrophilic oxygen in epoxidation is yet to be reached. The present study is a theoretical examination of the prerequisites necessary for direct epoxidation to occur on the Ag(100) surface, at varied monolayer concentrations. Additionally, the study investigates the characteristics of various oxygen species interacting with ethylene to promote the direct epoxidation pathway. Based on the effective charges and projected density of states (pDOS) analysis, three oxygen variants were identified on the Ag(100) surface: atomic oxygen, dissociatively adsorbed molecular oxygen, and O3 . The investigation reveals that all oxygen species, despite their physical and electronic differences, are electrophilic and undergo direct epoxidation.This work provides insights into the electronic factors influencing the epoxidation on Ag-O complexes.

Keywords: Direct epoxidation, electrophilic oxygen, Ag(100)

P-02

Computational Investigation of the Binding Affinity of 7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione with Cyclooxygenase Enzymes: A QM/MM Study

Amaze Mathe

Abstract: Tinospora cordifolia has a variety of compounds, and some of these compounds may have anti- inflammatory and antioxidant properties. In the present study, we identified the compounds in the leaf extract of T. cordifolia through Gas Chromatography-Mass Spectrometry (GC-MS) analysis and found the various metabolites. The compounds are screened virtually using a machine learning model, followed by molecular docking and simulation study to identify top-hit compounds as cyclooxygenase (COX) inhibitors. The molecular docking revealed that the compound 7,9-Di-tert- butyl-1-oxaspiro (4,5) deca-6,9-diene-2,8-dione (CID:545303) exhibited the lowest binding energies of −7.1 and −6.8 kcal/mol against COX 1 and COX 2 respectively. The interactions are favored by hydrogen bonding and hydrophobic interaction inside the binding pocket. The 100 ns MD simulation study for these compounds was performed to know the stability and found the RMSD around 2 Å and around 1.0 Å with minimal fluctuations indicating a stable complex throughout the simulation of 100 ns. Based on these findings, we proposed 7,9-Di-tertbutyl- 1-oxaspiro (4,5) deca-6,9-diene-2,8- dione could be used as a dual inhibitor of COX enzymes and a drug-like molecule for treating inflammation after evaluation of their biological properties. The methanolic extract of T. cordifolia was subjected to in vitro DPPH, ABTS, nitric oxide, anti-microbial, COX, and LOX inhibition activity. The results exhibited possible positive effects against the above activities.

P-03

Studying dynamics of collective motion from topological perspective

Anamika Roy[1,2,3]

[1] Physics Department, Charuchandra College, India

[2] Physics Department, St. Xavier's College, Kolkata 700016, India

[3] Condensed Matter Physics Research Centre, Jadavpur University, India

Abstract: This work focuses on studying the dynamical evolution of collective motion of living matter with the aid of algebraic topological tools. Simulated motion of living matter using standard Vicsek model is analyzed through the topological measure, Euler Characteristic. We construct Alpha complexes of the time varying distributions of the living matter and estimate their Euler Characteristic(χ) at different timesteps t and different scale of resolution r. The whole topological evolution of the dynamical system is thus summarized in a three dimensional phase space which we call the Euler Characteristic Surface($\chi s(r, t)$) or ECS. The effect of different parameters which are noise, radius of interaction, number density etc. are studied via these Euler Characteristic Surfaces to understand how they can control the flocking or aggregation in the collective motion. The similarity or dis- similarity between two motion is then quantified via a distance function called Euler metric(χ, dM) or EM which has a hilbert space structure. We thus use these topological tools to discover the dynamics of order disorder transition in these complex collective motions.

P-04

First-principle investigation of Janus SnSSe as a promising material for NO, NO 2 and NH3 gas sensing.

Anju Rajan[1], Raghu Chtanathodi[1]

[1] Department of Physics, NIT Calicut, Kerala 673601, India

Email: anjurajan2505@gmail.com

Abstract: Janus transition metal dichalcogenides (TMD) are a class of 2D materials that have attracted significant attention due to their unique electronic and optical properties. The quest for suitable materials to capture toxic gases, such as NO, NO2 , and NH3 , is of paramount importance as they are known to have detrimental effects on human health and the environment. Using DFT, we systematically investigated the gas-sensing properties of Janus SnSSe, for these toxi nitrogen-containing gases (NCG). Our study revealed that the three gases are adsorbed on the defective sulfur and selenium surfaces of Janus SnSSe with significant adsorption energy (, specifically it was found that a single chalcogen defect could significantly improve the adsorption energy. The electronic structure, charge transfer, and work function after adsorption is analyzed. Results showed a significant change in work function after adsorption as well as a decrease in energy gap (, indicating an improvement in conductivity. From Bader charge analysis, it is found that a significant amount of charge is transferred from the molecules to the monolayer. The results indicate that the material has high sensitivity for these gases, making it an excellent candidate for next-generation sensing applications.

Keywords: 2D material; sensor; DFT.

P-05

A Computational Study to Determine the Role of σ-Hole in nido-Heteroborane Binding Capabilities

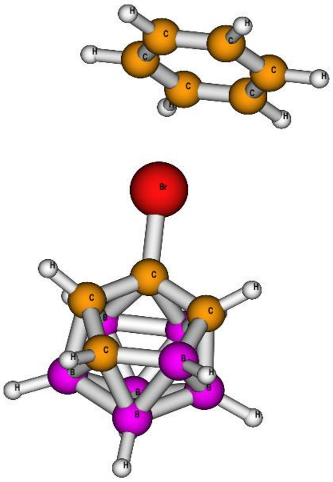
Archan Ravi Sankar[1], Sermarajan Arunachalam[1], Ramachandran Gnanasekaran[1,*]

[1] Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology-Chennai – 600127, India.

*(*presenting author) Email: archan.r2022@vitstudent.ac.in*

Abstract: A systematic quantum mechanical study of σ-hole on the halogen atom present in the nido-heteroboranes is performed. The potential of the halogen σ-hole was compared to that of its hydroxyl group counterpart. The hydrogen atom present in the -OH group had the maximum potential when compared to that of Br atom. The presence of a hetero-atom vertex like -CH, in a different position of a system, influenced the σ-hole and hence its binding abilities. Halogenated nido-carboranes had a weaker binding ability compared to their closo-counterparts; but were stronger than the halogenated hydrocarbons. The presence of solvent dampened the electrostatic interactions. The results of this study will be very useful for the rational engineering of halogen bonding in inorganic crystals as well as in bio-molecular complexes. This study also has many applications in drug delivery, pharmaceuticals, crystal engineering, etc.

Keywords: nido-carboranes; DFT; Binding energy; σ-hole;



Archan Ravi Sankar, Sermarajan Arunachalam, Ramachandran Gnanasekaran*, *Journal of Molecular Graphics and Modelling* **127** (2024) 108680.

P-06

Synergistic Niobium Doped Two-Dimensional Zirconium Diselenide: An Efficient Electrocatalyst for O2 Reduction Reaction

Ashok Singh[1] and Srimanta Pakhira[1,2*]

[1] Theoretical Condensed Matter Physics and Advanced Computational Materials Science Laboratory, Department of Physics, Indian Institute of Technology Indore (IIT Indore), Simrol, Khandwa Road, Indore-453552, Madhya Pradesh, India.

[2] Theoretical Condensed Matter Physics and Advanced Computational Materials Science Laboratory, Centre for Advanced Electronics (CAE), Indian Institute of Technology Indore (IIT Indore), Simrol, Khandwa Road, Indore-453552, Madhya Pradesh, India.

Email: phd2101151013@iiti.ac.in

Abstract: In the pursuit of advancing fuel cell technology for commercial applications, the imperative lies in the development of cathodic catalysts with heightened activity and cost- effectiveness, particularly in expediting the electrochemical sluggish oxygen reduction reaction (ORR). Here, we have investigated the electrocatalytic activity of the two-dimensional single- layer Nb-doped zirconium diselenide (2D Nb-ZrSe2) towards ORR by employing the dispersion corrected density functional theory (DFT-D) method. Through our study, we computed structural properties, electronic properties, and energetics of the 2D Nb-ZrSe2 and ORR intermediates to analyze the electrocatalytic performance of the 2D Nb-ZrSe2. The electronic properties calculations depict that the 2D monolayer ZrSe2 has a large band gap of 1.48 eV, which is not favorable for the ORR mechanism. After the doping of Nb, the electronic band gap vanishes and 2D Nb-ZrSe2 acts as a conductor. Our results show that the more favorable path for O2 reduction on the surface of the 2D Nb-ZrSe2 is the 4e- associative path. The detailed ORR mechanisms (both associated and dissociative) have been explored by computing the changes in Gibbs free energy (ΔG). All the ORR reaction intermediate's steps are thermodynamically stable and energetically favorable. The free energy profile for the associative path indicated a downward trajectory, signifying catalytic activity across all ORR intermediate structures and a notable preference for the 4ereduction pathway. Therefore, 2D Nb-ZrSe2 is a promising catalyst for the ORR, which can be used as an alternative ORR catalyst compared with expensive platinum (Pt).

Keywords: O2 reduction reaction; two-dimensional transition metal dichalcogenides (2D TMDs); associative and dissociative mechanism; adsorption energy; Gibbs free energy

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P-07

C_2 product formation over C_1 product and HER on 111 plane of specific Cu alloy nanoparticle identified through multiparameter optimization

Asif Iqbal[a], Anjana Tripathi[a], Ranjit Thapa*[a,b]

[a]Department of Physics, SRM University AP, Amaravati 522 240 Andhra Pradesh, India

[b]Centre for Computational and Integrative Sciences, SRM University – AP, Amaravati 522 240, Andhra Pradesh, India

* *Email: ranjit.phy@gmail.com*

Abstract: C_2 products are more desirable over C_1 products during CO_2 electroreduction (CO_2ER) because of the former acquires higher energy density and more industrial values. For CO_2ER, Cu is a well-known catalyst, but the selectivity towards C_2 product is still a big challenge in front of researchers due to complex intermediates, different final products and large space of catalyst due to morphology, plane, size, host surface, etc. Using DFT calculations, we find that alloying of Cu nanoparticles can help to enhance the selectivity towards C_2 products during CO_2ER with low overpotential. By systematical investigation on 111 planes (which prefer C_1 product in case of bulk Cu), the alloys show the generation of C_2 products via *CO-*CO dimerization. It also suppresses the counter pathway of hydrogenation of *CO to *CHO which leads to C_1 products. Further, we find $*CH_2CHO$ intermediate forficate the ethanol or ethylene as final product. We have used simple graphical construction to identify the catalyst for CO_2ER over HER, and vice versa. We have also defined the case of hydrogen poisoning and projected a parity plot to recognize the catalyst for C_2 product evolution over C_1 product. Our study reveals Cu-Ag and Cu-Zn catalysts selectively promote ethanol production on 111 planes. Moreover, edge doped $2SO_2$ graphene nanoribbon as host layer further lowers the barrier and selectively promote ethanol on Cu_{38} and Cu_{79} based alloys. This work provides new theoretical insight to design Cu based nano alloy catalysts for C_2 product formation on 111 plane.

Keywords: CO_2, Electrocatalyst, Nanoparticle, Ethanol Production, Adsorption, DFT

P-08

Comprehensive impedance and admittance spectroscopic investigation of MoS2-solar cells with exclusive Zn3P2 as HTL and least lattice mismatches

Atish Kumar Sharma[1,2], Ankita Srivastava[1], Keyur Sangani[3], Nitesh K. Chourasia[4,#], Ritesh Kumar Chourasia[2,*]

[1] University Department of Physics, L.N.M.U., Darbhanga-846004, Bihar, India.

[2] Post-Graduate Department of Physics, Samastipur College, Samastipur-848134 (A Constituent unit of L.N.M.U. Darbhanga-846004), Bihar, India.

[3] Electronics and Communication Engineering Department, Institute of Technology, Nirma University, Ahmedabad-382481, Gujrat, India.

[4] School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India.

Email: atishphyzics@gmail.com (Presenting Author); niteshphyzics@gmail.com#; riteshphyzics@gmail.com*

Abstract: In this analytical study, a four-layer molybdenum disulfide-based photovoltaic cell has been introduced first time using the SCAPS-1d universal open-source tool. The proposed cell has FTO as the window layer, ZnSe as the electron transport layer (ETL), MoS2 as the absorber layer, and exclusive Zn3P2 hole transport layer (HTL) with the least lattice mismatch of about 2.8% only. To explore the highest performance through the proposed novel solar cell configuration, simulation studies have been done on the best possible optimized physical and electrical parameters. The simulated power conversion efficiency, short circuit current, open circuit voltage, and fill factor is 32.55%, 37.75%, 1038.4mV, and 83.01% respectively. Further to investigate the defect states between the band levels, admittance, and impedance spectroscopic analysis has been done with an equivalent electrical circuit model obtained from the EIS module. The present studies help to identify the carrier accumulation behavior at various least-lattice mismatched interfaces and in the bulk of the four-layer solar device. For these analyses, the proposed solar device is simulated for characteristics such as capacitance-voltage (C-V), capacitance-frequency (C-F), conductance-voltage (G-V), and conductance-frequency (G-F) under different suitable and practical physical conditions. In this technique, a small AC signal is applied to the solutions obtained from the semiconductor and continuity equations in SCAPS-1d. Further, we have done an in-depth analysis through these measurements.

Keywords: molybdenum disulfide; Zn3P2; ZnSe; SCAPS-1d; admittance; impedance.

P-09

Enhancement of Quantum Efficiency in Perovskite Solar Cells through Whispering Gallery Modes from Titanium Oxide Micro-resonators

Ayusmin Panda[1,2], C Sudakar[2,*] and B. R. K. Nanda[1,3,†]

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

[2] Multifunctional Materials Lab, Department of Physics, IIT Madras, Chennai 600036, India

[3] Center for Atomistic Modelling and Materials Design, IIT Madras, Chennai 600036, India

(Dated: December 15, 2023)

Abstract: With the aid of 3D full-field finite difference time-domain simulations, we propose model configurations for CsPbI3 thin film solar cell devices that include periodically arranged TiO2 microspheres, exhibiting resonating WGMs. The TiO2 microspheres present, either immersed in perovskite or coated with perovskite layer, between the electron and hole transport layers show enhanced current conversion efficiency. The presence of WGMs lead to enhancement in the absorption of CsPbI3 layer. The incoming electromagnetic wave couples with TiO2 microsphere and forms confined resonating modes. Different designs have been examined for deciding the appropriate position of WGM spheres w.r.t thin-film PSC featuring back-reflector and optimized anti-reflectance coating. Since, the in-coupling element is lossless, energy stored in microspheres is absorbed efficiently by the underlying active material. This directly contributes to the increment in the current density of the solar cell. Thus, the devices show a higher current density of 23.62 mA/cm2, while that in planar solar cell device shows current density of 13.68 mA/cm2, for the same thickness of perovskite layer. This leads to more than 70% enhancement in the short-circuit current density than the conventional PSCs device of similar size.

P-10

α-Graphyne withUltra-low Diffusion Barriers as a Promising Sodium-ion BatteryAnode:Ab-initioDFT and MDStudies

Babuji Dandigunta[1,2], Abhijitha V G[1], Sharma S.R.K.C. Yamijala[2,3], B.R.K.Nanda[1,3]

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

[2] Computational Chemistry and Materials Science lab, Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, India

[3] Centre for Atomistic Modelling and Materials Design, Indian Institute of Technology Madras, Chennai-600036, India

Email: babujidandigunta19@gmail.com

Abstract: Sodium-ion batteries are considered as potential alternatives to conventional lithium ion batteries. To realize their large-scale practical applications, it is essential to identify suitable anode candidates exhibiting promising electrochemical properties such as high specific capacity, low diffusion energy barrier, and excellent cyclic stability. In this work, using density functional theory (DFT) calculations and ab initio molecular dynamics simulations, we examine α-graphyne (AGY) - a carbon-based 2D material - as a potential anode candidate. Our results show that AGY exhibits an ultra-low diffusion barrier of 0.09 eV along both the horizontal and vertical directions and a low average anodic voltage of 0.36 V. Our AIMD studies at 300K show excellent thermodynamical stability with the loading of four sodium atoms, resulting in a theoretical specific capacity (TSC) of 279 mAh/g. Doping studies show that varying the nature of acetylenic links of AGY with electron-rich (nitrogen) or electron-deficient (boron) elements, the adsorption strength and diffusion barriers for Na atoms on AGY can be tuned. Furthermore, treating AGY as a case study, we find that conventional DFT studies are expected to overestimate the TSC by a huge margin. Specific to AGY, this overestimation can be up to ~ 300 %. We identify that ignoring the probable formation of temperature-driven metal clusters is the main reason behind such overestimations. Here, we propose a scheme involving temperaturedependent AIMD simulation to substantially improve the accuracy of the TSC calculation using first-principles methods.
Keywords: α-graphyne, specific capacity, molecular dynamics, vertical diffusion, average adsorption energy.

P-11

Unveiling the Synergistic Performance of Double-atom Transition Metal Incorporation in Graphitic Surfaces as Electrocatalysts

Deeksha R, Deepak Kumar[1,*]

[1] Department of Chemistry, Faculty of Mathematical and Physical Sciences, M.S. Ramaiah
University of Applied Sciences, Bengaluru, Karnataka – 560058, India.

Email: deeksharamamurthy@gmail.com

Abstract: The hydrogen evolution reaction (HER) holds immense potential for sustainable energy generation, yet efficient and affordable catalysts remain a critical bottleneck. Herein, we explore the synergistic effects of incorporating 3d transition metals on two promising graphitic supports, g-C 3 N 4, and g-C 2 N, for enhanced HER activity using DFT calculations within the VASP framework. Initial screening of single-atom catalysts identified favorable candidates based on their binding energy and free energy for HER. Subsequently, we delve deeper into double-atom configurations considering both homogeneous and heterogeneous arrangements of the chosen transition metals. Our electronic structure calculations including Bader charge analysis, differential charge density analysis, and density of states analysis along with crystal orbital Hamilton population (COHP) and crystal orbital overlap population (COOP) provide detailed insights into the electronic and bonding interactions governing HER activity. We identify the most capable catalysts exhibiting optimal H binding strengths, favorable thermodynamics, and efficient electron transfer pathways. These findings pave the way for the rational design of highly active and stable transition metal-embedded graphitic electrocatalysts for next-generation hydrogen production.

Keywords: hydrogen evolution reaction; nitrogen g-C 3 N 4 and g-C 2 N; DFT, single-atom catalysts, double-atom catalysts

P-12

Improved Quantum Algorithm: A Crucial Stepping Stone in Quantum-Powered Drug Discovery

Thulasi Bikku[1], Malligunta Kiran Kumar[2], Srinivasarao Thota[3], Surapaneni Phani Praveen[4]

[1] Department of Computer Science and Engineering, School of Computing Amaravati, Amrita Vishwa Vidyapeetham, Kuragallu Village, Mangalagiri (M), Guntur, Andhra Pradesh – 522503

[2] Associate Professor, Department of Electrical and Electronics Engineering, Koneru Lakshmaiah Education Foundation, Green Fields, Vaddeswaram, A.P. – 522302.

[3] Department of Mathematics, Amrita School of Physical Sciences, Amrita Vishwa Vidyapeetham, Amaravati, Andhra Pradesh - 522503, India

[4] Department of Computer Science & Engineering, PVP Siddhartha Institute of Technology, Kanuru, Vijayawada 520007, Andhra Pradesh, INDIA. Department of Computer Science and Engineering, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

Email: b_thulasi@av.amrita.edu

Abstract: Quantum computing is revolutionizing drug discovery by introducing a robust system to accelerate the improvement of new and effective treatments. Quantum mechanics enables the implementation of quantum algorithms, surpassing the constraints of traditional computing methods. QNNs facilitate the creation of simulations that illustrate molecular interactions, thereby assisting in the identification of potential candidates for drug development. This research work exhibits the difficulties of molecular dynamics and Quantum chemistry and gives excellent insights. Recently, the world has been paying interest in quantum algorithms due to their perfect results, but modifications and upgrades are still required to improve accuracy and precision. The proposed quantum neural network algorithm skillfully addresses the hurdles that must be surmounted to assess the importance of quantum computing in the realm of drug discovery. Given the inherent susceptibility of quantum structures to noise, noise reduction is paramount. Quantum neural networks excel in managing intricate molecular interactions encompassing numerous atoms and electrons, necessitating a shift in approach. Moreover, optimizing the arrangement of algorithms needs complex paradigms to enhance the overall performance of quantum algorithms aimed at drug discovery. To handle all the above challenges, researchers are looking towards quantum algorithms tailored for drug discovery, allowing correct molecular interaction simulations and providing the groundwork for faster, world-class, targeted drug discovery. The company's drug development software can alter drug discovery as quantum computing matures. Hence, when applied to different datasets, the proposed QNN algorithm is more reliable and provides more accurate results than traditional machine learning algorithms.

Keywords: Quantum computing, drug discovery, neural networks, scalability, algorithm optimization.

P-13

Synergistic MoS 2 -TiO 2 Nanocomposite for Efficient H 2 Evolution, Dye Degradation, and Supercapacitor Applications

M. Chandra Sekhar[1], B. Purusottam Reddy[2], Charan Kuchi[1], B. Jagadeesh Babu[1], C. Kamal Basha[3], N. Reddeppa[1], C. Madhavi[4], Si-Hyun Park[2]

[1] Department of Physics, Madanapalle Institute of Technology and Science, Madanapalle, 517325, India

[2] Department of Electronic Engineering, Yeungnam University, 280 Daehak-ro, Gyeongsan-si,

Gyeongsanbuk-do, South Korea

[3] Department of EEE, Madanapalle Institute of Technology and Science, Madanapalle, 517325, India

[4] Department of Polymer Science and Technology, S.K.University, Anantapur, 515003, India

Email: drcahrank@mits.ac.in

Abstract: In this study, we explore the multifunctional applications of a novel MoS 2 -TiO 2 nanocomposite, synthesizing and characterizing its properties for efficient hydrogen (H 2) evolution, dye degradation, and supercapacitor performance. The integration of MoS 2 , a two- dimensional transition metal dichalcogenide (TMD), and TiO 2 , a wide-bandgap metal oxide semiconductor, addresses challenges in clean energy, environmental remediation, and energy storage. X-ray diffraction (XRD) confirms successful MoS 2 -TiO 2 integration, maintaining characteristic peaks of both materials. Scanning and Transmission Electron Microscopy (SEM and TEM) reveal a synergistic architecture with TiO 2 nanoparticles uniformly dispersed within porous MoS 2 microspheres, indicating strong interfacial interactions. X-ray Photoelectron Spectroscopy (XPS) elucidates the electronic states and chemical composition of the nanocomposite, validating the presence of MoS 2 and TiO 2 . Brunauer-Emmett-Teller (BET) analysis demonstrates enhanced surface area and porosity, attributed to the synergistic effect. Photocatalytic studies show superior dye degradation, and hydrogen evolution experiments exhibit a threefold rate increase with incorporated TiO 2 , emphasizing efficient photon absorption. The nanocomposite demonstrates stability over cycles, promising for solar-driven hydrogen production. Electrochemical analyses reveal pseudocapacitive behavior, surpassing pure MoS 2 in specific capacitance, energy density, and power density. Electrochemical impedance spectroscopy (EIS) indicates comparable charge transfer kinetics, highlighting TiO 2's positive effect without significantly affecting resistance. The MoS 2 -TiO 2 nanocomposite emerges as a transformative material with multifaceted applications, showcasing versatility in addressing global challenges related to clean energy and environmental sustainability.

Keywords: MoS2-TiO2 nanocomposite, Hydrogen evolution, Dye degradation, Supercapacitor,

Clean Energy, Environmental sustainability

P-14

Unveiling the potential of two-dimensional V2S2 monolayer as a high-performance anode material for metal-ion batteries: A first-principles study

Somnath Chowdhury[1,2], Tuya Dey[1], Sung Gu Kang[2], Jagadish Chandra Mahato[1] and Bikash C. Gupta[1]

[1] Department of Physics, Visva-Bharati, Santiniketan- 731235, West Bengal, India

[2] School of Chemical Engineering, University of Ulsan, 93 Daehak-ro, Nam-gu, Ulsan, Republic of Korea

Email: jagadishc.mahato@visva-bharati.ac.in

Abstract: In this present report, using first principle calculation we have predicted for the first time that the V2S2 monolayer may be an efficient anode material for metal (Li, Na, K)-ion batteries. We have investigated the pristine V2S2 monolayer system's energetical, dynamical, and thermal stability using first principle density functional theory (DFT) VASP code. The intrinsic metallicity of the pristine V2S2 monolayer facilitates its electrical conductivity as an electrode material. We also investigated the structural and electrical properties of the metal (Li, Na, K)-adsorbed V2S2 monolayer. It is observed that Metal-atoms prefer to get intercalated on top of the buckled hexagon of the pristine V 2 S 2 monolayer, and the metallicity of the 2D nanosheet is preserved.

Out of four possible adsorption sites namely-hollow site (h-site), vanadium site (V-site), sulfur site (S-site) and vanadium-sulfur site (V-S site), the hollow site is the most favorable one. In the hollow-site adsorption process, Bader charge analysis provides 0.99, 0.99, and 0.87 electronic charge transferred from the Metal (Li, Na, K) atom to the V 2 S 2 monolayer. Furthermore, this system exhibits a high storage capacity of 968.9 mAh/g for both Li and Na and 322.9 mAh/g for K. This V2S2 system manifests moderately low diffusion energy barrier of 0.55 eV, 0.25V, and 0.27eV for Li, Na and K respectively. The calculated open-circuit voltage of 0.68 V, 0.71 V and 1.40 V for Li, Na and K respectively. Our results suggest that the V 2 S 2 monolayer may be a potential candidate for anode material for rechargeable monovalent (Li, Na, K)-ion batteries.

Keywords: Metal-ion battery, Lithium ion battery, Sodium ion battery, first principle calculation.

P-15

What is the viscosity of liquid water confined in a hydrophobic nanotube? Estimation using a novel approach

Golam Rosul Khan[1], SnehasisDaschakraborty[2]

[1,2] Department of Chemistry, Indian Institute of Technology Patna, Bihar 801106, India

Email: golam_2121ch08@iitp.ac.in

Abstract: Computation of the shear viscosity (η) of liquid water under nanoconfinement is a daunting task, albeit crucial in different areas related to nanofluidics. The viscosity of bulk water is computed using the Green-Kubo (GK) formula or Stokes-Einstein (SE) relation. However, these relations are less useful in the case of water confined in a cylindrical nanotube since the stress tensors are asymmetric and the SE relation breaks down. Using a novel method, based on translational Jump-Corrected SE (JCSE) relation that takes into account the breakdown of SE relation, we compute the viscosity of water inside some hydrophobic carbon nanotubes (CNT) at a wide range of temperatures including supercooled regime. The viscosity of water in narrow CNT (10,10) is seen to be surprisingly higher compared to bulk water at the same thermodynamic condition. This contradicts the usual notion and the past theoretical observation suggesting significantly low viscosity of water inside hydrophobic CNT.

Keywords: shear viscosity, nanoconfinement, Stokes-Einstein, supercooled

P-16

Unveiling the Electrocatalytic Activity of Cobaloxime Metallolinker in UU-100(Co) Metal-Organic Framework towards H2 Evolution Reaction: A DFT Study

Himani Joshi[1], Nilima Sinha[2], Kahkasha Parveen[1], Srimanta Pakhira[1,2,3*]

[1] Theoretical Condensed Matter Physics & Advanced Computational Materials Science Laboratory,
Department of Physics, Indian Institute of Technology Indore (IIT Indore), Simrol, Khandwa Road,
Indore, Madhya Pradesh 453552, India.

[2] Theoretical Condensed Matter Physics & Advanced Computational Materials Science
Laboratory, Department of Metallurgical Engineering and Materials Science (MEMS), Indian
Institute of Technology Indore, Simrol, Khandwa Road, Indore Madhya Pradesh 453552, India.

[3] Theoretical Condensed Matter Physics & Advanced Computational Materials Science
Laboratory, Centre for Advanced Electronics (CAE), Indian Institute of Technology Indore,
Simrol, Khandwa Road, Indore, Madhya Pradesh 453552, India.

Email: phd2001251004@iiti.ac.in

Abstract: Developing an efficient electrocatalyst for water splitting is one of the leading and challenging tasks for modern renewable energy technology and sustainable fuels. Exploring non precious, highly efficient, and stable alternative catalysts for Hydrogen evolution reactions (HER) is desirable. Here, we have studied the HER catalytic activity of the cobaloxime linker in UU-100(Co) Metal-Organic Framework (MOF)1 using the hybrid-density functional theory. Our study shows that 3D cobaloxime linker is a semiconducting material where cobalt (Co) acts as an active metal site for efficient electrocatalysis. The existence of Co metal atoms in this UU 100(Co) MOF has spurred a lot of attention due to its electron-accepting ability. The electrochemical HER mechanism has been explored by considering a finite molecular model and it found cobaloxime linker follows the Volmer-Tafel pathway for HER.[2] During the Volmer and Tafel reactions, the calculated barrier energies are 36.12 kcal/mol and 33.10 kcal/mol respectively, in the DMF solvent. Also, N-N coordination in the structure of the cobaloxime linker supports electron transfer, this charge transfer mechanism between the central metal atom Co and N atoms not only drives the initial HER steps but also contributes to the overall stability of the cobaloxime linker during the catalytic cycle. It enables electron reduction, and protonation along with H2 production, ultimately contributing to the advancement of sustainable hydrogen production technologies. This study highlights the capability of MOF as an emerging material for electrochemical reactions in fuel cell applications.

Keywords: Cobaloxime Linker; Density Functional Theory; Hydrogen Evolution Reaction.

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P-17

Quantum monodromy in effective polyad breaking Hamiltonian

Ishita Ghorai[1]

[1] School of Physical Sciences, Indian Institution of Technology – Mandi, Himachal Pradesh, India

Email: d20068@students.iitmandi.ac.in

Abstract: Monodromy is a classical property of two or more degrees of freedom of integrable dynamical systems that creates a distinctive pattern in the distribution of quantum mechanical eigenvalues. The concept of quantum monodromy was recently developed and demonstrated to be an important qualitative feature of numerous realistic models. From these examples, new qualitative features of molecular systems are used to naturally lead to generalized monodromy notions. Finally, in extremely complex systems, a relationship or link between phyllotaxis and monodromy is possible. As spectroscopy becomes more advanced and also the theory of anharmonic systems and nonlinear systems has resulted in a renewed and acute appreciation of the complexity and subtlety of molecular vibrational motion in recent years. Quantum monodromy concept will play a crucial role in the understanding of these complex motions. As most of the realistic models do not conserve polyad quantum numbers, quantum monodromy in effective polyad breaking Hamiltonian can give an insightful perspective to study and analyze classical models.

Keywords: Quantum Monodromy; Effective Hamiltonian; Polyad breaking

P-18

Theoretical Insights into Impact of Solid-State Environment on hot-exciton TADF Emitter Properties

Jesni M Jacob[1], Mahesh Kumar Ravva[2,*]

[1] Department of Chemistry, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

[2] Centre for Computational and Integrative Sciences, SRM University-AP, Amaravati, India

Email: jesni_jacob@srmap.edu.in

Abstract: Understanding Thermally Activated Delayed Fluorescence (TADF) in solid-state environments is crucial for practical applications. However, limited research focuses on how the medium affects hot-exciton-based TADF materials. In our study, we calculated and compared reverse intersystem crossing, radiative, and non-radiative decay rates of TADF emitters in gas, solvent, and solid phases. The emitters designed have a donor-acceptor-donor (D-A-D) structure, with donors like triphenylamine (TPA) and diphenyl amine thiophene (ThPA), paired with acceptors such as benzothiadiazole (BT), pyridine thiadiazole (PT), thiadiazolobenzopyridine (NPT), and benzobisthiadiazole (dBT). We model the solvent and solid phases with the polarizable continuum model (PCM) and quantum mechanical/molecular mechanics (QM/MM) methods, respectively. Using density functional theory (DFT) and time-dependent DFT, we analyze how TADF emitters'; geometrical, electronic, and excited-state properties vary in these phases. Our results show that the solid-state environment significantly influences emitter geometries and TADF properties. In the presence of a solid medium, our study indicates that non-radiative decay rates tend to be slower. On the other hand, radiative emission rates are found to be less influenced by the properties of the surrounding medium. TPA-based donors exhibit slower non-radiative decay than ThPA-based donors, while acceptor choice has a marginal effect on non-radiative decay. Achieving long-wavelength hot-exciton-TADF emitters requires a strategic combination of donors and acceptors. Our study connects emitter chemical structure and the surrounding environment's impact on excited-state characteristics and photochemical properties.

Keywords: TADF; Hot-excitons; multiple channels; solid-state effect; energy-gap law

P-19

CARBONE SUPPORTED DIBERYLLIUM COMPOUNDS Be2 (CL2)2, L=NHC, PMe3, cAAC and CO A THEORETICAL STUDY

Abstract: Diberyllium is characterized as a weakly bonded system. It is of interest to investigate the stabilization of Be2 using donor ligands like carbones. Carbones (CL2) are expected to interact with Be2 in the excited states and donate both σ and π lone pairs. A detailed bonding study of carbone supported diberyllium compounds, L2C-Be2-CL2, with L = NHC (A), PMe3 (B), cAAC (C) and CO (D) has been carried out at the M06/def2-TZVPP//BP86/def2-TZVPP level of theory. Compound A possess a singlet trans-bent geometry, while B is most stable in triplet allenic geometry having D2d point group symmetry. On the other hand, compound C is the most stable in a triplet planar geometry with D2h point group symmetry. Compound D possess a non-planar structure. The MO analysis of all compounds shows that there is a single bond between Be and carbone carbon which is formed by the donation of σ lone pair of carbone to Be. The π lone pair of carbone is not involved in bonding interaction with Be2. The natural charge from the NBO analysis further indicates that carbone is not acting as a double donor ligand in these compounds. However, σ-donation from carbone stabilizes the Be—Be bonding as indicated by the shorter Be-Be bond length.

P-20

Tri-Atom Metal Cluster Decorated Nb 2 CO 2 MXene: Comparative Insights for Efficient Hydrogen Evolution Reaction

Jose Antony V J[1], Maneesha M[1], Sai Raj Ali[2], Praveen C S[1]

[1] International School of Photonics, CUSAT, Ernakulum, Kerala, India, 682022

[2] Department of Physics, Jamia Millia Islamia University, New Delhi, India, 110025

Email: joseantonyvj@cusat.ac.in

Abstract: Cost-effective catalysts derived from non-noble metals play a crucial role in enabling the hydrogen evolution reaction (HER) as a sustainable source of renewable energy in the form of hydrogen. Among the emerging 2D materials, MXene has gained significant attention owing to its promising catalytic properties. Using density functional theory (DFT), we systematically compared the impact of anchoring a series of Tri-Atom Metal Clusters (TAMC) - Ag, Cu, Ir, Pd,Ru, and Rh - onto Nb 2 CO 2 MXene for assessing its HER activity of clusters@MXene. Within the evaluated clusters@MXene, Cu 3 @Nb 2 CO 2 emerged as the best, exhibiting notably superior HER activity, with a Gibbs free energy of hydrogen adsorption (ΔG H) of -0.01eV, highlighting its remarkable adsorption capabilities. Conversely, the other TAMCs, Ir, Pd, Ru, Rh, and Ag, demonstrated comparatively lower HER activity than Cu 3 @Nb 2 CO 2 MXene. A detailed examination of the catalysts' electronic structure and bonding nature revealed that the enhanced catalytic performance can be attributed to the accumulated charge at the core of the Cu 3 cluster within Cu 3 @Nb 2 CO 2 . This analysis underscores Cu 3 @Nb 2 CO 2 as a superior choice for the HER process, emphasizing its potential as a highly effective and cost-efficient catalyst.

Keywords: Mxene: Hydrogen evolution reaction: Density functional theory; Tri-Atom Metal Cluster.

P-21

Treatment of Van der Waals dispersion forces for layered MXenes in the framework of DFT

Rajashekhar Vaibhava K M[1,2,3], Rajappan Vetrivel[2], Ganapati V. Shanbhag[1,2*]

[1] Materials Science and Catalysis Division, Poornaprajna Institute of Scientific Research,
Bidalur, Devanahalli, Bengaluru, 562164, India

[2] Center for Quantum and Computational Studies, Poornaprajna Institute of Scientific Research,
Bidalur, Devanahalli, Bengaluru, 562164, India

[3] Graduate Studies, Manipal Academy of Higher Education (MAHE), Manipal, 576104,
Karnataka, India

Email: vaibhav@ppisr.res.in

Abstract: The Two-dimensional metal carbides and nitrides are known as the MXenes and they are part of a large family of layered materials. Since the discovery of two-dimensional Ti 3 C 2 in 2011, MXenes have shown fascinating physical and chemical properties that possess tremendous promise for applications ranging from electronic devices to photo and electrocatalysis and also in the fields of sustainable energy storage and conversion. The large range of possibilities of these materials makes the first principle simulation a vital step in the developmental stage of these materials alongside conventional experiments. Since each of these materials possesses unique properties, this requires methodologies with good approximations that account for all most of the interactions occurring in these materials at a reasonable computational cost. In this regard, Density Functional Theory (DFT) has been a successful approach to the study of real-life materials and has become a routine procedure. Within the intralayer, 2D layered materials are typically firmly bound via covalent and ionic forces, which are well modeled by semi-local DFT. Thus, essential energetic characteristics of a 2D layered material relate to the weak VdW- related forces between layers that are ultimately responsible for the stability. The work focuses on studying the VdW interaction present in 2D layered MXenes and their effect on electronic structure, and physical and chemical properties while exploring the available methods to incorporate VdW interaction and extending the work to develop a dispersion correction for accurate considerations of VdW interaction present in these materials.

Keywords: MXenes; Density Functional Theory (DFT); Van der Waals forces; Long range correlation

P-22

Experimental Investigation and Thermodynamic Reassessment of Mg-Sr-Zn Ternary System

K. Santhy[1,*], B. Rajasekaran[2] and Sujoy K. Chaudhury[1]

[1] Department of Materials and Metallurgical Engineering, IITE, Indus University,

Ahmedabad – 382115, India

[2] Department of Metallurgical and Materials Engineering, National Institute of Technology,
Surathkal - 575025, India

Email: santhyk.mt@indusuni.ac.in

Abstract: Magnesium-zinc (Mg-Zn) alloys are gaining attention as promising biomaterials due to their superior biocompatibility. Researchers are actively seeking to enhance their properties through the addition of alloying elements such as strontium. Recent investigations have unveiled the presence of ternary intermediate phases in the ternary MgSr0.5ZnX (X=2 to 18) alloy using analytical techniques like X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS) and Differential Thermal Analysis (DTA). However, there is a lack of understanding on its thermodynamic assessment in the literature. To gain deeper insights into the evolution of various ternary intermediate phases in Mg-Sr-Zn system, a comprehensive reassessment is undertaken by combining the CALPHAD approach with first principle calculations. Enthalpy of formation of various binary compounds are calculated using first principle methods and compared with the available literature data. By accounting for the solubility of the third element in binary compounds, the energy of formation for hypothetical end members is determined through first principle calculations, which are then integrated into phase modeling. In this study, Gibbs free energy value for various equilibrium phases of the Mg-Sr-Zn system is calculated by combining the thermodynamic principles in conjunction with the experimental data. Further, the reassessed thermodynamic data are employed to construct liquid projections, isothermal sections, and vertical sections of the Mg- Sr-Zn system and compared with experimental observations. In summary, this research makes an attempt to advance the thermodynamic understanding of Mg-Sr-Zn alloys, with a specific focus on the presence of ternary intermediate phases. It combines experimental characterization and advanced thermodynamic modeling to provide insights that may impact the development and optimization of these alloys for potential biomaterial applications.

Keywords: Mg-Sr-Zn system; Characterization; First principle calculation; CALPHAD Approach, Phase diagram.

P-23

Abstract: Semiconductor to Metal transition in single and double polyyne chains Polyynes represent the thinnest and most robust carbon allotrope, demonstrating significant potential in emerging low-dimensional devices of the next generation. This potential arises from their possession of a band gap. Theoretical propositions have been made regarding double carbon chain systems, indicating the tunability of their band gap through structural modifications. In this study, we demonstrate the manipulation of the band gap and the transition from a semiconductor to a metal state in both single and double polyynes when subjected to a transverse electric field. To support this transition and comprehend its spin-related implications, we conducted analyses of spin-polarized band structures and partial densities of states. Furthermore, we assessed the thermodynamic stability using phonon dispersion curves, employing Density-Functional Perturbation Theory. In addition, we employed ab initio molecular dynamics simulations to evaluate thermal stability at room temperature and calculated formation energies to ensure structural integrity before and after the application of the electric field. This research introduces an innovative approach to modulating the band gap in low-dimensional systems, aiming to elucidate the fundamental factors responsible for this effect. The material under investigation holds significant promise for the advancement of flexible andnano-electronic devices in the future.

P-24

Atomistic Insights on FacetDependent Functional Properties in CdSe Nanocrystals

Kushal Samanta[1], Priyanka Deswal[2], Dibyajyoti Ghosh[1,3]

[1] Department of Materials Science and Engineering, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi 110016, India

[2] Department of Physics, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi 110016, India

[3] Department of Chemistry, Indian Institute of Technology, Delhi, Hauz Khas, New Delhi 110016, India

Email: msz218503@mse.iitd.ac.in

Abstract: Semiconductor nanocrystals (NCs) are used for various optoelectronic devices ranging from electronic displays to solar cells to quantum emitters. Owing to the large surface-to-volume ratio, photophysics is dominantly controlled by the atomistic details of NC surfaces. The insights into NC surface geometry, defects, and their impact on the functional properties remain largely limited due to the lack of experimental probes. Here, we combine multiple first-principles- based computational techniques to gain insights into the crystal facet-specific electronic, optical, and catalytic properties of stoichiometric cadmium selenide (CdSe) NCs. The undercoordinated Se atoms on the pristine NC surface give rise to strongly localized trap states near the edge of occupied levels. The inorganic salts can selectively bind and passivate these anionic sites, efficiently mitigating the trap states. The band edge states are primarily delocalized on the polar facets of the trap-free CdSe NC. However, excess passivation can reintroduce the trap states above the delocalized occupied states. The computed absorption spectra reveal that precise surface passivation can improve the optical characteristics of passivated CdSe NC. We further find that the exact location and facet-polarity of active atomic sites play a critical role in their catalytic performance. Our comprehensive study pins down the predominant influence of facet properties on the electronic, optical, and catalytic characteristics of CdSe NCs. These atomistic details will guide the experimental efforts to control the shape, size, and surface geometry of semiconductor NCs for their optimum performance.

Keywords: semiconductor nanocrystals, cadmium selenide, surface passivation, optoelectronic properties

P-25

Atomistic simulation studies of ion transport in NASICON using molecular dynamics simulations

Likun Pradhan[1] and Padma Kumar Padmanabhan[2]

[1] Department of Physics, Indian Institute of Technology Guwahati, 781039, Guwahati, India.

Email: lpradhan @iitg.ac.in

Abstract: In recent decades, lithium-ion batteries have dominated the realm of portable electronic devices due to their high energy densities. However, the quest for cost-effective alternatives for larger-scale energy storage has led to the emergence of sodium-ion batteries. To address safety concerns linked with liquid electrolytes, there is a growing emphasis on exploring solid-state electrolytes, highlighting their necessity in advancing battery technology. NASICONs (Na Super Ionic CONductors), Na1+xZr2SixP3-xO12, x=0-3, discovered by Hong and Goodenough in 1976, stand out as promising materials for solid-state electrolytes. Specifically, the composition with x=2 demonstrates impressive conductivities of about 0.67 mS/cm at room temperature and 200 mS/cm at elevated temperatures (573 K). There exists potential to further enhance conductivity by introducing di- and tri-valent dopants partially into the Zr sites. This study employs molecular dynamics simulations technique to probe the impact of Si/P ordering and various factors on Na ion transport across the entire composition range of NASICONs. The objective is to unveil microscopic insights into the favored migration channels and energy barriers governing high Na mobility within the system. Our research contributes essential information for refining the design and performance of NASICON-based solid-state electrolytes, offering valuable advancements in energy storage applications.

Keywords: NASICON, Solid-state electrolyte, Molecular dynamics simulation

P-26

Enriched Optical Dielectric and Magnetic Properties of Praseodymium and Bismuth substituted Yttrium iron Garnet (Pr: BYIG) nanoparticles by sol-gel Technique

Bhargavi M[1], P Vanitha[1], Salla Gangi Reddy[1], Annapureddy venkateswarlu[2]

[1] department of physics, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

[2] department of physics, National institution of technology, Tiruchirappalli, Tamil Nadu.

Email: bhargavi_m@srmap.edu.in

Abstract: We have prepared Praseodymium and Bismuth doped yttrium iron garnet (YIG) nanoparticles with a compositional variation of Pr x BiY 2-x Fe 5 O 12 ($x = 0.1, 0.25, 0.5, 1.0$, and 1.25) using sol-gel; auto-combustion method and studied their suitability for high-frequency device as well as field sensing device applications. Using X-ray diffraction, Fourier-transform infrared spectroscopy, and UV-visible spectroscope, we have analyzed the structural and optical properties along with the confirmation of the garnet phase. For surface morphology, we have used microscopic images and found that the grain size decreases with the increase in the value of Pr concentration x. Further, we found that the ceramic sample with $x = 0.5$ has frequency frequency-independent dielectric response along with low tangent loss which can be utilized for high-frequency device applications. We have also observed that there two parameters in the dielectric response are varying in the presence of an applied magnetic field, namely, frequency bandwidth and magneto-capacitance coefficient. This variation can be used for sensing the field and found that for $x = 0.25$, the frequency bandwidth shows a maximum variation of 19 % at 0.5 T. We have correlated the magneto-dielectric and dielectric properties with structural and oxygen deficit states obtained using X-ray photo-electron spectroscopy.

Keywords: Yttrium iron garnet, Sol-Gel, auto-combustion, High-Frequency Device Applications, Magneto-Dielectric Properties

P-27

Understanding the effect of O_2 in the growth mechanism of 2D MoS_2 in a chemical vapor deposition reactor

Madhavan Nampoothiri[1], D K[1] and Ananth Govind Rajan[1]

[1] Department of Chemical Engineering, Indian Institute of Science, Bengaluru, 560012 Karnataka, India

Email: madhavann@iisc.ac.in

Abstract: Two-dimensional (2D) transition metal dichalcogenides, such as molybdenum disulfide (MoS_2), are emerging candidates for varied applications, including neuromorphic computing, catalysis, gas separations, and optoelectronic devices. Powder-based chemical vapor deposition (CVD) techniques with MoO_3 (s) and S(s) as molecular precursors are commonly employed for the growth of MoS_2 monolayers. Experimental studies suggest that passing O_2 along with the typical carrier gas plays a catalytic role in the crystallization of MoS_2. In this study, we track the detailed gas-phase reaction pathway towards the formation of MoS_2 with and without O_2 assist to understand the mechanism by which O_2 affects the reaction. We propose a reaction mechanism from first principles by observing the key intermediates obtained by running prolonged ab initio molecular dynamics (AIMD) simulations for both pathways. The reaction energies and activation barriers for these reaction steps were calculated using density functional theory (DFT) methods. The ensuing results indicate that the formation of unstable sulfur oxides such as SO and SO_3 drives the chemistry in the O_2 -assisted pathway while S_2 drives the process in the standard pathway. Both reaction pathways proceed similarly with SO/S_2 insertion into $(MoO_3)_3$ ring trimer, followed by ring opening and chain breaking. The smaller MoO_xS_y chains then continuously sulfurize by S_2 /SO attack and S_2O and SO_2 removal to form MoS_6 in the gas phase. Our work is expected to shed light on the precise mechanism of CVD growth of 2D MoS_2 using first-principles calculations.

Keywords: CVD, MoS_2 , growth mechanism, reaction pathway, thermodynamics, kinetics, DFT

P-28

Prediction of significant biomarkers by network analysis for breast cancer bone metastasis

Mahima Bhardwaj[1], Thanvi Sri[1], K. Abraham Peele[1*], Sachidanand Singh[2*]

[1] Department of Biotechnology, Vignan's Foundation for Science, Technology and Research (Deemed to be University), Vadlamudi, Guntur-522213, Andhra Pradesh, India

[2] Department of Biotechnology, Faculty of Engineering and Technology, Pandit Deendayal Energy University, Gandhinagar - 382426 Gujarat, INDIA

*Corresponding Authors: drsachinbioinfo@gmail.com

Abstract: Background: Breast cancer is one of the most common cancers in women. About 70% of breast cancer patients have bone metastasis, and in the present growing world bone metastasi is common for breast cancer patients. The prediction of target genes or biomarkers for bon metastasis from breast cancer would aid in classifying individuals at high risk and would also be used to guide focused treatment for bone metastasis.

Objective: This research aims to identify the key targets or biomarkers that lead to bone metastasis from breast cancer. The workflow involves with meta-analysis, network studies and functional enrichment studies.

Design: Analysis of microarray data has become the standard method in this study. In this study, the datasets (GSE103357, GSE55715, GSE2034, GSE14776 and GSE137842) were retrieved from the Gene Expression Omnibus (GEO), and differentially expressed genes were identified using the tool ImaGEO. A protein-protein interaction (PPI) network was constructed from high throughput experiments using STRING (Search Tool for the Retrieval of Interacting Genes). Some of the gene in the network shows direct connections in the string and the network was transferred to Cytoscape 3.9.1. Analysis of the network and hub gene identification was done by plug-ins of Cytoscape. The functional enrichment analysis, Pathway analysis and Gene Ontology (GO) studies of the target genes or biomarkers was performed by Funrich 3.1.3, KEGG and GeneCards.

Result: In consonance with our study, there were 90 differentially expressed genes acquired. Where among these 90 genes 18 genes were showing direct connection with each other in STRING database. The network was analyzed with Network analyzer a plug-in of Cytosacpe3.9.1. As a result of Network analyzer 12 genes were common from all the centrality parameters. These genes were given rank by CytoHubba another plug-in of Cytoscape and the resultant hub genes are RACGAP1, PPP1CC, RAG23A, PSMD1 and RPL26L1. Further these genes were used for Functional enrichment analysis, Pathway analysis and GO studies with the help of Funrich 3.1.3.

Keywords: Bone metastasis, differentially expressed genes Network analysis and hub genes

P-29

An Understanding into the CO_2 Reduction on Homo and Hetero atom doped V_2CO_2

Maneesha M[1], Jose Antony V J[1], Sai Raj Ali[2], *C S Praveen[1]

[1] International School of Photonics, Cochin University of Science and Technology, University Road, South Kalamassery, Kalamassery, Ernakulam, Kerala 682022, India

[2] Department of Physics, Jamia Millia Islamia, New Delhi 110025, India.

*Corresponding author e-mail: mnrpraveen@cusat.ac.in

Abstract: Carbon Dioxide(CO_2), a notorious green house gas, is a global concern in recent times, whose concentration in the atmosphere is increasing abruptly. In order to mitigate the negative effects of CO_2 and make use of it in a sustainable manner, conversion of CO_2 into useful green fuels is a best choice. Seeking for a good catalysts towards the reduction of CO_2, we observed an intriguing family of non-noble 2D layered materials, Mxenes. It shows excellent performance as an electrocatalyst for heterogenous catalysis such as hydrogen evolution reaction (HER), carbon dioxide reduction reaction (CO_2RR) and so on[1]. Here, in this work, the mechanistic reaction pathway towards the formation of formate by Electrochemical Reduction(ECR) of CO_2 is being carried out on different active sites of vanadium carbide with fully oxygen terminated surface (V_2CO_2), doped with non-metals such as Boron(B) and Nitrogen(N)[2]. This is achieved using Density Functional Theory with BEEF-vdW functional for accurate forecast. The enhancement in the CO_2RR activity is being observed when the V_2CO_2 is doped with heteroatom rather than homo atoms. To achieve high performing electrocatalyst for CO_2 reduction, we studied the reaction pathway of corresponding hydrogenated derivatives of doped V_2CO_2. This work predicts new opportunities for cost effective catalytic materials for CO_2 reduction.

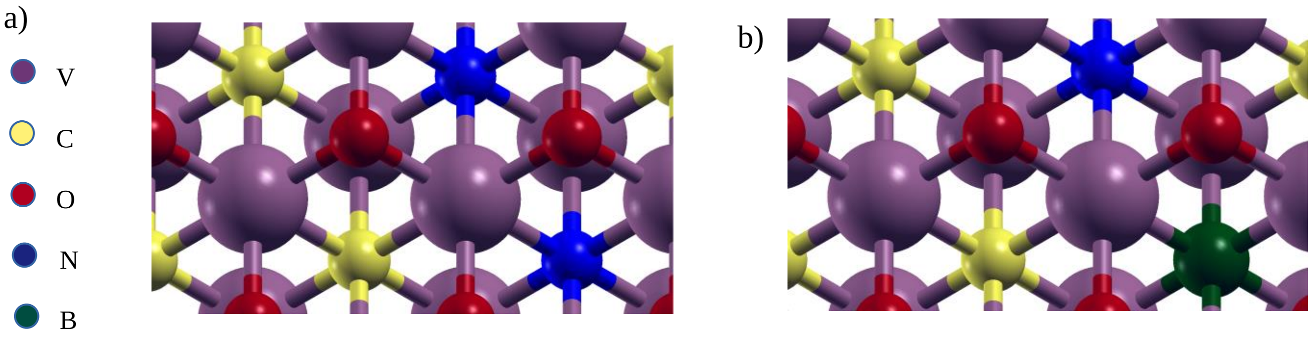

Figure 1: Top view of the a) Homo atoms doped V_2CO_2 (b) Hetero atom doped V_2CO_2

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P-30

Traversing the role of nonpolar surfaces of ZnO in industrial catalysts form CO2 reduction to methanol synthesis: A Periodic DFT Investigation

Meema Bhati[1,2], Shweta Mehta[1,2], Kavita Joshi[1,2*]

[1] Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India.

[2] Academy of Scientifc and Innovative Research (AcSIR), Ghaziabad-201002, India.

Email: m.bhati@ncl.res.in

Abstract: ZnO, a promotor in the catalyst Cu-ZnO/Al2O3, is employed in industrial processes to synthesize methanol from CO2 hydrogenation. Polymorphism of ZnO affects the catalytic performance for methanol synthesis. The low conversion rate of CO2 to methanol is still debatable, and the exact role of ZnO during CO2 hydrogenation still needs to be determined. In this work, we systematically investigated the interaction of carbon dioxide (CO2) and H2 with five nonpolar facets of ZnO by employing periodic density functional theory (DFT). We report the formation of tridentate carbonate and spontaneous dissociation of CO2 on the (1010) facet, whereas bidentate carbonate formation on the (1122) surface. Interestingly, spontaneous dissociation of H2 is observed only on flat facets ((1010) and (1011)) with H2O formation on the 1011)) surface.

Further, we demonstrated CO2 hydrogenation with molecular and atomic hydrogen. CO2 is hydrogenated by atomic hydrogen on the (1122) facet and forms metal carboxyl (MCOOH), an active intermediate for methanol synthesis. In contrast, the physisorption of CO2 and H2 is the only outcome on three facets. The underlying electronic structure is investigated to understand the adsorption behavior of CO2, H2, and H species on the various surfaces of ZnO. Analyzing structural arrangements of ZnO surfaces, Mulliken charges, and pDOS, we establish a correlation between the electron density of ZnO surfaces and the nature of adsorbate(CO2 and H2), explaining the variation in adsorption phenomena. This work suggests that controlling the polymorphism of ZnO doping for structural stability in the industrial catalyst may improve the reaction rate.

Keywords: Density functional theory(DFT), Metal carbonyl (MCOOH), Carbon dioxide (CO2)

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Enhanced Catalytic Activity in Nb-Doped TiO_2 for Electrochemical Oxygen Reduction Reaction

Muhammed Fasil Puthiyaparambath[1] and Raghu Chatanathodi[1]

[1] Department of Physics, National Institute of Technology Calicut, 673601, Kerala, India

Email: fasilmuhammed121@gmail.com

Abstract: TiO_2 has wide applications in catalysis and photocatalysis and is an attractive alternative to Pt or Pt-based catalysts due to its abundance, low cost, and non-toxicity. However, it does not display any worthwhile catalytic activity as far as the Oxygen Reduction Reaction (ORR) is concerned. Attempts have been made to improve the activity of TiO_2 by doping and creating defects on the surface. Nb-doped TiO2 is experimentally found to have good conductivity and electrochemical activity for low Nb concentrations. This work presents a systematic modelling study of how Nb doping influences the ORR activity of anatase TiO_2 using plane wave Density Functional Theory (DFT) method. We elucidate the probable dopant sites, the effect of Nb doping on the oxygen binding capability at active sites, the favored reaction pathway and the transition state. We find a remarkable enhancement in the capability of TiO_2 to catalyze ORR upon doping with Nb. We have also modeled the effect of solvation on the binding of oxygen and other reaction intermediates, using a model where water molecules are added as a monolayer over Nb-doped TiO_2. Solvation introduces additional hydrogen bonding, which improves the binding of intermediates to the active site and lowers activation barriers. Our model for ORR in Nb-doped TiO_2 agrees with recent experimental results on the same.

Keywords: DFT, ORR, Activation barrier, Solvation

P-32

Charge contortion due to bridge oxygen vacancy in SnO_2 lattice manipulate the nature of N_2 adsorption towards a kinetically-driven ammonia electrosynthesis

Ashmita Biswas,[†a] Narad Barman,[†b] Avinash Nambron,[a] Ranjit Thapa,[b,c] Ramendra Sundar Dey*[a]

Abstract: Oxygen vacancy engineering has been a less-explored avenue in the electrochemical nitrogen reduction reaction (NRR). Till date, this field has been superficially investigated for NRR performance of the materials. However, this work concerns the synthesis of oxygen vacancy-engineered SnO_2 displaying a structural transformation owing to in-plane (io_v) to bridge oxygen vacancy (bo_v) dominancy. Resultantly, the electron occupancy of the sp^3d hybrid orbital changed leading to an upshifted valence band maxima towards Fermi level. This has profound effect on the end-on followed by side-on N_2 adsorption and charge-transfer kinetics from active site (site A and B-Sn atoms adjacent to bo_v) to N_2 across the electrode-electrolyte interface, investigated with rotating ring disc electrode (RRDE) technique. The N_2 bond polarization was further arrested by the in-situ ATR-FTIR studies along with the obscured NRR intermediates formed during the alternating NRR mechanism. A restricted hydrogen evolution reaction on Sn-site (favored over O-atoms) results in 48.5% Faradaic efficiency, better than all the literature reports on SnO_2 for NRR. This study thus unveils sufficient insights into the role of oxygen vacancy in the crystal as well as electronic structural alteration of SnO_2 and the identification and distinct role of active site impacting the rate kinetics of NRR.

Keywords: Oxygen Vacancy (In-plane and bridge), adsorption, NRR, Fermi level, Faradaic efficiency.

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A first-principles study of the topological phase in Zintl compound KCd4As3

Nidhi[1*], Ramesh Kumar[1], Mukhtiyar Singh[1#]

[1] Department of Applied Physics, Delhi Technological University, New Delhi, 110042, India

*Email: # mukhtiyarsingh@dtu.ac.in; * kadyannidhi6@gmail.com*

Abstract: Topological materials (TMs) are exotic materials which are insulating in bulk but have exotic metallic states present at their surfaces attracting significant research efforts in condensed matter physics. These materials have potential applications in Spintronics, Quantum computing, Chemical catalysts, and thermoelectric energy harvesting. TMs can be divided into several categories e.g., topological Insulators (TI), topological semimetals (TSM), topological crystalline insulators (TCI) and many more. Time reversal symmetry (TRS) and spin-orbit coupling (SOC) play an important role in TIs. Consequently, inversion in bulk bands is observed at high symmetric points in the bulk Brillion zone which are protected by TRS and inversion symmetry. The calculation of Z 2 topological invariants and surface Dirac cone are used to identify the topological nature of materials. These surface states are doubly protected and do not allow the backscattering in absence of a magnetic field.

In this work, we report the topological phase in the centrosymmetric layered arsenide KCd4As3 using first-principles calculations. It was reported that KCd 4 As 3 exists in a rhombohedral structure with space group (166). This material has a similar crystal structure to experimentally synthesized RbCd4As3 which shows topological character at ambient conditions. We investigated the topological nature of KCd 4 As 3 and identified that this material exhibits a topological non-trivial nature. The Z 2 topological invariants are calculated with the help of product of parities at time reversal invariant momenta (TRIM) points and found of non-zero value. The Surface density of states (SDOS) is also calculated where a Dirac cone is observed near the Fermi level. The existence of topological band inversion and the Dirac cone confirms that KCd4As3 is topologically non-trivial.

Keywords: first-principle calculations, Topological phase, Zintl, SOC, Dirac cone, surface state

P-34

HYST 2.0: Analysis and interpretations of machine learning model trained on an updated database

Nikhil Wilson[1], Piyush Maharana[1], Ashwini Verma[1,2], Kavita Joshi[1,2]

[1] Physical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pashan, Pune-411008,India

[2] Academy of Scientific and Innovative Research (AcSIR), Sector 19, Kamla Nehru Nagar, Ghaziabad, Uttar Pradesh-201002, India

Email: n.wilson@ncl.res.in

Abstract: Hydrogen absorption in metal alloys is a more realistic alternative as storage systems due to its reversible hydrogen storage with high volumetric energy density at ambient conditions.[1] Experimental screening of chemical spaces for different alloy compositions is a herculean task which limits the study of all possible potential alloy compositions. Statistical tools like machine learning helps to reduce the search space to find the best performing alloys. In our previous work [2], we developed HYST (hydrogen storage capacity) model to predict the hydrogen weight capacity of metal alloys as a function of temperature. The majority of the database used consisted of points from HydPark database. In this work, we have updated our database with new points from literature which also consists information about high entropy alloys thus broadening the scope of the model. We also added element's hydriding properties as features and retrained the HYST model. We validated the models predictability on different families of multicomponent metal alloys. The model performs well for all the different families including high entropy alloys with a mean absolute error of 0.32 H2wt% and an R2 score of 0.76. We also predict the hydrogen weight capacity for 6.4 million binary, ternary, and quaternary alloy compositions and compare it to the predictions of our previous model.

Keywords: Solid state hydrogen storage; Machine learning; Metal hydrides

P-35

Effect of Mn Doping on the Electrical Conduction Properties of BiFeO3 Thin-Films

Nilofar Naaz[1], Sruthi Sudhakaran[2], Sanket Goel[3*], Kannan Ramaswamy[1*]

[1] Department of Physics, BITS – Pilani, Hyderabad Campus, Jawahar Nagar, Medchal District, Hyderabad, Telangana 500078, India

[2] School of Physics, IISER Thiruvananthapuram, Maruthamala, Vithura Thiruvananthapuram, Kerala, 695551, India

[3] MEMS, Microfluidics and Nanoelectronics Lab, Department of Electrical and Electronics Engineering, BITS – Pilani, Hyderabad Campus, Jawahar Nagar, Medchal District, Hyderabad, Telangana 500078, India

** Corresponding Authors: kannan@hyderabad.bits-pilani.ac.in; sgoel@hyderabad.bits-pilani.ac.in*

Email: p20200474@hyderabad.bits-pilani.ac.in

Abstract: BiFeO3 (BFO) and Mn-doped BiFeO3 thin films were prepared using spin coating. The optimal concentration of Mn doping to obtain the least leakage current density in BFO thin films was investigated. The FESEM images revealed that the grain size remained constant with increased Mn concentration, and the film deposition was uniform and crack-free. The X-ray diffraction pattern shows that the BFO gets modified from a rhombohedral to an orthorhombic structure on Mn doping. The Goldschmidt tolerance factor (t) displayed a monotonous increase in structural stability with Mn doping. The X-ray photoelectron spectroscopy revealed that Fe exists in Fe2+ and Fe3+ states and Mn exists in Mn3+ and Mn4+ states. The J-V plots showed that the leakage current density decreased by four orders of magnitude from 10-5 A/cm2 for BFO to 10-9 A/cm2 for Mn concentration of 15% by weight. However, a further increase in the Mn doping revealed increased leakage current density. In summary, it appears from these investigations that an optimum concentration of Mn doping in the BFO thin-film matrix is useful for fabricating devices such as solar cells where low leakage current density is desirable.

Keywords: Bismuth ferrite; leakage current, solar cell; thin films

P-36

Water dissociation on (0001) surface of α-Titanium: a first principles investigation.

Pallavi Chame[1], Kyosuke Ueda[2], Takayuki Narushima[2], Ryoji Sahara[3] and Prasenjit Ghosh[1,4]

[1] Department of Chemistry, Indian Institute of Science Education and Research, Pune 411008, India

[2] Department of Materials Processing, Tohoku University, Aoba-ku, Sendai 980-8579, Japan; Research Center for Structural Materials, National Institute for Materials Sc, Tsukuba, Ibaraki 305-0047, Japan

[3] Research Center for Structural Materials, National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan; Department of Materials Processing, Tohoku University, Aoba-ku, Sendai 980-8579, Japan

[4] Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India

Email: chame.pallavi@students.iiserpune.ac.in

Abstract: High strength, low density and corrosion resistance of α-Ti make it an ideal material for jet engines. However, titanium is prone to oxidation at high operating temperatures resulting in of its mechanical properties. Hence, there has been lot of efforts to develop Ti- based oxidation resistant alloys that retain the mechanical properties of Ti. However, for rational designing of such alloys it is important to develop microscopic understanding of the oxidation process. In a recent study by some of the authors of this work, the early oxidation of Ti in presence of different alloying elements were studied using density functional theory (DFT) based calculations.[1] However, under operating condition, there is presence of moisture and hence it is imperative to understand how water vapor affects the oxidation process. Though experimental studies indicate that the presence of water vapor accelerates the oxidation rate of Ti compound, [2-4] there are no mechanistic studies of the process. As a first step towards developing such an understanding, in this work, we have studied dissociation of a water molecule on Ti(0001) surface using DFT based calculations. We find that water prefers to adsorb on the top site. From our nudged elastic band calculations, we have found that the OH bonds of water dissociate sequentially resulting in two H atoms and an O atom bound to the surface. Further, the dissociated H atoms prefer to diffuse from surface to subsurface rather than forming H2 gas.

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Keywords: Ti oxidation, DFT, nudged elastic band

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A Real-Time Study of Charge-Transfer Dynamics in Metal Nanoparticle-Perfluorooctaniod Acid (PFOA) and Degradation of PFOA

P. K. Verma[1,2,*], Samir Kumar Nayak[1,3], Sharma S. R. K. C. Yamijala[1,3,4,5,*]

[1] Department of Chemistry, Indian Institute of Technology Madras, Chennai, 600036 India

[2] Department of Physics, Indian Institute of Technology Madras, Chennai, 600036 India

[3] Centre for Atomistic Modelling and Materials Design, IIT Madras, Chennai 600036, India

[4] Centre for Molecular Materials and Functions, IIT Madras, Chennai 600036, India

[5] Centre for Quantum Information, Communication, and Computing, IIT Madras, Chennai 600036, India

**Email: ic38804@imail.iitm.ac.in, yamijala@iitm.ac.in*

Abstract: Due to their unique properties, Per- and poly-fluoroalkyl substances (PFAS) are used in various places such as fire-fighting foams, non-stick cookware, room-polisher, shampoos, food packaging, and masks, to name a few. But, at the same time, they are very harmful to many species, including humans [1]. Recently, there have been several attempts to dissociate them [1]. However, there is no precise understanding of how to dissociate these forever chemical species efficiently. Plasmon-induced molecular dissociation has received great attention in present times [2]. The underlying mechanism behind this process lies in the charge transfer from metal to the attached semiconductor or molecule via the decay of plasmons into the hot carriers (HCs) (a process known as Landau damping). In our work, we aimed to use the metal nanoparticle plasmons to study the dissociation of one of the PFASs, namely the perfluorooctanoic acid (PFOA). We used the real-time time-dependent density functional theory (RT-TDDFT) [3-4] to study the real-time dynamics of plasmon formation, their decay into HCs, the interfacial charge transfer dynamics, and the subsequent decay of PFOA in the combined systems of Ag55-PFOA and Au55-PFOA. Interestingly, we observed that the direct hot-hole transfer from NP to PFOA competes with the intra-NP excitations. Direct hot-electron transfer from NP to PFOA also occurs with a finite probability. These HC transfers from NP to PFOA could in principle lead to the dissociation of PFOA, which is under investigation. These studies are not only fundamentally important but also will have huge practical implications in the area of degradation of PFAS and other photochemical and photovoltaic applications.

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P-38

Entropy stabilized HfZrNiCoSnSb half-Heusler alloy for thermoelectric application: a theoretical prediction

Rajeev Ranjan[1], Prasenjit Ghosh[1,2]

[1] Department of Physics, IISER Pune, Pashan, Pune, 411008

[2] Department of Chemistry, IISER Pune, Pashan, Pune, 411008

Email: *rajeev.ranjan@students.iiserpune.ac.in*

Abstract: Half-Heusler (hH) alloys are potential thermoelectric materials for use at elevated temperatures because of their high Seebeck coefficient, and superior mechanical and thermal stability. However, their enhanced lattice thermal conductivity is detrimental for thermoelectric applications. One way to circumvent this problem is to introduce mass disorder at lattice sites through mixing of two or more alloys. Such systems are usually stabilized by the entropy of mixing. In this work, using computational tools we propose a mixed hH, namely, HfZrNiCoSnSb which can be formed by mixing ZrNiSn/HfNiSn and HfCoSb/ZrCoSb. We propose that this new compound can be synthesized at high temperatures due to the lowering of its Gibbs free energy because of an increased configurational entropy. Our calculations show that it is a dynamically stable semiconductor with a band gap of 0.61 eV. Its lattice thermal conductivity at room temperature is found to be 5.08 W/mK which is much smaller than those of the parent compounds. The peak value of the figure of merit (zT) of this alloy is found to be 0.99 for the n- type carriers at 1100 K which is 77 % more than the best figure of merit obtained for the parent compounds. For the p-type carriers, the zT value of HfZrNiCoSnSb is 0.87, which is comparable to that observed in parent HfNiSn.

Keywords: Half-Heusler, Thermoelectric materials, Entropy of mixing, Figure of merit,

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First principle studies of novel Mg(NH2)2 and LiH for enhancing kinetics for hydrogen storage along with LiBH4 as additive under the ambient condition

Rakesh Kumar[1,2], Ankita Srivastava[2], Keyur Sangani[3], Nitesh K. Chourasia[4,#], Ritesh Kumar Chourasia[2,*]

[1] University Department of Physics, L.N.M.U., Darbhanga-846004, Bihar, India.

[2] Post-Graduate Department of Physics, Samastipur College, Samastipur-848134 (A Constituent unit of L.N.M.U. Darbhanga-846004), Bihar, India.

[3] Electronics and Communication Engineering Department, Institute of Technology, Nirma University,

Ahmedabad-382481, Gujrat, India.

[4] School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India.

*Email: rakeshphyzics@gmail.com (Presenting Author); niteshphyzics@gmail.com[#];riteshphyzics@gmail.com**

Abstract: In the global quest for sustainable development, hydrogen energy storage is becoming recognized as a key component in reaching clean and sustainable energy solutions. To fulfil the aforementioned need, we have utilized quantum mechanical modelling with the full potential linearized augmented plane waves (FP-LAPW) technique integrated into the WIEN2k code based on the first principle treatment. Magnesium amide [Mg(NH2)2] and Lithium hydride (LiH) are being valued for their high hydrogen storage capacity of 8.2 wt% and 12.6 wt.% hydrogen theoretically which are appealing for uses in hydrogen storage and fuel cell technologies due to their reversible hydrogen absorption and desorption processes. It is critical to create such hydrogen storage materials under an ambient environment with reversible cycling to overcome its unfavorable thermodynamics and kinetics barrier. To enhance the kinetics, we proposed and employed the additive LiBH4,which releases hydrogen at a relatively moderate temperature compared to all other metal hydrides increasing the stability and enhancing the energy storage.

Keywords: Quantum mechanical; Density Functional Theory; Hydrogen energy storage; WIEN2k; Ambient temperature and pressure.

P-40

An ab-initio study of topological phase tuning in Zintl compound RbZn4P3

Ramesh Kumar[1,*], Rajesh Kumar[1], Mukhtiyar Singh[1]

[1] Department of Applied Physics, Delhi Technological University, New Delhi, Delhi 110042, India

Email: ramesh_2k19phdap506@dtu.ac.in

Abstract: Topological phase of matter is becoming increasingly popular after the discovery of topological insulators (TIs). Exploring a topologically trivial material that can be made topologically non-trivial by strengthening spin-orbit coupling (SOC) is quite interesting. The external pressure is a particularly advantageous tool because it has no effect on the system's charge neutrality. Both theoretically and experimentally, numerous types of Zintl compounds including binary, ternary, and quaternary have been investigated. According to first-principles calculations, the structural phase transition leads the topological phase transition in NaCd4As3, which changes it from a topological crystalline insulator (TCI) to a topological insulator (TI). The topological phase transition has been attributed to the breaking of mirror symmetry. RbZn 4P3 have isoelectronic structure with NaCd 4 As 3 but with different space group. Presently, using first-principles calculations, we examined the topological phase characteristics of the ternary Zintl compound RbZn4P3 under the influence of hydrostatic pressure and epitaxial strain. RbZn 4 P 3 shows topological phase transition under hydrostatic pressure of 10.5 GPa and under axial strain of 2% topologically non-trivial phase can be seen. Further, non-trivial phase can be verified with the help of parity table and observed surface states.

Keywords: DFT, topological phase transition, zintl

P-41

Unlocking the Potential of Mo2CO2 MXenes for the Hydrogen Evolution Reaction via Single Atom Doping.

Sai Raj Ali[1], Lekha Nair[1], CS Praveen[2]

[1] Department of Physics, Jamia Millia Islamia, New Delhi 110025, India

[2] International School of Photonics, Cochin University of Science and Technology, University Road, South Kalamassery, Kalamassery, Ernakulam, Kerala 682022, India

Email: rs.sairajdrea@jmi.ac.in

Abstract: The development of sustainable and efficient electrocatalysts for the hydrogen evolution reaction (HER) is paramount for clean energy technologies reliant on water splitting. However, the efficiency of state-of-the-art HER catalysts like Pt is insufficient for wide-scale adoption. In our work, we computationally explore molybdenum carbide MXenes with Oxygen termination (Mo2CO2), as a promising class of earth-abundant HER catalysts. Using density functional theory calculations, we demonstrate that doping Mo2CO2 monolayers with Ir significantly strengthens hydrogen adsorption and improves HER kinetics compared to Pt doping. Modifying the Mo-O-Mo center with an Ir dopant is found to be the optimal configuration, bringing the hydrogen binding energetics closer to ideal values. Further tuning of the composition and architecture of Mo2C materials will likely be required to fully attain Pt-equivalent efficiency. Nonetheless, the insights from this computational investigation provide an important framework and starting point to guide the rational design of Mo2C electrocatalysts with optimized efficiency. Our findings underscore the promise of suitably engineered Mo2C MXenes for enabling scalable and sustainable hydrogen production from water electrolysis.

Keywords: MXene; Hydrogen Evolution Reaction; Density Functional Theory; 2D-Materials

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Non fullerene acceptors with Enhanced Photostability for Organic Solar Cells applications

Sairathna Choppella[1], Sheik Haseena[2], Mahesh Kumar Ravva[1,2,3*]

1 Ph.D. Research Scholar

2 Project assistant-SRF

3 Associate Professor

1,2,3 Department of Chemistry, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

Email: *sairathna_choppella@srmap.edu.in*

Abstract: The development of non-fullerene acceptors (NFAs) with enhanced stability and photovoltaic performance is crucial for the advancement of organic solar cells (OSCs). This study introduces a novel design strategy for fused NFAs (FNFAs) that eliminates the vinylene bridge between donor and acceptor units, a known source of photochemical degradation and photoisomerization. The proposed FNFAs incorporate molecular cores of high- performance acceptors, Y6 (FY6) and ITIC (FITIC), fused with end groups from well- established acceptor units (Im, SN, F, etc.). Density functional theory (DFT) calculations at the LC-whpbe (SRSH)/6-31g(d,p) level in solvent phase reveal promising properties for the designed molecules, particularly those with imidazole end groups (FITIC_Im and FY6_Im).

These molecules exhibit a red-shifted absorption spectrum, a high quadrupole moment, and reduced hole and electron reorganization energies. Molecular dynamics (MD) simulations and DFT calculations of acceptor dimers and DA complexes with D18 as the donor demonstrate highly ordered packing of acceptor dimers and efficient hole and electron transport. Additionally, the study investigates the energetic disorder in the electron affinities of the acceptor molecules. The outcomes of this work suggest that the proposed FNFAs hold promise as stable and high-performance acceptor materials for OSCs.

Keywords: Non-fullerene acceptors; Density functional theory (DFT); Molecular dynamics (MD) simulations; SRSH;

P-43

Computing accurate bond dissociation energies of emerging per- and polyfluoroalkyl substances: Achieving chemical accuracy using connectivity-based hierarchy schemes

Per- and polyfluoroalkyl substances (PFASs) are a group of chemical compounds with several industrial applications, and they have been widely used since the 1950s. The widespread usage of PFASs in various industries stems from the fact these molecules possess the strongest organic bond, namely, the carbon-fluorine (C–F) bond. Despite their widespread usage, unfortunately, PFASs are pretty dangerous to all forms of life, including humans. Diet and drinking water are the primary routes of human exposure to PFASs. In recent years, the environmental persistence of PFASs and their biomagnification in food webs have generated significant interest in degrading these substances. However, the presence of strong C–F bonds makes their degradation extremely difficult. Since finding accurate bond dissociation energies (BDEs) of different carbon-fluorine bonds in PFASs would help to find feasible degradation pathways, in this work, we propose to calculate the BDEs of hundreds of PFASs at near chemical accuracy (~ 1 kcal/mol). However, there is only limited experimental data on the PFAS BDEs, and there are uncertainties associated with the BDEs computed using density functional theory. Although quantum chemical methods like the G4 composite method can provide highly accurate BDEs (< 1 kcal mol-1), they are limited to small system sizes. To address DFT's accuracy limitations and G4's system size constraints, we examined the connectivity-based hierarchy (CBH) scheme and found that it can provide BDEs that are reasonably close to the G4 accuracy while retaining the computational efficiency of DFT. To further improve the accuracy, we modified the CBH scheme and demonstrated that BDEs calculated using it have a mean-absolute deviation of 0.7 kcal mol-1 from G4 BDEs. To validate the reliability of this new scheme, we computed the ground state free energies of seven PFAS compounds and BDEs for 44 C–C and C–F bonds at the G4 level of theory. Our results suggest that the modified CBH scheme can accurately compute the BDEs of both small and large PFAS at near G4 level accuracy, offering promise for more effective PFAS degradation strategies.

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P-44

Exploring the Thermoelectric Potential of CsGaSb 2 Zintl Phase Compound: A Computational Study

Sangeeta[1], Rajesh Kumar[2], Mukhtiyar Singh[3]

[1] Department of Applied Physics, Delhi Technological University, Delhi, 110042, India

Email: sangeetadhull_2k20phdap02@dtu.ac.in

Abstract: Thermoelectric (TE) materials have attracted significant attention for their potential in converting waste heat into useful electrical energy, holding promise for various energy harvesting applications. Achieving high TE performance of a material requires a high power factor and a low thermal conductivity. The recent discovery of antimonide based Zintl phase compounds has prompted exploration in the search of high-performance TE materials, as they exhibit phonon-glass electron-crystal behaviour. Thus, the present study systematically examines the transport properties of a ternary antimonide Zintl phase CsGaSb 2 , which crystalizes in the tetragonal structure, using first-principles calculations in conjunction with Boltzmann transport theory. Our computed structural parameters, agree well with the available experimental reports, authenticating the robustness of our theoretical framework. This compound is found to be thermodynamically and mechanically stable. CsGaSb 2 is found to be direct band gap semiconductor employing Tran Blaha modified Becke Johnson functional. We propose a strategy to improve the power factor and TE performance by optimizing carrier concentration. The high power factor and low thermal conductivity, resulting in high figure of merit of the investigated compound. Thus, the present study may provide valuable insights in exploring the effect of carrier concentration on transport properties of Zintl phases and their prospective energy harvesting applications.

Keywords: Thermoelectric material; Zintl compounds; First-principles; Figure of merit

P-45

Role of framework flexibility and local cationic environments on oxide ion transport in Sr-doped LaFeO3

Sanjib Ray[1], P. Padma Kumar[1]

[1] A Department of Physics, Indian Institute of Technology Guwahati, Guwahati, 781039, Assam, India

Email: sray@iitg.ac.in

Abstract: Sr-doped LaFeO 3 is a promising mixed ionic electronic cathode material for IT-SOFC. Classical molecular dynamics simulation is employed to study La 1-x Sr x FeO 3-δ at 1200 K for a range of dopant concentration (x=0.1-0.6). Having established the structural stability of the system, we dive in to understand the mechanism of oxide ion transport in these systems. Microscopic energy barriers of oxide ion diffusion between its two nearest sites are calculated and are found to be in agreement with observed conductivity behavior. The effect of Sr-dopant on the gross nature of oxygen diffusion is also studied.

Keywords: Perovskites ; Fuel Cells ; Molecular dynamics

P-46

Bond Exchange Mechanism Drives Volmer-Tafel route and Electronic Descriptor to Predict HER Activity of Borophene

Erakulan E. Siddharthan[1], Sourav Ghosh[1], Ranjit Thapa[1,*]

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

*Corresponding Author email: ranjit.t@srmap.edu.in

* Presenting Author email: sourav_ghosh@srmap.edu.in

Abstract: Hydrogen is considered an excellent alternative to fossil fuels because it is a clean and versatile energy carrier. It can be produced from a variety of sources, such as water and renewable energy, and when used in fuel cells, it only emits water vapor as a byproduct, making it an environmentally friendly option. The electrocatalytic hydrogen evolution reaction (HER) plays a crucial role in the production of hydrogen through water electrolysis. In HER, an electrochemical process occurs at the cathode, where water molecules are split into hydrogen ions (H+) and electrons (e^-). These hydrogen ions then combine to form hydrogen gas (H2). Understanding the complete reaction that aligns with experimental results has been a longstanding challenge in the field, lacking a comprehensive theoretical solution. In this work, the Volmer-Tafel (V-T) pathway is investigated on borophene sheets utilizing Density Functional Theory (DFT) as a computational method. The study demonstrates that the hydrogen (H2) evolution occurring in the Tafel step exhibits a lower activation energy due to bond-exchange mechanism. This finding suggests that H2 evolves through this mechanism, challenging the existing model that assumes direct H2 evolution. This is proven to work in other HER catalysts such as nitrogen-doped graphene, 2H-MoS2 and Pt(111) as well. A descriptor, Bader charge 2 /p z at E F 2 (Ep z) is also proposed that shows better correlation towards HER activity on the borophene sheets.

This research provides valuable insights into the theoretical modeling of the hydrogen evolution reaction (HER), offering improved methods for understanding the underlying mechanisms of the reaction. The proposed descriptor can be further investigated for its applicability to other boron allotropes and similar reactions, expanding our understanding of these systems.

DFT, HER, Bond-exchange mechanism, Borophene

The Impact of Strain on the Thermoelectric Properties of HfNBr Monolayer: A First- Principles Study

Stephen Shaiju Mathew[1], Sangeeta[1], Mukhtiyar Singh[1,*]

[1] Department of Applied Physics, Delhi Technological University, Delhi, India, 110042

Email: Stephensmathew07@gmail.com

Abstract: Two-dimensional (2D) materials have garnered significant interest and research due to their unique properties and potential for thermoelectric (TE) energy harvesting. Most of the investigated compounds for TE applications are binary and exhibit isotropic behavior. Here, in this study, we investigate the TE properties of ternary transition metal halide HfNBr monolayer under varying strain using first-principles calculation in conjunction with semiclassical Boltzmann transport theory. We examined the impact of uniaxial compressive and tensile strain on the electronic, mechanical and transport properties of the HfNBr monolayer. We focused on the orthorhombic form of HfNBr, exhibiting the anisotropic transport properties. HfNBr is found to be an indirect band gap semiconductor by employing the Heyd-Scuderia-Ernzerhof (HSE06) exchange-correlation functional. Due to its layered structure, HfNBr exhibits highly anisotropic values of Seeback coefficient, electrical and thermal conductivity. A high power factor and low thermal conductivity of the investigated monolayer is obtained via strain engineering. This contributes a reasonably high thermoelectric figure of merit (ZT), making HfNBr very promising in thermoelectric energy harvesting. Thus, the present study may provide valuable insights in exploring the impact of compressive and tensile strain on the transport properties of ternary transition metal nitrides and their prospective energy harvesting applications.

Keywords: Thermoelectric figure of merit ; Monolayer ; Electronic properties ; Transport properties

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Efficient Water–Gas shift catalysts for H2O and CO dissociation using Cu–Ni step alloy surfaces

Sudipta Roy[1], Ashwani K. Tiwari[2]

[1] Department of Physics, IISER Pune, Pashan Pune, Maharashtra 411008, India

[2] Department of Chemical Sciences, IISER Kolkata, Mohanpur, West Bengal 741246, India

Email: sudipta218@gmail.com

Abstract: Density functional theory (DFT) has been used to study H 2 O and CO dissociation on a series of step (211) bimetallic alloy surfaces consisting of Cu and Ni metals. The water dissociation process was seen to be more facile on (211) step surfaces than on (111) flat surfaces. But CO dissociation on the (211) step surfaces was less reactive than that on its close-packed (111) counterparts. Depending on the initial-state structures, the transition states for H2O dissociation were located at different sites available on a (211) step surface. The introduction of Cu atoms on a bare Ni(211) surface (Ni-based alloy) reduces the reactivity of H2O dissociation, whereas the introduction of Ni atoms on a bare Cu(211) surface (Cu-based alloy) increases the reactivity. Different surface-based properties such as surface energy, work function, d-band center energy, and H adsorption energy were calculated and qualified as descriptors for H2O dissociation on the alloy surfaces. The transition state toward a given dissociation pathway is modified by the motion of top-layer lattice atom over which H2O gets adsorbed. The effect of surface temperature on the reactivity, which has been calculated using semiclassical methods, showed that the reactivity increased with surface temperature on all of the alloy surfaces. C2 dimer formation, the first step of coke formation on any catalyst surface, was less reactive for Cu-based alloy surfaces. Overall, considering all of the aspects of H2O and CO dissociation and C2 dimer formation, Cu-based (211) step alloy surfaces showed improved performance as the WGS reaction catalyst.

Keywords: WGS; DFT; Semi-classical Tunneling; Step Surfaces.

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Understanding Ammonia Gas Sensing Mechanism in n-Type Conducting Polymer

Sushri Soumya Jena[1], Sonu Sunny[1], Mohit Garg[1], Sarbani Ghosh[1,*]

[1] Department of Chemical Engineering, Birla Institute of Technology and Science, Pilani,
Rajasthan, 333031 India

Email: p20210013@pilani.bits-pilani.ac.in

Abstract: Conducting polymers (CP) have gained significant attention in gas sensing due to their flexibility, ease of processing, and low-temperature operation. However, the most commonly used chemo-resistive sensors are based on p-type conducting polymers when it comes to sensing the reducing gas such as ammonia (NH 3), the conductivity decreases, and they often suffer from inherent limitations of selectivity, stability, and sensitivity. Here we report an n-type conducting polymer, i.e., benzimidazobenzophenanthroline (BBL), for NH 3 sensing studied using density functional theory (DFT) and molecular dynamics (MD) simulations to unravel the mechanism of NH 3 sensing. In gas sensing, the most common mechanism is the adsorption of a gas by the polymer, followed by a redox reaction. First, we calculated the adsorption energy and the charge transfer states of NH 3 on BBL using DFT. Next, we studied the redox reaction of NH3 , which shows BBL can be reduced by NH 3, leading to the change in (opto)electronic properties. We have also investigated the diffusion coefficient of the gas molecule using MD simulations, as it plays a crucial role in influencing the sensitivity of the sensor. We found that the adsorption and diffusion of NH 3 take place in the void spaces inside the films without affecting the crystallinity of the BBL, which suggests the conductivity and, eventually the sensitivity will not decrease. These characteristics of BBL polymer studied from DFT and MD simulations suggest that it is a promising candidate material to be used as an active material of room-temperature NH3 sensor.

Keywords: Gas Sensor; Conducting Polymer; Density Functional Theory; Molecular Dynamic; Redox Reaction

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Applicability of Polyurethane Foam Filled Thin-Walled Composite Columns in Structural Engineering

Mahesh Kumar Tangudupalli[1], Nishant Sharma[1]

[1] Department of Civil Engineering, SRM University – AP, Amaravati 522502, Andhra Pradesh, India

Email: maheshkumar_tangudupalli@srmap.edu.in

Abstract: The remarkable mechanical properties and low density of polyurethane makes its usage an integral component in several modern-day world applications. Polyurethanes have made significant contributions to our daily lives, whether it is through leisure pursuits such as sports or through energy conservation. Specifically, in the automotive sector, foam-filled thin-walled composite tube members are frequently used to protect vehicles against impact or sudden loads and to reduce the weight of the vehicles. In the field of structural engineering also, one of the major objectives is associated with designing light weight structural members with adequate strength. One way by which this can be fulfilled is by designing the members as concrete-filled tubular (CFT) columns rather than as conventionally utilized RC members. This approach, although, can reduce the weight, however, it may not provide high strength-to-weight ratios in the members. Therefore, it is worth exploring sustainable options to achieve a further reduction in weight without significantly compromising on strength, and thereby achieve high strength-to-weight ratios. Polyurethane foam is one such material that could be utilized in place of CFT columns for achieving the same. The present study investigates, numerically, the capability of Polyurethane Foam Filled Thin-Walled Composite (PUFTW) Columns in exhibiting similar structural action compared to the CFT columns. Pushdown analysis in carried out to evaluate the strength and failure characteristics of PUFTW Composite Columns. Based on the results, the applicability of PUFTW Columns in structural engineering is discussed.

Keywords: Polyurethane; Foam-filled; Thin-walled columns; Composite

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Enhancing Photochemical Reactivity and Large Solar Thermal Energy Storage with Polycyclic Heteroaromatic π-Linkers in Dithienylethene Molecular Switches

Thillaiarasi S[1], D. Sravanakumar Perumalla[2], Baswanth Oruganti[1,*] and Bo Durbeej[2,*]

[1] Department of Chemistry, SRM University – AP, Andhra Pradesh, India.

[2] Division of Theoretical Chemistry, Linkoping University, Sweden.

E.mail: thillaiarasi_s@srmap.edu.in

Abstract: Dithienylethene photoswitches, featuring an aromatic π-linker connecting two thiophene units, give interesting results for advancing Molecular Solar Thermal energy (MOST) storage technologies.[1-3] Their inherent aromaticity in the ring-open state enhances energy storage densities when transitioning to the ring-closed form via photoinduced electrocyclization (photocyclization) reactions.[4,5] However, this often results in unfavorable low barriers for thermal cycloreversion reactions. The present work utilized computational methodologies to propose a solution by employing polycyclic heteroaromatic π-linkers. Moreover, this work demonstrates that by fine-tuning the aromatic characteristics of individual rings within the π-linker, such as indole or isoindole, it is feasible to strike a delicate balance that simultaneously achieves high energy-storage density and substantial cycloreversion barriers. Additionally, this design facilitates a rapid and efficient photocyclization reaction, owing to the emergence of excited-state antiaromaticity in the π-linker upon absorption of light by the ring-open form. Dithienylethenes incorporating polycyclic heteroaromatic π-linkers exhibit promising thermal and photochemical properties, rendering them suitable candidates for further development in Molecular Solar Thermal energy (MOST) systems.

Keywords: Heterocycles, Molecular dynamics, Molecular photoswitches.

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Impact of ball milling duration, phase transformation and processing on the thermoelectric performance of Cu2Se

M Uday Kumar[1,2], R Swetha[1,2], B V Sahana[1,2], Ramappa S Kuri[1,2,3], Bogdan Popescu[4], Ilhame Assahsahi[d] and Latha Kumari[1,5]

[1] Department of Physics, B.M.S. College of Engineering, Bull Temple Road, Bengaluru-560019, India

[2] Department of Physics, Mangalore University, Mangalagangothri-574199, India

[3] Department of Physics, Government First Grade College, Bagalkot-587103, India

[4] National Institute of Materials Physics, Atomistilor Street 405A, Magurele, Ilfov 077125, Romania

[5] BSN Centre for Nano-Materials and Displays, B.M.S. College of Engineering, Bull Temple Road, Bengaluru 560019, India

Email:udaykumarm@bmsce.ac.in

Abstract: In the present work, the effects of ball milling duration and sintering on the thermoelectric properties of bulk Cu2Se were investigated. The X-ray diffraction (XRD) analysis confirms that ball-milled powders show phase transformation with increasing milling duration. The XRD results also reveals that ball-milled powders for 2 h show the mixed phases of Cu3Se2 and Cu2Se. On further increasing the ball milling duration (5 h and 10 h), the β-cubic Cu2Se phase was obtained. Also, ball milling duration was correlated to the formation of microstructure, and was confirmed by Scanning electron microscopy (SEM) analysis. The powders were consolidated into dense pellets by Spark Plasma Sintering (SPS). The SPS sample indicates that the β-cubic Cu2Se phase is transformed to the α-monoclinic Cu2Se phase. The electrical conductivity of all samples decreased with increasing temperature, indicating a heavily doped semiconducting nature, and the positive sign of the Seebeck coefficient shows p-type conduction. The maximum Seebeck coefficients of 133 μV/K, 129 μV/K and 136 μV/K were obtained for samples milled at 2, 5 and 10 h, respectively. The highest power factor of 838 μWm -1 K-2 was achieved at 823 K for 10 h sample. Cu2Se ball-milled samples were expected to show better thermoelectric performance with controlled sample processing.

Keywords: Cu 2 Se; Ball milling; Spark Plasma Sintering; Seebeck coefficient; Power factor.

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Temporal Evolution of Avalanches in the Fiber Bundle Model of Disordered Solids

Narendra Kumar Bodaballa[1], Soumyajyoti Biswas[1], Parongama Sen[2]

[1] Department of Physics, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

[2] Department of Physics, University of Calcutta, Kolkata 700 009, India

Email: narendrakumar_b@srmap.edu.in

Abstract: In this study we analyze the evolution of avalanche shapes in the fiber bundle model, which simulates failure processes in materials. Here, two loading mechanisms namingly discrete (fixed loading components) and quasi-static (single fiber failure triggering) are followed. Analyzing the asymmetry of the avalanche shapes over time, measured by a specific metric (A), we find that under quasi-static loading type, the shapes initially lean leftwards but become symmetrical as the system approaches critical breakdown. This follows a universal scaling law, $A \sim (\sigma_c - \sigma)^{\frac{1}{4}}$, independent of the internal threshold distributions of the system. This makes it possible to use this asymmetry measure as tool for indicator of imminent failure. Whereas in discrete loading, it is always asymmetric. We also try to show a case where the loading mechanism was varied over a interaction range, which results seems to be qualitatively similar.

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Prediction of imminent breakdown using Gini and Kolkata indices

Diksha[1], Soumyajyoti Biswas[1]

[1] Department of Physics, SRM University - AP, Andhra Pradesh - 522502, India

Abstract: Prediction of an imminent catastrophic event in a driven disordered system is of paramount importance—from the laboratory scale controlled fracture experiment to the largest scale of mechanical failure, i.e., earthquakes. It has long been conjectured that the statistical regularities in the energy emission time series mirror the "health" of such driven systems and hence have the potential for forecasting imminent catastrophe. Among other statistical regularities, a measure of how unequal avalanche sizes are is potentially a crucial indicator of imminent failure[1,2,3,4,5]. The inequalities of avalanche sizes are quantified using inequality indices traditionally used in socioeconomic systems: the Gini index g, and the Kolkata index k. In this work, we outline a framework that can give a precursory signal of imminent failure by monitoring the variations in sizes or the inequality of the intermittent responses of a system seen before the failure point. The crossing point of these two indices serves as a precursor to imminent breakdown. Given a scale-free size distribution of the responses, we calculate the expressions for these indices, evaluate their crossing points, and give a recipe for forecasting imminent breakdown. We compare these with simulation results from the Fiber Bundle Model, BTW Model, and Manna model with variable interaction strength and lab scale fracture experiment results from the different charcoal samples. The results also explain previously observed near-universal values of Gini and Kolkata indices in self-organized critical systems.

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[5] Diksha, G. Eswar, Soumyajyoti Biswas, Prediction of depinning transitions in interface models using Gini and Kolkata indices, arXiv:2310.03682 (2023).

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Abstract: Understanding the dynamics of driven interfaces through disordered media is crucial for various systems, ranging from fracture in materials to fluid invasion in porous media. The depinning transition, a critical phenomenon, marks a transformative point for these systems. In this work, we propose a novel framework leveraging supervised machine learning to predict the onset of depinning transitions. Our approach involves monitoring variations in the sizes and inequality of intermittent responses preceding the depinning point. Drawing inspiration from economic inequality measures, specifically the Gini index and the Kolkata index, we identify a precursor to imminent depinning— the crossing point of these indices. This serves as a valuable signal of the depinning transition To validate our framework, we apply it to simulations of different interface dynamics models, including Edwards-Wilkinson, KPZ, and the Fiber bundle model with variable interaction strength. The results demonstrate the universality of our approach, making it applicable to a broad range of systems undergoing depinning transitions. We focus on understanding the importance of "g" and how this significance varies with "γ," while also exploring system size dependence and the impact of an increased training set using supervised machine learning. This research contributes not only to the understanding of depinning transitions but also underscores the broader applicability of machine learning in predicting critical phenomena in diverse systems. Our work stands at the intersection of physics, machine learning, and predictive modeling, offering valuable insights for researchers across disciplines.

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Understanding the effect of alignment interaction on spatio-temporal patterns in a active matter system.

Ravitheja Kandalam[1], Dr. Supravat Dey[1,*]

[1] Department of Physics, SRM University – AP, Amaravati 522502, Andhra Pradesh, India

Email: ravitheja_Kandalam@srmap.edu.in

Abstract: Active matter systems such as school of fish, flock of birds or living tissues can show remarkable phase transition like phenomenon from disordered to ordered state through interactions with neighbors. Contact inhibition of locomotion (CIL) is a fundamental process in cell-cell interactions and plays a crucial role in biological phenomena such as wound healing, cancer metastasis, tissue development etc. Similar to Vicsek model, we simulate the effect of CIL by modeling the cells as self-propelled disks which obey overdamped Langevin dynamics in crowded environment. We update the positions and orientations of cells through computer simulations using the mathematical model we designed. This kind of alignment interaction shows many interesting spatio-temporal patterns whose dynamics we would like to discuss as a poster presentation in the conference.

Keywords: Contact Inhibition of locomotion; Alignment interaction; Collective behaviour.

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Fracture Networks: Topology, Geometry and Evolution

Ruhul Amin Ibne Haque 1,2

[1] Physics Department, St. Xavier's College, Kolkata 700 016, India

[2] Condensed Matter Physics Research Centre, Jadavpur University, Kolkata 700032, India

Abstract: The space of planar surface fracture networks is mapped into a four-parameter mathematical space, summarizing the average topological connectivity and geometrical properties of a network idealized as a convex polygonal mesh. The four parameters are identified as the average number of nodes and edges, the angular defect with respect to regular polygons, and the isoperimetric ratio. The map serves as a low-dimensional signature of the fracture network and is visually presented as a pair of three-dimensional graphs. A systematic study is made of a wide collection of real crack networks for various materials, collected from different sources. To identify the characteristics of the real materials, several well-known mathematical models of convex polygonal networks are presented and worked out. These geometric models may correspond to different physical fracturing processes. The proposed map is shown to be discriminative, and the points corresponding to materials of similar properties are found to form closely spaced groups in the parameter space. While most desiccation crack mosaics in nature were Gilbert-like, there were crack mosaics that started from Gilbert-like and finally equilibrated to Voronoi-like patterns, such as columnar joints. Here, molten volcanic lava, by the sea, cools and cracks under appropriate thermal and elastic conditions, causing the crack system to grow downward, creating long, vertical columns with polygonal cross-sections. As the columns grow downward to lengths of several meters (in natural systems), their outline continuously changes, and the center may shift, causing the column to twist. The trajectory of the columnar joint systems in the four-parameter space is found to depend on the crack seed distribution and crack orientation. An empirical relationship between the system energy and the crack mosaic shape parameter λ has been proposed based on principles of fracture mechanics.

Keywords: crack geometry, tessellation, 3-dimensional cracks, dynamics, energy minimization

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Critical scaling through Gini index

Soumyaditya Das[1] and Soumyajyoti Biswas[1,*]

[1] Department of Physics, SRM University - AP, Andhra Pradesh - 522502, India

Email: soumyaditya_das@srmap.edu.in

Abstract: In the systems showing critical behavior, various response functions have a singularity at the critical point. Therefore, as the driving field is tuned toward its critical value, the response functions change drastically, typically diverging with universal critical exponents. We can quantify the inequality of response functions with measures traditionally used in economics, namely by constructing a Lorenz curve and calculating the corresponding Gini index. The scaling of such a response function, when written in terms of the Gini index, shows singularity at a point that is at least as universal as the corresponding critical exponent. The critical scaling, therefore, becomes a single parameter fit, which is a considerable simplification from the usual form where the critical point and critical exponents are independent. Another measure of inequality, the Kolkata index, crosses the Gini index at a point just prior to the critical point. Therefore, monitoring these two inequality indices for a system where the critical point is not known can produce a precursory signal for the imminent criticality. This could be useful in many systems, including that in condensed matter, bio- and geophysics to atmospheric physics. The generality and numerical validity of the calculations can be verified with the Monte Carlo simulations of the two-dimensional Ising model, site percolation on square lattice, and the fiber bundle model of fracture.

Keywords: Gini index, critical scaling, universal critical exponent, Ising model .

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Viscoelastic effect on oscillation and synchronization of biological oscillators

Subhajit Gupta[1], Supravat Day[1]

[1] Department of Physics, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

Email: subhajit_g@srmap.edu.in

Abstract: When it comes to biological transportation, such as mucociliary transport, synchronized beating among a group of cilia is crucial. Biological fluids where such collective movements occur are mostly viscoelastic. Past studies mainly consider the fluid purely viscous, and the effect of viscoelasticity on synchronized oscillations is unclear. Viscoelasticity can create a delayed response in the dynamics, which is absent in the purely viscous fluid. We investigate the synchronization between two oscillators using a toy model that only takes care of the time delayed response and we also discuss the effect of noise. The rower model is one of the simplest models which is experimentally realized by an oscillatory motion of a colloid driven by an external force to study synchronization due to hydrodynamic coupling. Previously it was shown that assuming purely viscous medium two rowers establish an anti-phase synchronization. Considering different type of memory effect in the coupling, our study shows that two rowers can oscillate with in-phase synchronization. We also investigate the robustness of synchronization phenomenon in the presence of noise.

Keywords: Oscillation; Hydrodynamic Synchronization; viscoelasticity

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Studying the final values of inequality indexes for creep ruptures using the fiber bundle model

Tarun Ram Kanuri[1], Subhadeep Roy[2], Soumyajyoti Biswas[1]

[1] Department of Physics, SRM University – AP, Amaravati, Andhra Pradesh, India

[2] Department of Physics, BITS Hyderabad, Telangana, India

Email IDs: tarun_kanuri@srmap.edu.in, soumyajyoti.b@srmap.edu.in, subhadeep.r@hyderabad.bits-pilani.ac.in

Abstract: Disordered solids, even when loaded below their critical strengths, can fail due to long-term structural degradation or creep ruptures if exposed to external noises such as temperature. The Fiber Bundle Model (FBM) is a generic model to study fractures of disordered material under stress. We studied the creep behavior appearing in the FBM while exposed to external (thermal) noise. Inequality indexes such as the Gini index and Kolkata index proved to be good indicators for failure time forecasting. We investigated the relationship between the final values of the Gini index and Kolkata index and applied load and temperature in creep statistics. We calculated the theoretical final values for the Gini index and the Kolkata index and compared them with simulations. We also compared the predictivity of rule-based predictions with that of inequality indexes.

Keywords: Fiber Bundle Model; Creep behavior; Fractures; Disorder; Critical phenomena; Statistical Physics

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Critical crack length during fracture

Viswakannan R. K.[1,*], Subhadeep Roy[1]

[1] Dept. of Physics, Birla Institute of Technology and Sciences Pilani, Hyderabad Campus,
Secunderabad 500078, Telangana, India.

* Email: p20230074@hyderabad.bits-pilani.ac.in

Abstract: We have studied a statistical heterogeneous media [1] to understand the relation between the critical crack length and nominal stress during a failure process and how such a correlation is affected by two main parameters that dictate the nature of a failure process: (i) the strength of disorder and (ii) the range of stress relaxation - the former controls the failure abruptness [2] while the latter is responsible for spatial correlation during crack propagation [3]. Through controlled numerical simulation in a one dimensional fiber bundle model [4], a statistical model guided by threshold activated dynamics, we have explicitly showed an inverse relation between critical stress and critical crack length where the distribution of critical crack length exhibits a gamma distribution with its mode being a function of both the disorder and the dimension of the medium. Finally, a phase diagram on the 'disorder vs stress relaxation range' plane demarcates between a region where the largest crack is the most vulnerable one vs where they differ from one another.

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Keywords: disordered systems, avalanches, fracture, fiber bundle model, critical crack length, nominal stress.

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Dynamics of path opening during multi-phase flow: Rheological study in capillary fiber bundle model.

Anjali Vajigi[1], Subhadeep Roy[1]

[1] Department of Physics, Birla Institute of Technology and Science, Hyderabad Campus,

Secunderabad 500078.

Email: 2023proj055@hyderabad.bits-pilani.ac.in

Abstract: The knowledge of multi-phase flow has relevance to a wide variety of different systems in the industrial, geophysical, and medical sectors [1, 2]. Recently it has become a main interest from the point of view of theory, simulations, and experiments as well as to understand its various applications, such as bubble generation in microfluidics, blood flow in capillary vessels, catalyst supports used in the automotive industry, transport in fuel cells, oil recovery, groundwater management, and CO2 sequestration. Such studies deal with the flow of bubble trains in different types of systems, ranging from single capillaries to more complex porous media. In this work, we have adopted a 1D prototype for multi-phase flow in porous media, the capillary fiber bundle model (CFBM), to understand its rheology. CFBM has been explored in earlier literature [3] briefly discussing the influence of path-opening dynamics on effective rheology (pressure gradient vs flow rate) during a steady-state flow. A similar notation of such path- opening dynamics has been presented earlier by Talakstad et al. [4] in 2D porous media. In 1D due to less complexity, it's much more convenient to keep track of the flowing channels. Here we explicitly demonstrated that by disjoining the contribution of existing paths and newly opened paths we can understand these dynamics more clearly. The flow rate then can be split into two parts: Darcy flow [5] through the existing path multiplied by the number of active paths. Through a controlled numerical simulation, it is possible to show the contribution of each element separately.

Keywords: Effective Rheology; Multi-Phase Flow; Disordered Porous Media; Capillary Fiber Bundle Model (CFBM); Path Opening Dynamics.

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Electronic transport across the Radial π-conjugated Molecules

Sneigitha G[1] and Sabyasachi Mukhopadhyay[1]

[1] Department of Physics, SRM University-AP, Andhra Pradesh, India - 522240

Abstract: Molecules exhibiting radial π-conjugation, contrasting the more conventional linear π-conjugation, have garnered significant interest in recent years. Phenylene ethynylene macrocycles and Pico tubes stand as notable examples, yet their synthesis often involves laborious multistep routes with low yields. To address this, alternative synthetic methodologies have emerged, incorporating new arylene units to form belt-like structures. Oligothiophenes, polythiophenes, and thiophene-phenylene hybrids exemplify such approaches, leveraging the self-assembling nature of π-conjugation to tailor material properties [1]. While linear π-conjugation characterizes thiophene-based materials, cyclic π-conjugated compounds also play a vital role[2]. In our theoretical exploration, we investigated the charge transport properties of macrocycles integrating 2,5-dihydropyrrolo[3,4-c] pyrrole-1,4-dione, benzo[c][1,2,5]thiadiazole, thiophene, and benzene molecular units, denoted as CDPPN2, CpolyBDTN2, CpolyBTBCN2, CpolyIDTBD2, and CpolyPTN2. Employing Density Functional Theory with Non-Equilibrium Green's Function (DFT-NEGF) methodology, our findings unveil their manifestation of negative differential resistance. This behavior in the current-voltage characteristics (I-V) was elucidated through the evolution of the transmission spectrum with the projected density of states under applied bias.

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Quantitative estimation of the thermodynamic and kinetic properties of the Cytoskeletal protein- inhibitors interaction employing molecular dynamics simulation

Anuj Kumar[1], Debabrata Pramanik[1,2]

[1] Department of Physics, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

[2] Centre for Computational and Integrative Sciences, SRM University – AP, Amaravati 522 502, Andhra Pradesh, India

Email: anuj_kumar@srmap.edu.in

Abstract: Cytoskeletal proteins make a dynamic and sophisticated network of protein filaments within the cell. These protein filaments help cells to spatially organize the organelles, transport cargo materials, and deliberate cell motility. Actin and MreB are well-known globular shaped cytoskeletal proteins primarily found in eucaryotic cells and rod-shaped bacterial cells. Inhibiting these proteins by small chemical molecules can affect the functionalities and in turn various cell activities. Therefore, understanding the structural, thermodynamic, and kinetic properties of these protein – ligand systems is very useful from biological perspectives. One such important MreB inhibitor is A22 (S-(3, 4-dichlorobenzyl) isothiourea). Since Eukaryotic Actin is structurally analogue to bacterial MreB, we first investigate the effect of A22 inhibitor on the Actin protein. Using all-atom classical molecular dynamics simulation and enhanced sampling techniques, we explored binding affinities of A22 with these proteins and their dominant interactions at the binding site. For MreB and A22, crystal structure is available in literature. However, for MreB homologue, till now there is no crystal structure available in the literature. Since finding out the important binding pockets are important to study its interaction with ligands, we used computational tools to predict the binding site/s of Actin protein suitable for A22 molecule. We perform molecular docking to get initial binding pockets for A22 in Actin. Later, we performed all-atom molecular dynamics simulation to calculate the key interactions and interacting residues, responsible for protein-ligand binding. Employing the well-tempered metadynamics, we compute the free energy profile of A22 unbinding from different binding pockets of Actin. Insights of structural and dynamical properties of protein and ligand binding will help us in discovery and development of therapeutic drugs for cytoskeletal proteins. It will also shed some light towards the understanding of the mechanism of protein assembly and disassembly processes to form protein filaments.

Keywords: Cytoskeletal Proteins; Molecular Dynamics; Well-Tempered Metadynamics; Actin/MreB