NATIONAL CONFERENCE

COMPUTATIONAL & DATA-DRIVEN ADVANCED MATERIALS (CDAM)

Book of Abstracts

April 7-8, 2026

CSIR-Central Glass & Ceramic Research Institute

Kolkata

Book of Abstracts

National Conference

Computational and Data-Driven Advanced Materials

CDAM 2026

April 7–8, 2026

Organized by

CSIR-Central Glass and Ceramic Research Institute, Kolkata

KEY TOPICS

Multi-scale Modeling of Materials

High-throughput Computational Screening

Data-Driven & AI-Based Materials Discovery

Digital Twins & Integrated Computational Materials Engineering (ICME)

Emerging Directions in Computational Material Research

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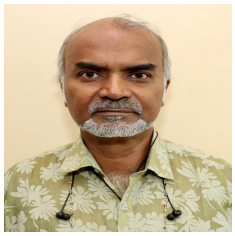

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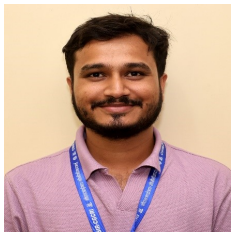

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COMPUTATIONAL AND DATA-DRIVEN ADVANCED MATERIALS (CDAM)

CSIR-Central Glass & Ceramic Research Institute, Kolkata

Venue: A.P.C Roy Seminar Hall, CSIR-CGCRI

Dates: April 07–08, 2026

Day 1: April 07, 2026

Time	**Program**
08:30 hrs–09:15 hrs	Registration
Inaugural Session	
09:15 hrs–09:20 hrs	Inauguration and the Ceremonial lighting of a lamp
09:20 hrs–09:30 hrs	Welcome Address and Setting the Context, **Prof. Bikramjit Basu**, Director, CSIR-CGCRI and Patron, CDAM 2026
09:30 hrs–09:40hrs	Introductory Remarks by Guest of Honour, **Dr. G. K. Patra**, Director, CSIR-4PI, Bangalore
09:40 hrs–09:50 hrs	Introductory Remarks by Chief Guest, **Prof. Tanusri Saha Dasgupta**, Director, SNBNCBS, Kolkata
09:50 hrs–09:55 hrs	Vote of thanks by **Dr. Indrajit Tah** , Scientist-C, CSIR-CGCRI
09:55 hrs–10:00 hrs	Group Photo Session

Day 1: April 07, 2026

Time	Program
Technical Session 1	
10:00 hrs–10:30 hrs	**Prof. Tanusri Saha Dasgupta**, Director, SNBNCBS, Kolkata *Title: Intelligent Materials Design & Understanding: ML in action*
10:30 hrs–11:00 hrs	**Prof. Srikanth Sastry**, JNCASR, Bangalore *Title: Seeing through glass failure: Prediction of fatigue failure in glasses from damage quantification and machine learning*
11:00 hrs–11:30 hrs	**Dr. G. K. Patra**, Director, CSIR-4PI, Bangalore *Becoming a Scientist in the Age of AI: Opportunities in Advanced Materials Research*
11:30 hrs–12:00 hrs	Inauguration of the Computational Materials Section at CSIR-CGCRI
12:00 hrs–12:25 hrs	**Prof. Priya Mahadevan**, SNBNCBS, Kolkata *Title: Determining rules for distortions in complex systems – case of hybrid perovskites*
12:25 hrs–12:50 hrs	**Prof. Suman Chakrabarty**, SNBNCBS, Kolkata *Title: Navigating Pathways in Free Energy Landscape: Adaptive (Machine) Learning Strategies in Molecular Simulation*
12:50 hrs–13:15 hrs	**Prof. Sankha Mukherjee**, IIT (Kharagpur) *Title: From Configurational Disorder to Anharmonic Lattice Softening: Mechanistic Origins of Superionic Conduction in Ge-Free Sulfide Solid Electrolytes*

Time	Program
Workshop Session	
14:30 hrs–15:45 hrs	Hands-on Workshop by **Prof. Srikanth Sastry**, JNCASR Bangalore *Title: Aneesur Rahman and the beginnings of molecular dynamics*
16:00 hrs–17:15 hrs	Hands-on Workshop by **Prof. Gautam Anand**, IIT (BHU) *Title: Entropy as a computational design tool for structure-property correlations in materials*
17:30 hrs–18:30 hrs	**Poster Session & Evaluation**

COMPUTATIONAL AND DATA-DRIVEN ADVANCED MATERIALS (CDAM)

CSIR-Central Glass & Ceramic Research Institute, Kolkata

Venue: A.P.C Roy Seminar Hall, CSIR-CGCRI

Dates: April 07–08, 2026

Day 2: April 08, 2026

Time	Program
Technical Session 3	
10:00 hrs–10:30 hrs	**Prof. D. D. Sarma**, IISc Bangalore *Title: Synergy between experiment and theory in materials science: A few examples*
10:30 hrs–11:00 hrs	**Prof. Partha Pratim Chakrabarti**, IIT (Kharagpur) *Title: Artificial Intelligence: The Emerging Face of Modern Scientific Discovery and Technological Innovation*
11:00 hrs–11:30 hrs	**Prof. Asim Tewari**, IIT Bombay *Title: The Changing Role of Human Researchers in the Age of AI-Enabled Materials Discovery*

Day 2: April 08, 2026

Time	Program
Technical Session 4	
12:00 hrs–12:30 hrs	**Prof. Smarajit Karmakar**, TIFR, Hyderabad *Title: Yielding Transition in Amorphous solids: Effect of Fragility*
12:30 hrs–13:15 hrs	Panel discussion on *"Emerging Computational tools for acceleratedddiscovery of materials"*
Workshop Session	
14:15 hrs–15:30 hrs	Hands-on Workshop by **Prof. Asim Tewari**, IIT (Bombay) *Title: Hands-on Tutorial on Cloud-Based Open-Source Finite Element Analysis and AI-Driven Topology Optimization*
15:45 hrs–17:00 hrs	Hands-on Workshop by **Dr. Bishwajit Ganguly**, Emeritus Scientist, CSIR-CGCRI,Jadavpur, Kolkata *Title: Computational Methods for Exploring Structural and Electronic Effects in Molecules and Materials*
Valedictory Session	
17:00 hrs–17:10 hrs	Concluding Remarks by **Mr. Jyotirmay Sikder**, Scientist G, CSIR-CGCRI
17:10 hrs–17:25 hrs	**Poster Prize Distribution**
17:25–17:30	Vote of thanks by **Mr. Ankush Pratap Singh**, Scientist-C, CSIR-CGCRI

Director's Message

It is with great pleasure and enthusiasm that I welcome you all to the "Conference on Computational and Data-driven Advanced Materials" (CDAM 2026), to be held at CSIR-Central Glass and Ceramic Research Institute, Kolkata during April 7-8, 2026. This conference represents a unique opportunity to engage in stimulating intellectual discourse, share ground-breaking research, and forge valuable connections that will undoubtedly play a pivotal role in shaping the future of computational and data-driven design and research of advanced materials and their diverse applications.

A galaxy of luminaries from the premier academic and research institutions across India, including CSIR, IISc, JNCASR, TIFR, SNBNCBS, and IITs will grace the occasion. Through a series of thought-provoking sessions, interactive panels, and insightful lectures, we aim to explore innovative ideas, stimulate the curious young minds and push the boundaries of our collective understanding.

One of the hallmarks of this conference is its commitment to fostering cross-disciplinary collaboration and communication among the active researchers in this field. Over the two days, the leading professors, researchers, and scholars will brainstorm on recent advances in multiscale simulations, machine learning, high-throughput experiments, and integrated computational–experimental frameworks for advanced materials. I trust that CDAM 2026 will, in particular, excite many young minds to peruse their research in the broad area of computational and data-driven materials.

May this conference be an intellectually enriching experience for each of you. I welcome you once again to the CSIR-CGCRI and look forward to witnessing the exchange of innovative ideas and fostering collaborations during this event. Thank you.

Prof. Bikramjit Basu
Director, CSIR-Central Glass & Ceramic Research Institute

Chairperson's Message

हमारे संस्थान में इस प्रकार का एक अत्याधुनिक सुविधा का होना अपने आप में एक वरदान स्वरूप है। यह व्यवस्था संस्थान और आसपास के शोधकर्ताओं को AI-ML और उच्च गणनात्मक कंप्यूटिंग जैसे उन्नत प्रणालियों का उपयोग करके उपलब्ध डेटा का संगणनात्मक रूप से विश्लेषण कर नई उन्नत पदार्थ खोजने और बनाने में मदद करेगा।

हालांकि CSIR के पास CSIR-4PI, CSIR-NAL और अन्य जैसी प्रयोगशालाओं में भी उच्च गणनात्मक कंप्यूटिंग की व्यवस्था हैं। पर यह पहली बार होगा जब CSIR-CGCRI द्वारा उन्नत पदार्थ के विकास के लिए अपनी खुद की व्यवस्था होगी। शोधकर्ता OQMD, ICSD, NOMAD इत्यादि जैसे विभिन्न डेटाबेस का उपयोग कर सकेंगे और उनका गणनात्मक रूप से विश्लेषण कर सकेंगे।

मैं इस सुविधा का उपयोग करने वाले सभी लोगों की सफलता की कामना करता हूं और उम्मीद करता हूं कि वे AI-ML जैसी आधुनिक तकनीकों की मदद से अपनी खुद की नई उन्नत पदार्थ का निर्माण कर सकेंगे, जो बदले में भविष्य में मानवता के लिए उपयोगी होगी।

ज्योतिर्मय सिकदर
Scientist "G"
Head: ITCMS & HR

DISTINGUISHED SPEAKERS

Prof. Dipankar Das Sarma
IISc, Bangalore

Prof. Partha Pratim Chakrabarti
IIT, Kharagpur

Prof. Tanusri Saha Dasgupta
SNBNCBS, Kolkata

Dr. G. K. Patra
CSIR-4PI, Bangalore

Prof. Srikanth Sastry
JNCASR, Bangalore

Prof. Smarajit Karmakar
TIFR, Hyderabad

Prof. Asim Tewari
IIT, Bombay

Dr. Bishwajit Ganguly
Emeritus Scientist, CSIR-CGCRI, Kolkata

Prof. Gautam Anand
IIT (BHU), Varanasi

Prof. Suman Chakrabarty
SNBNCBS, Kolkata

Prof. Priya Mahadevan
SNBNCBS, Kolkata

Prof. Sankha Mukherjee
IIT, Kharagpur

ABSTRACTS OF DISTINGUISHED SPEAKERS

Synergy between experiment and theory in materials science: A few examples

Prof. Dipankar Das Sarma
Solid State and Structural Chemistry Unit
Indian Institute of Science, Bengaluru 560012, India
sarma@iisc.ac.in

The intrinsic link between theoretical considerations and experimental practice in materials research is well established and requires no further justification. The dynamic interplay between these two research methodologies has significantly advanced the field, sometimes through mutual challenges and at other times through cooperative efforts. This synergy will be illustrated with three examples from our work. First, I shall address the paradoxical achievement of thermal conductivity below the expected minimum in a specific system, namely, 3D hybrid halide perovskites.[1] Then, I shall discuss the discovery of a 2-dimensional hybrid halide material, derived from its 3-dimensional perovskite analogue, with the smallest bandgap and exciton binding energy in this class of compounds.[2] Finally, I shall briefly discuss the mechanism of Mn emission in doped 3D hybrid halide perovskite nanocrystals.[3] This way, I shall cover materials research across three-, two-, and zero-dimensional objects in terms of structural connectivity.

References

1. Debasmita Pariari, Paribesh Acharyya, Arijit Sinha, Ashutosh Mohanty, Shaili Sett, Navkiranjot Kaur Gill, Arindam Ghosh, Umesh V Waghmare, Kanishka Biswas, and D. D. Sarma, ACS Energy Letters 9, 2128 (2024).
2. Debasmita Pariari, Sakshi Mehta, Sayak Mandal, Arup Mahata, Titas Pramanik, Sujit Kamilya, Arya Vidhan, Tayur N. Guru Row, Pralay K. Santra, Shaibal K. Sarkar, Filippo De Angelis, Abhishake Mondal, and D. D. Sarma, J. Am. Chem. Soc. 145, 15896 (2023).
3. Poulomi Mukherjee, Ranjan Das, Debasmita Pariari, Koushik Das, Priya Mahadevan, and D. D. Sarma, ACS Energy Lett. 10, 6381 (2025).

Artificial Intelligence: The Emerging Face of Modern Scientific Discovery and Technological Innovation

Prof. Partha Pratim Chakrabarti
Indian Institute of Technology, Kharagpur
ppchak@adm.iitkgp.ac.in

This lecture will explore the architecture and methodologies of modern Artificial Intelligence (AI), illustrating its role in accelerating the integration and advancement of scientific knowledge and technological innovation. The discussion will cover the foundational frameworks of Artificial Intelligence and Machine Learning (AI/ML), with a specific focus on foundation and large language models. Through illustrations, the talk will demonstrate how AI enables cross-domain assimilation and reasoning. These capabilities rapidly generate recommendations that expedite the derivation of scientific equations and mathematical proofs, propose novel experiments, predict material compositions and optimized processes, and facilitate the creation of complex engineering designs. Furthermore, the presentation will examine AI's capacity for intelligent human interaction—particularly with students, researchers, creators, and innovators—frequently yielding insights and collaborative outcomes that surpass the capabilities of individual experts or groups. Alongside these advancements, the lecture will critically address the potential pitfalls of AI/ML methodologies. It will highlight the profound risks associated with utilizing AI without sufficient knowledge and critical discernment, including the depletion of both physical and intellectual resources. Finally, the talk will outline the necessary pathways to improve current iterations of AI, ensuring that its future deployment remains inherently trustworthy, ethical, and responsible.

Intelligent Materials Design & Understanding: ML in action

Prof. Tanusri Saha Dasgupta
Department of Condensed Matter Physics & Materials Science
Thematic Unit of Computational Materials Science
S. N. Bose National Centre for Basic Sciences, Kolkata, India
t.sahadasgupta@gmail.com

One of the strong pillars in advancement of designed materials, with targeted properties like magnetism, superconductivity, topological characters is computation of materials. The synthesis and optimization of properties of real materials in experiment is both time-consuming and costly, being mostly based on trial and error. Computational approach in this connection is of natural interest to screen materials, before they can be suggested and tested in the laboratory. For the prediction of new materials, a powerful tool is the machine-learning assisted high throughput computation. In this approach new materials have been computationally predicted by combining electronic-structure methods with intelligent machine learning technique based on data mining and database construction. In this talk we discuss application of this method for prediction of new magnetic double perovskites [1], low cost rare earth based permanent magnets [2] and semiconductor heterostructures,[3] binary nanoalloys.[4] We will also touch upon machine-learning prediction of the formation of atomic gold wires by mechanically controlled break junctions.[5] Finally, we will demonstrate how machine learning helps in understanding the deformation properties in layered MAX compounds.[6]

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Becoming a Scientist in the Age of AI: Opportunities in Advanced Materials Research

Dr. G. K. Patra
CSIR-4PI, Bangalore
gkpatra.4pi@csir.res.in

Scientific progress has historically been driven by the evolution of instruments that extend human capability to observe, model, and understand nature. In this context, Artificial Intelligence (AI) is emerging as a universal scientific instrument, reshaping how research is conducted. This talk revisits science from first principles and examines the recent surge in AI capabilities arising from the convergence of data, compute, and advanced algorithms. Focusing on the post-2022 era, it highlights the impact of Generative AI, Foundation Models (FMs), and Large Language Models (LLMs) in enabling knowledge synthesis and hypothesis generation. The transition from AI tools to agentic systems is discussed, with emphasis on applications in materials science, including materials design, property prediction, and accelerated discovery pipelines. The talk also presents practical AI tools, while critically examining opportunities and challenges such as reliability, interpretability, and integration into scientific workflows, concluding with key takeaways for researchers in the CSIR ecosystem.

Seeing through glass failure: Prediction of fatigue failure in glasses from damage quantification and machine learning

Prof. Srikanth Sastry
Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India
sastry@jncasr.ac.in

When solids are subjected to repeated cycles of stress or deformation, they can fail after several such cycles, as a result of accumulated plasticity and internal structural changes. Such behaviour has been investigated actively in recent years in amorphous solids, wherein the nature of the internal changes leading to failure, and the mechanism of failure, are more elusive than the crystalline counterparts. Glasses exhibit interesting non-monotonic behaviour, with deformation induced annealing preceding failure, which cannot be neatly fit into conventional descriptions of fatigue failure, e. g., in metals. The extent to which the description of fatigue failure in amorphous solids may differ from that in crystalline, metallic, solids, is thus an open question of interest. We investigate several measures of damage, from microscopic to macroscopic length scales, which enable prediction of failure time, or fatigue life, accurately. However, several questions remain regarding the best quantification of damage, as well as a rationalization of the empirical results, remain to be addressed. As a step towards these goals, we employ machine learning approaches to explore key properties relevant for fatigue life prediction. Results from these investigations, as well as approaches to developing a microscopic picture of fatigue failure in amorphous solids, will be discussed.

References

1. S. Maity, H. Bhaumik, S. Athani and S. Sastry, Fatigue failure in glasses under cyclic shear Deformation, Nature Physics, `https://doi.org/10.1038/s41567-026-03174-x(2026)`.

Yielding Transition in Amorphous solids: Effect of Fragility

Prof. Smarajit Karmakar
Tata Institute of Fundamental Research, Hyderabad
smarajit@tifrh.res.in

Amorphous materials, particularly metallic glasses, exhibit remarkable mechanical properties, including high yield strength and large yield strain. Research continues to unravel the relationship between their microscopic failure mechanisms and the yielding transition. Notably, yielding behaviour varies with the sample's initial age and material characteristics, like fragility. In poorly annealed conditions, both strong and fragile glass formers show a consistent critical yield strain, γ_c, but fragile glasses experience a significant increase in yield point with further annealing, unlike strong glasses. In this talk, I will elucidate a universal behaviour across diverse glassy systems, controlled by glass fragility, including metallic and molecular glasses, and explain it using a modified mean-field elastoplastic model, emphasising the role of changing energy barriers during yielding.

References

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The Changing Role of Human Researchers in the Age of AI-Enabled Materials Discovery

Prof. Asim Tewari
Center for Machine Intelligence and Data Science (C-MInDS)
Department of Mechanical Engineering
IIT Bombay, Powai, Mumbai 400 076, India

Artificial Intelligence (AI) and Machine Learning (ML) are rapidly transforming the landscape of computational materials science, redefining both the pace of discovery and the role of the human researcher. Traditionally, materials development relied on a combination of physical intuition, empirical experimentation, and computational modeling. Today, AI-driven approaches are enabling a shift from sequential and expert-dependent workflows to adaptive, data-rich, and highly accelerated discovery frameworks. Across the full spectrum of materials research, from new alloy development and physical metallurgy to process optimization and property prediction, ML models are being used to uncover complex structure-process-property relationships that were previously difficult to resolve. More advanced paradigms, including mixture-of-experts models, chain-of-thought reasoning, and agentic AI frameworks, are beginning to integrate scientific knowledge, simulation tools, and decision-making into unified systems capable of proposing, evaluating, and refining hypotheses with minimal human intervention. In this setting, computational tools are no longer merely instruments operated by researchers; increasingly, they are becoming components of intelligent discovery engines guided by AI. This transformation extends beyond simulation. With the rise of AI-directed combinatorial experimentation, it is now possible to envision discovery pipelines in which candidate materials, process pathways, and validation strategies are first conceived computationally and then verified experimentally in an autonomous or semi-autonomous loop. Similar paradigms have already demonstrated major impact in pharmaceutical discovery, where AI-assisted methods have accelerated the identification of novel compounds and therapeutic leads. Looking ahead, AI-based computational models are poised to play an even more significant role in the design of both structural and functional materials. As a result, the role of the human researcher is also evolving—from one of direct manual exploration to one of framing questions, guiding objectives, interpreting outcomes, and ensuring scientific validity. Computational materials science is thus entering a new era in which human creativity and machine intelligence will work in close partnership to enable deeper and faster materials innovation.

Computational Methods for Exploring Structural and Electronic Effects in Materials

Dr. Bishwajit Ganguly
Emeritus Scientist, CSIR-CGCRI, Jadavpur, Kolkata
compmat.89@rediffmail.com

Quantum chemical calculations are a powerful toolkit for understanding and predicting the behavior of molecules and materials at the atomic level. The central challenge is always a trade-off between accuracy, computational cost, and system size. This session would overview with examples and practical insights into selecting the right approach.

Entropy as a computational design tool for structure-property correlations in materials

Prof. Gautam Anand
Indian Institute of Technology (BHU), Varanasi
gautamanand.mst@itbhu.ac.in

The discovery and development of high-entropy alloys (HEAs)—a comparatively new class of materials comprising multicomponent, compositionally concentrated solid solutions with simple underlying crystal structures—has opened new avenues for materials design with tunable properties. However, the immense compositional complexity of these materials presents significant computational challenges. Conventional brute-force, trial-and-error approaches become impractical due to the combinatorial explosion of possible configurations, necessitating the development of more efficient computational strategies for materials discovery. In this talk, we will present an innovative framework for atomistic sampling of multicomponent materials. Specifically, we introduce the Genetic Algorithm for Atomistic Sampling Protocol (GAASP) [1–3], an alchemical Monte Carlo–based approach designed to efficiently explore the thermodynamically relevant regions of the potential energy landscape of high-entropy materials. We demonstrate the effectiveness of this method by integrating it with a graph neural network–based machine learning architecture, enabling rapid and accurate exploration of the potential energy surface of high-entropy alloys. Furthermore, we will show how information entropy can be employed as a descriptor of the sampled potential energy landscape to predict phase stability across a wide range of alloy systems, including HEAs. The role of chemical short-range order in high-entropy materials is examined using a complementary combinatorial sampling framework, namely Order Parameter Engineering for Random Systems (OPERA) [4]. Finally, we discuss the broader applicability of the information entropy–based approach for property prediction in high-entropy alloys, highlighting potential limitations and strategies to mitigate them.

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Navigating Pathways in Free Energy Landscape: Adaptive (Machine) Learning Strategies in Molecular Simulation

Prof. Suman Chakrabarty
Department of Chemical and Biological Sciences
S. N. Bose National Centre for Basic Sciences, Kolkata, India
sumanc@bose.res.in

Computation of the underlying free energy landscapes for any complex chemical or biophysical processes provides quantitative insights into the thermodynamics and kinetics of the process, including the mechanistic pathways. However, several important (bio)chemical processes occur on timescales not accessible to standard computational methods like atomistic molecular dynamics (MD) simulations. This motivates the development of enhanced sampling methods to accelerate rare events. However, identification of suitable reaction coordinate(s) or a mechanistic hypothesis is crucial to the success of such methods.

In this talk, we shall discuss a few computational methods developed in our group for adaptive navigation of rugged energy landscapes to generate reactive pathways. We shall demonstrate how we can efficiently compute rare event kinetics, e.g. drug unbinding kinetics (residence time; k_{off}), which is an effective parameter in drug discovery research, at a reasonable computational cost. Modern machine learning approaches combined with physics-based simulations provide a powerful avenue towards quantitative estimation of kinetics in complex (bio)chemical/physical processes.

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Distortions in Complex Materials: Insights from First-Principles Studies

Prof. Priya Mahadevan
Department of Condensed Matter and Materials Physics
S.N. Bose National Centre for Basic Sciences, Kolkata India
priya@bose.res.in

The hybrid perovskites are of interest in recent times because of their multifarious nature. The close correlation between the structure and the ensuing properties requires an understanding of the factors that drive the structural distortions. These are well understood among the inorganic perovskites in terms of a geometric quantity dependent on the radii of the atoms making up the materials. However, this is more complex in the hybrid perovskites, where the molecule interacts with the inorganic cage. Considering the three dimensional members which are few in a number we had identified the factors [1] that determine the distortions. However, this becomes more complex in the context of the two dimensional perovskites where the number is large. In this talk I will present our recent results [2] in which we identify few descriptors and explore their correlations with the structural distortions.

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From Configurational Disorder to Anharmonic Lattice Softening: Mechanistic Origins of Superionic Conduction in Ge-Free Sulfide Solid Electrolytes

Vinay Maithani, Sankha Mukherjee*
Department of Metallurgical and Materials Engineering
Indian Institute of Technology Kharagpur, Kharagpur 721302, West Bengal, India
sankha@metal.iitkgp.ac.in

All-solid-state batteries require solid electrolytes that combine fast Li-ion transport with chemical and mechanical robustness while avoiding scarce elements such as Ge. Herein, I will discuss a first-principles investigation of two Ge-free sulfide electrolyte families, disordered $Li_{10}MP_2S_{12}$ (M = Sn, Si) and $Li_{11}AlP_2S_{12}$ (LAPS), to show how superionic conduction emerges from two complementary materials-design motifs: configurational disorder and dynamic lattice softness. For disordered $Li_{10}MP_2S_{12}$, ensemble-statistical sampling of representative ordered configurations combined with isothermal-isobaric Car–Parrinello molecular dynamics reveals a strong configuration dependence of transport. The most probable $Li_{10}SiP_2S_{12}$ configuration exhibits lower Li-ion migration barriers than $Li_{10}SnP_2S_{12}$, with tracer and charged activation energies of 0.11 ± 0.05 and 0.12 ± 0.05 eV, respectively, indicating that local cation arrangement can actively promote cooperative Li transport [1]. These results show that disorder in thio-LISICON frameworks is not merely a structural complication, but a functional degree of freedom that reshapes diffusion pathways and bonding landscapes. Building on this disorder-centric picture, computations show that LAPS is a promising earth-abundant LGPS analogue whose high intrinsic conductivity is governed by finite-temperature lattice dynamics. *NpT ab initio* molecular dynamics predicts room-temperature ionic conductivities of 7–11 $mS\,cm^{-1}$ with activation energies of 0.22–0.24 eV, arising from a three-dimensional, weakly correlated diffusion network. Vibrational analysis further indicates that anharmonic lattice softening and liquid-like low-frequency Li dynamics underpin this superionic response. Complementary thermodynamic analysis suggests that LAPS possesses an intrinsic electrochemical stability window of 1.55–2.04 V vs. Li/Li^+, forms electronically insulating self-passivating interphases, and shows moderate elastic anisotropy favorable for stress accommodation. Taken together, these results establish a unified design principle for Ge-free sulfide electrolytes: high Li mobility can be engineered either through statistically favorable disordered sublattices or through soft, anharmonic host frameworks, and the most promising candidates are those that combine fast transport with chemomechanical compatibility for next-generation all-solid-state batteries.

Keywords: sulfide solid electrolytes; $Li_{10}MP_2S_{12}$; $Li_{11}AlP_2S_{12}$; superionic conduction; disorder; anharmonicity; all-solid-state batteries

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ABSTRACTS FOR POSTER PRESENTATION

Decoding the Local Atomic Structure of Amorphous ZrO_2 Fibers via Correlated Pair Distribution Function Analysis, Molecular Dynamics Simulations, and First-Principles Calculations

Debjani Niyogi[1], Sanjiban Das[1], Soupitak Pal[1]*

[1]Advanced Ceramics and Composites Division, CSIR-Central Glass and Ceramic Research Institute, 196 Raja S.C. Mullick Road, Jadavpur, Kolkata, West Bengal, 700032

soupitak.cgcri@csir.res.in

Sol–gel-derived, solution-blown ZrO_2 fibers are amorphous in the as-blown condition and transform to tetragonal ZrO_2 upon heat treatment at 800°C, followed by transformation to monoclinic ZrO_2 at 1200°C. This behaviour contradicts the conventional phase transformation sequence of ZrO_2, where monoclinic is stable at room temperature and transforms to tetragonal above ∼1170°C. To understand this anomalous behaviour, the local atomic arrangement in amorphous ZrO_2 fibers and their phase evolution during heat treatment are investigated using an integrated experimental–computational approach combining X-ray total scattering, pair distribution function (PDF) analysis, molecular dynamics (MD) simulations, and density functional theory (DFT) calculations. Experimental PDFs reveal short-range structural correlations characteristic of disordered zirconia, evolving progressively during thermal treatment. Comparison with MD-simulated PDFs enables accurate identification of local atomic configurations and cluster-size distributions. Amorphous zirconia networks consist of distorted ZrO_6 polyhedral units with limited correlation length and structural resemblance to the tetragonal phase. These gradually reorganize into nanocrystalline domains, following a transformation pathway from amorphous → metastable tetragonal → monoclinic ZrO_2. DFT calculations indicate that the tetragonal phase is stabilized at nanoscale cluster sizes due to reduced strain energy, whereas the monoclinic phase becomes thermodynamically favourable at larger domain sizes.

Keywords: Pair distribution function (PDF); Molecular dynamics simulation; Density functional theory; Phase transformation.

Computational and Data-Driven Investigation of Solid-State Electrolytes for Sodium-Ion Batteries

Sankha Mukherjee[1], Srijita Chakraborty[1]*

[1]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Kharagpur, Kharagpur, India

srijitachakraborty.24@kgpian.iitkgp.ac.in

The development of next-generation energy storage technologies requires electrolyte materials that exhibit high ionic conductivity, strong chemical stability, and robust mechanical integrity. Solid-state electrolytes for sodium-ion batteries have emerged as promising candidates due to the abundance and low cost of sodium resources. However, understanding the relationship between atomic-scale structure and macroscopic material properties remains a major challenge. Computational modelling and data-driven approaches provide powerful tools to accelerate the discovery and optimization of such advanced materials.

In this work, we employ a multiscale computational framework combining density functional theory (DFT), molecular dynamics (MD) simulations, and artificial intelligence–assisted machine learning (AI/ML) techniques to investigate the structural, mechanical, thermal, and chemical properties of solid-state sodium-ion electrolytes. First-principles DFT calculations are used to analyze the electronic structure, thermodynamic stability, and ion-migration pathways of candidate electrolyte materials. Molecular dynamics simulations further provide insight into temperature-dependent ionic diffusion, lattice dynamics, and thermal stability under realistic operating conditions.

Additionally, data-driven methodologies are employed to identify structure–property relationships and expedite the screening of potential electrolyte materials. The integration of physics-based simulations with machine learning enables efficient prediction of key performance metrics, including ionic conductivity, mechanical robustness, and chemical compatibility with electrode materials.The results provide a comprehensive understanding of how atomic-level structural features influence macroscopic material properties that determine the performance and safety of sodium-ion batteries. This study demonstrates the effectiveness of combining DFT, molecular dynamics, and AI-assisted modelling for the rational design of advanced solid-state electrolytes and highlights promising directions for the development of high-performance and sustainable sodium-ion battery technologies.

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Unified pathway of flat band engineering, quantum transport of low-dimensional model lattices and optical analogue

Atanu Nandy[1]*

[1]Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata, West Bengal – 700 131, India

atanunandy1989@gmail.com

We have addressed the problem of flat band engineering in different quasi-one dimensional networks through a generalized analytical proposition worked out within the tight-binding methodology. Exact fabrication of single particle eigenstates with localized as well as diffusive modes is reported through the demonstration of such unified pathway by virtue of a simple 'real space decimation' formalism in these flat band models. The description provides a common platform to investigate the band dispersion including the overall spectral portrait, quantum transport and associated physical aspects for those quasi-one dimensional lattices. Analytical work out is justified through the numerical evaluation of density of eigenstates, electronic transmission behavior, inverse participation ratio, persistent current study, Aharanov-Bohm oscillation in the transmittance and other related issues. Electronic models can be easily extended to the photonic realm which has a direct application to the slow-light, optical caging and related quantum memory devices.

Keywords: Flat band; Aharonov-Bohm effect; compact localization; slow light.

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A Structural Approach to Predict Dynamics in Supercooled Glassy Liquid

Surajit Maji[1], Indrajit Tah[1]*

[1]CSIR-Central Glass and Ceramic Research Institute, Kolkata-700032, India

indrajittah@cgcri.res.in

In contrast to crystalline solids, disordered systems do not possess well-defined structural defects that govern atomic rearrangements; instead, rearrangements occur due to thermal fluctuations, applied stress, or external perturbations. One of the major challenges in the scientific community is to understand how structural features control the dynamics of supercooled liquids, where disorder prevails and no clear structural signatures of defects exist. For a long time, considerable effort has been devoted to identifying a structural quantity that can reliably predict atomic dynamics in supercooled liquids.

Several approaches based on statistical mechanics and machine learning have been developed to correlate dynamics directly with structural information [1]. While machine learning methods often provide accurate predictions, their internal decision-making processes remain largely opaque due to the high-dimensional nature of the correlations involved. In this context, we propose a simple and physically interpretable structural descriptor, the shape index that captures atomic dynamics in model supercooled liquid systems. In this study, we investigate the functional dependence of the probability of rearrangement on the shape index, its associated information-loss timescale, and compare its predictive capability with that of a machine-learning-derived structural quantity, softness.

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Learning Structural Signatures of Plasticity in Disordered Solids

Bipasha Bhowmick[1], Indrajit Tah[1]*

[1]CSIR–Central Glass and Ceramic Research Institute, Kolkata 700032, India

indrajittah.cgcri@csir.res.in

Catastrophic failure events in disordered materials, engineered structures, and natural systems such as avalanches often occur without clear warning, leading to large-scale disasters and significant loss of life. Understanding the microscopic and mesoscopic processes that precede such failures therefore remains a critical challenge for both science and society. A central question is whether reliable precursors of material yielding, particularly for disordered materials, exist that can be identified well before macroscopic failure occurs. Unlike crystalline solids, disordered materials such as glasses do not possess regular lattices or well-defined defects that indicate where failure will occur. Instead, plastic deformation arises from rare and highly localized rearrangements involving only a few particles. Identifying these weak regions before deformation remains one of the most important challenges in the physics of disordered matter. A central objective of current research is to identify spatially localized regions susceptible to plastic rearrangements by analyzing structural descriptors that encode incipient mechanical instability well in advance of the onset of plastic deformation. In this work, we examine this possibility using a simple geometric descriptor derived from Voronoi tessellations: the shape index, which quantifies how compact or distorted a particle's local environment is.Under applied shear in amorphous solids, particles with extreme shape-index values exhibit only a weak statistical propensity for plastic activity, with substantial overlap between plastic and non-plastic populations. The absence of a clear threshold underscores the fundamental limitations of low-dimensional structural descriptors for predicting plastic rearrangements.Motivated by this result, we turn to machine-learning approaches that can combine multiple local structural features and capture complex, high-dimensional correlations between structure and plastic response. Our results provide a clear motivation for data-driven methods as a powerful route to uncover the hidden structural signatures of plasticity in amorphous materials.

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Structural, Thermal and Optical Property Modulation in CeO_2-Doped Bi_2O_3–B_2O_3–SiO_2–Na_2O–Y_2O_3–Al_2O_3 Multicomponent Glass

Saikh Rafiuddin[1], Srikrishna Manna[1]* and Sourav Nag[1]*

[1]Specialty Glass Division, CSIR-Central Glass and Ceramic Research Institute, Kolkata 700032, India

souravnag.cgcri@csir.res.in /srikrishna.cgcri@csir.res.in

CeO_2-doped multicomponent (Bi_2O_3–B_2O_3–SiO_2–Na_2O–Y_2O_3–Al_2O_3) bismuth glasses are synthesized using the conventional melt–quenching technique to investigate the influence of rare-earth-induced network modification on the structural, thermal, and optical properties of the glass matrix. X-ray diffraction analysis confirms the predominantly amorphous nature of all prepared compositions. Structural investigations using Raman and FTIR spectroscopy reveal systematic changes in borate structural units, particularly the conversion between BO_3 and BO_4 groups, along with distortion of Bi-centred polyhedra such as BiO_6 and BiO_3 within the glass matrix. This contributes to enhanced network compactness, resulting in a more rigid glass structure. X-ray photoelectron spectroscopy further indicates the presence of mixed Ce^{3+}/Ce^{4+} oxidation states, which influence oxygen coordination environments and stabilize the Bi^{3+} oxidation state.

Compositional variation demonstrates that increasing Bi_2O_3 content enhances electronic polarizability and optical basicity of the glass network, while simultaneously promoting non-bridging oxygen formation that slightly reduces thermal stability. In contrast, the incorporation of Y_2O_3 strengthens the glass network by increasing structural compactness and stabilizing BO_4 units, leading to an improved glass transition temperature. The prepared glasses exhibit moderate visible transparency (∼75–80%), a high refractive index, and tunable optical band gap values in the range of approximately 2.38–2.44 eV.

The results highlight that controlled adjustment of Bi_2O_3 and Y_2O_3 concentrations under optimized CeO_2 doping effectively tunes the structure–property relationships of the multicomponent glass system. Such compositional engineering provides a promising pathway for developing lead-free, optically transparent heavy-metal oxide glasses with potential applications including radiation-shielding windows and optoelectronic devices[1,2].

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Strain-Tuneable Lattice Thermal Conductivity in Ferromagnetic VS2

Zimmi Singh[1], Sankha Mukherjee[1]*

[1]Metallurgical and Materials Engineering Department, Indian Institute of Technology Kharagpur,India

sankha@metal.iitkgp.ac.in

This work examines the lattice thermal conductivity (κ_{lat}) of 2H-phase VS_2 in both unstrained and equi-biaxial tensile-strained configurations using first-principles calculations. Strong electron correlation effects were treated within the DFT+U+V framework to obtain the electronic band structure and to quantify the magnetic exchange interactions. The Curie temperature (T_{c}) was subsequently evaluated via Monte Carlo simulations of the Heisenberg model, with exchange parameters extracted from a localized-orbital projection scheme. Lattice thermal transport was computed by iteratively solving the phonon Boltzmann transport equation under the constant relaxation-time approximation. The calculated κ_{lat} exhibits a clear temperature dependence that varies systematically with applied strain. These results demonstrate the decisive role of spin–lattice coupling in 2H$-VS_2$, opening avenues for strain-controlled spintronic devices, high-performance thermoelectrics, and on-chip thermal management at the nanoscale.

Keywords: DFT; 2H-phase VS_2; Phonon dispersions; Curie temperature; DFT+U; Lattice thermal conductivity; Cophonicity.

First-Principles study on SC2P as a promising anode material for metal ion batteries

Soutrik Banerjee[1]*, Mousumi Parvin[1], Bikash Chandra Gupta[1]

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

soutrikphysics04@gmail.com

Energy plays a pivotal role in the effective functioning of modern society and is indispensable for daily life. However, the availability of conventional energy resources is limited and increasingly constrained. To address this challenge, researchers have shifted their focus toward renewable energy sources for sustainable power generation, along with the development of efficient energy storage systems to ensure reliable future use. The development of efficient anode materials for alkali metal-ion batteries (MIBs) has become imperative in response to the growing demand for high-performance energy storage systems. The effectiveness of an electrode material is primarily determined by three critical parameters: high storage capacity, excellent electrical conductivity, and rapid ion diffusion capability. Extensive research efforts have been devoted to the discovery and development of novel materials, particularly two-dimensional (2D) materials [1-3], that are suitable for use as electrode materials in battery technologies. In this study, we consider a two-dimensional transition metal phosphide (TMP), specifically the Sc_2P monolayer, to examine its feasibility as an efficient electrode material. Our theoretical investigation reveals that the Sc_2P monolayer possesses a structurally stable honeycomb-like lattice with intrinsic metallic character, ensuring excellent electrical conductivity. Furthermore, the monolayer demonstrates strong adsorption toward Li/Na/Mg atoms, which facilitates efficient charge transfer and sustains good electronic conductivity, while maintaining moderate ion diffusion barriers. To elucidate the charge transfer mechanism and quantify the extent of electron exchange between Li/Na/Mg and the Sc_2P sheet, charge density difference (CDD) analysis combined with Bader charge calculations has been systematically performed. A detailed layer-by-layer adsorption analysis reveals remarkable theoretical storage capacities of approximately 1330.675 $mAh\,g^{-1}$ for Na, 887.12 $mAh\,g^{-1}$ for Li, and 887.11 $mAh\,g^{-1}$ for Mg. These values significantly surpass that of the conventional graphite anode. In light of these outstanding electrochemical characteristics, we propose the Sc_2P monolayer as a potential high-performance anode material for next-generation Li-, Na-, and Mg-ion batteries.

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PO_4 and Ho^{3+} ions effects in phosphate glass for radiation protection applications

Anu K John[1]*, P. Vinothkumar[1]

[1]Department of Physics, Saveetha Engineering College, Anna University, Chennai, Tamilnadu, 602105, India

kjohnanu91@gmail.com

The structural, optical, and physical properties of holmium-doped phosphate glass, which is composed of 55% P_2O_5, 5% Al_2O_3, 4% MgO, 5% NaF, 10% $LiCO_3$, 5% CaO, 10% $SrCO_3$, 5% ZnO, and 1% Ho_2O_3, are analyzed and described through the melt-quench process. The amorphous character is confirmed by XRD, while the significant phosphate functional groups are revealed by FTIR. The optical band gap energy was 3.02 eV after the acquisition of UV absorption spectra. Ho^{3+} transitions were represented by three peaks in the PL spectra: $^5I_8 \rightarrow {}^5G_6$, $^5I_8 \rightarrow {}^3K_8$, and $^5I_8 \rightarrow {}^5F_3$. Furthermore, the glass demonstrated radiation shielding properties in accordance with a variety of critical factors. The role of O = P–O, P=O bond, PO_4 tetrahedra, and Ho–O bonding vibrations shows a critical role in radiation shielding applications. Gamma radiation shielding characteristics, including the Mean Free Path (MFP), Effective Atomic Number (Z_{eff}), Linear Attenuation Coefficient (μ), and Mass Attenuation Coefficient (μ/ρ), were determined using the Phy-X program. According to MAC data, the area of prominence of Compton scattering (CS) decreases when CS alters in the intermediate photon energy zone ($E > 3$ MeV). The material can induce the photoelectric effect at lower energies, Compton scattering at intermediate energies, and pair creation at higher energies. Holmium-doped glasses exhibited shortened MFP values, which implies a greater degree of shielding effectiveness.

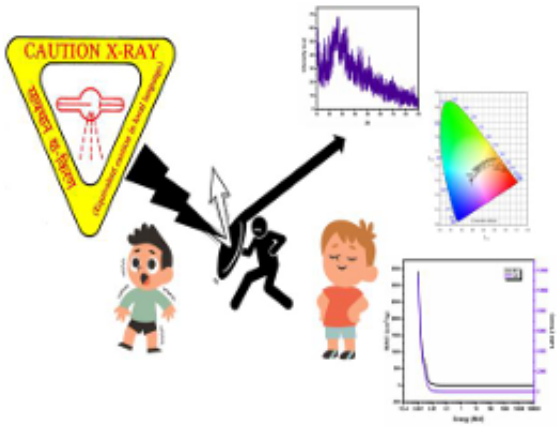

Fig. 1: Radiation Shielding

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Predicting Shear Modulus of Glass Using Machine Learning

Soumyadeep Rooj[1], Indrajit Tah[2]*

[1]Siksha Bhavana, Visva-Bharati, Santiniketan, Bolpur, Birbhum, 731235.

[2]Specialty Glass Division, CSIR-Central Glass and Ceramic Research Institute, Kolkata-700032

indrajittah.cgcri@csir.res.in

The mechanical properties of glassy materials, particularly the shear modulus, play a critical role in determining their suitability for a wide range of technological applications. In this study, we investigate the predictive modelling of the shear modulus for Calcium Aluminosilicate (CAS) glass using different machine learning models. A dataset comprising composition and experimentally measured shear modulus values was employed to develop machine learning models. The performance of each model was evaluated based on statistical metrics such as the coefficient of determination (R^2 score) and mean square error (MSE). Among the models examined, the linear regression provides the most accurate predictions, indicating a predominantly linear compositional dependence of the shear modulus in CAS glasses within the studied range. These findings highlight the potential of data-driven models to support materials design and accelerate the development of glass compositions with tailored mechanical properties.

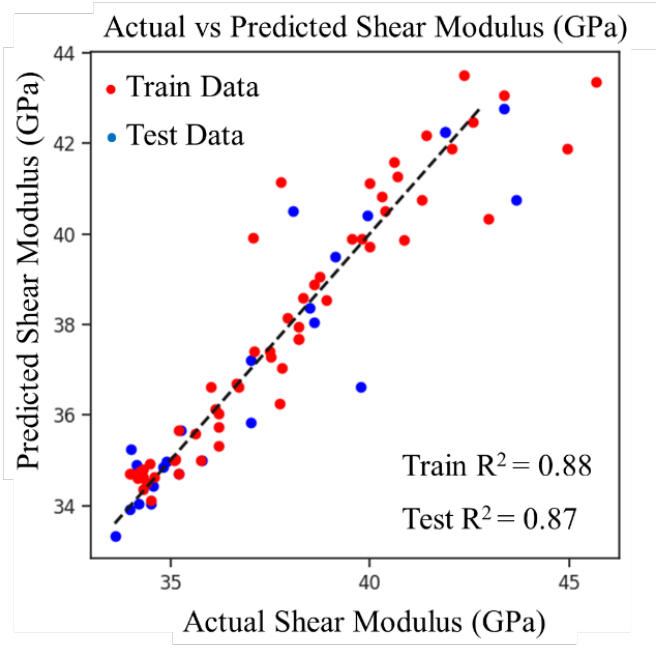

Fig. 1: Actual vs predicted shear modulus plot for linear regression

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Tuning Fragility in Sodium Lead Borate Glasses: Unveiling the Interplay Between Compositions, Stokes-Einstein Breakdown, and Dynamical Heterogeneity

Azhar Uddin Mallick[1], Roni Chatterjee[2], Jagannath Gangareddy[1], Smarajit Karmakar[2], and Indrajit Tah[1]*

[1]Specialty Glass Division, CSIR-Central Glass and Ceramic Research Institute, Kolkata-700032. [2]Tata Institute of Fundamental Research, 36/P, Gopanpally Village, Serilingampally Mandal, Ranga Reddy District, Hyderabad 500046, Telangana.

indrajittah.cgcri@csir.res.in

The rapid increase in viscosity or relaxation as supercooled liquids approach their glass transition temperature is a universal hallmark of all glass-forming liquids. The temperature dependence of viscosity is characterized by fragility, which varies widely among glassy liquids. Some show Arrhenius temperature dependence of viscosity or relaxation time (strong liquids), while others exhibit super-Arrhenius behavior (fragile liquids).

In this work, we performed extensive molecular dynamics simulations on a realistic glass-forming system, sodium–lead–borate glasses (Na_2O–PbO–B_2O_3), to investigate how systematically increasing the PbO concentration, at the expense of B_2O_3, influences viscosity growth and kinetic fragility. The results reveal a clear strong-to-fragile transition with increasing PbO concentration (Figure 1). To further characterize the dynamics, we analyzed the breakdown of the Stokes–Einstein (SE) relation, the Kohlrausch–Williams–Watts (KWW) stretching exponent (β_{kww}), and dynamical heterogeneity using the four-point susceptibility, $\chi_4(t)$, and the non-Gaussian parameter, $\alpha_2(t)$. Our results show that strong glass exhibits slightly higher heterogeneity, despite weaker SE breakdown and larger β_{kww} values. We also quantified the associated dynamical and structural correlation length scales. Overall, the results highlight the interplay between fragility, Stokes–Einstein breakdown, and dynamical heterogeneity, emphasizing the critical role of glass composition in controlling viscosity and dynamics in glass-forming systems.

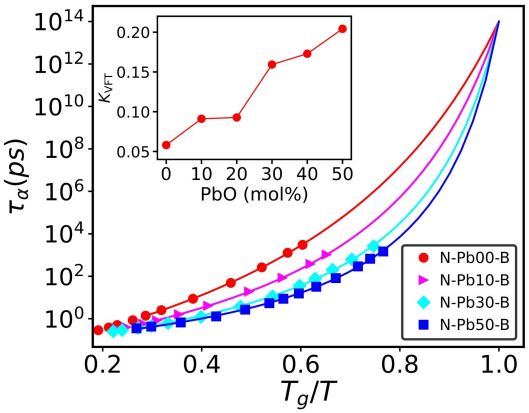

Fig. 1: Angell plot showing strong-to-fragile transition in Na_2O–PbO–B_2O_3 glasses with increasing PbO concentration

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Near-Surface Buried Plasmonic Silver Nanoparticles in Sodium Aluminium Silicate Glass as a new SERS Substrate for Trace Detection of Organic Molecules

Jagannath Gangareddy[1]*

[1]Specialty Glass Division, CSIR-Central Glass and Ceramics Research Institute (CSIR-CGCRI), Kolkata, West Bengal, 700032, India

jagannath.cgcri@csir.res.in

Surface-enhanced Raman scattering (SERS) is one of the most sensitive methods for the detection of adsorbed molecules on the nanostructured coinage-metal surface. The enhancements in the order of 104–106 are routinely observed. Such an effect makes SERS spectroscopy a technique applicable to the study the adsorption of analytes in the sub-monolayer regime. Novel SERS sensors require novel substrates with high activity for great sensibility detection of different molecules applied in many fields, such as detections of narcotics, explosives, and molecules with biological interest.

In this work, silver (Ag) nanoparticles (NPs) buried near the surface of sodium aluminium silicate glasses are explored as a new SERS substrate for the trace detection of Nile blue and Rhodamine 6G (R6G). The glass substrates were characterized by R optical absorption, scanning electron microscopy (SEM) techniques. This work contributes to the development of simple approach in obtaining an efficient glass-based SERS substrate.

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Dynamic Electron Density Analysis of α-KNO_3

Anagha Ghosh[1]* and Swastik Mondal[1,2]

[1]CSIR-Central Glass and Ceramic Research Institute, 196, Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India.

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

anaghagsh@gmail.com

Understanding the microscopic mechanisms of temperature dependent structural phase transitions requires direct insight into the thermal evolution of electron density in crystalline materials. In this work, temperature-dependent dynamic electron density of α-KNO_3 is reconstructed from high-resolution synchrotron X-ray diffraction data using multipole electron-density models [1]. The thermally averaged density incorporates atomic displacement effects and enables examination of bonding topology at 100, 200, 290, and 380 K. Topological analysis reveals pronounced temperature-dependent variations in the electron density and Laplacian at the N–O bond critical points. The initially non-equivalent N–O bonds progressively evolve with temperature and become nearly equivalent at 380 K, preceding the $\alpha \rightarrow \beta$ phase transition [2]. To quantify this electronic symmetry breaking, a microscopic order parameter (η) is defined from the topological parameters of the N–O bond critical points. These results demonstrate that dynamic electron density provides a sensitive probe of electronic precursors to structural phase transitions. Further theoretical electron density analysis is currently in progress and compare it with the experimental one.

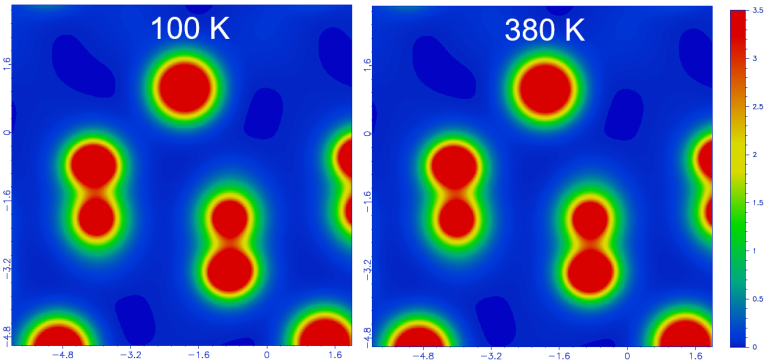

Fig. 1: Dynamic electron density distribution through atoms O1, N1, and O2 at 100 K and 380 K.

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Development and Characterization of a Novel Inorganic/Organic Eutectic PCM Composite for Thermal Energy Storage

Imran Sk[1]*, Swastik Mondal[1,2]

[1]CSIR-Central Glass and Ceramic Research Institute, 196, Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India.

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

immu.ju.1065@gmail.com

Phase Change Materials (PCMs) are promising for thermal energy storage; however, single component PCMs often suffer from limited tunability and stability issues. In this study, a eutectic PCM based on magnesium nitrate hexahydrate (MNH) and Acetamide was developed and reinforced with expanded graphite (EG) for enhanced thermal performance.

The eutectic composition and phase transition temperature were theoretically predicted using the Schröder-Van Laar equation and subsequently validated through experimental analysis. The theoretical prediction indicated a eutectic temperature of approximately 36.8°C, while experiments revealed a melting range of 34.7-37.9°C. The optimized PCM exhibited a latent heat of fusion of 76.68 J/g, reasonably close to the theoretical value (87.23 J/g), indicating effectiveness of the theoretical calculations. Incorporation of EG improved thermal conductivity and structural stability, reducing leakage typically associated with salt hydrate PCMs. The near-ambient phase transition temperature highlights the potential of this composite PCM for passive building cooling and energy-efficient thermal management applications.

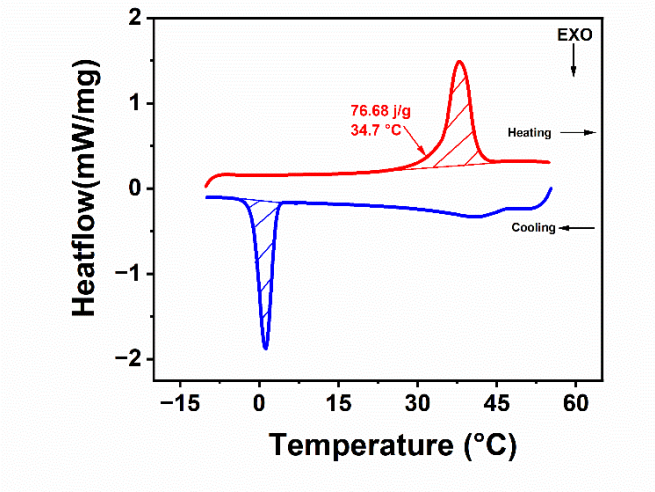

Fig. 1: DSC curve of the final composite, incorporating EG, demonstrates successful thermal stabilization and performance

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Exploring the dynamics of grain growth and coarsening in polycrystalline materials through finite-element method and multiphase-field simulation

Jayee Sinha[1], Atanu Ghosh[2]*

[1]Department of Electronic Science, University of Calcutta, 92 A.P.C. Road, Kolkata, 700009, India

[2]Department of Electronic Science, Rishi Bankim Chandra College, West Bengal State University, Berunanpukuria, North 24 Parganas, Kolkata, 700126, India

jselc@caluniv.ac.in

A two-dimensional multiphase-field model has been developed using finite-element based technique to study temporal evolution of grain growth and coarsening in polycrystalline materials. This work, for the first time, demonstrates a simple programming-based approach to simulate complex microstructure evolution during polycrystalline grain formation developed using finite-element software suite, popularly known as COMSOL Multiphysics. Effect of initial nucleation condition on the evolution of final polycrystalline microstructure has been systematically investigated. Moreover, optimization study has been performed to compare the computational efficiency of adaptive mesh over default triangular shaped static mesh available in COMSOL Multiphysics. In addition, this study also investigates the temperature dependence of grain growth in polycrystalline materials. A comparative analysis between our simulated results and experimental observations demonstrates good agreement and thus, validates our proposed method.

Multiphysics Simulation Assisted CO_2 Adsorption Bed Design

Satya Prakash Pandey[1], **Ankush Pratap Singh**[1]*

[1]CSIR-Central Glass and Ceramic Research Institute, 196, Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India

apsingh@cgcri.res.in

The performance of adsorption-based carbon capture systems is strongly governed by the coupled transport of momentum, mass, and heat within porous adsorption beds. Conventional adsorption columns typically employ straight or planar geometries, which can limit interfacial contact area and reduce mass transfer efficiency between the gas phase and the adsorbent surface. In this study, a geometry-driven intensification strategy is proposed by introducing a wavy axisymmetric adsorption channel to enhance the surface-area-to-volume ratio and improve transport characteristics within the adsorption bed. A comprehensive two-dimensional non-isothermal numerical model is developed to investigate CO_2 adsorption dynamics in the structured porous bed. The model simultaneously solves the governing equations for fluid flow, mass transport, and energy conservation under non-thermal local equilibrium conditions. Adsorption equilibrium is described using the Toth isotherm, while adsorption kinetics are modelled through the linear driving force (LDF) formulation to account for intra-particle mass transfer resistance. The exothermic nature of CO_2 adsorption is incorporated through coupled gas–solid energy equations, enabling accurate prediction of thermal effects during the adsorption cycle. The conventional planar axisymmetric configuration is extended to a wavy axisymmetric geometry to promote enhanced mixing, increased adsorbent–gas interfacial area, and improved axial transport characteristics. Numerical simulations are performed to examine the influence of geometric waviness on flow structure, adsorption breakthrough behaviour, and temperature evolution within the bed. The results reveal that the wavy configuration significantly enhances adsorption performance by delaying CO_2 breakthrough and improving adsorbent utilization due to intensified convective transport and better heat dissipation. The findings demonstrate that geometric structuring of adsorption beds provides an effective pathway for process intensification in carbon capture systems. The proposed wavy axisymmetric adsorption configuration offers a promising design strategy for next-generation compact adsorption reactors and structured adsorption columns aimed at improving the efficiency of gas separation and post-combustion CO_2 capture technologies.

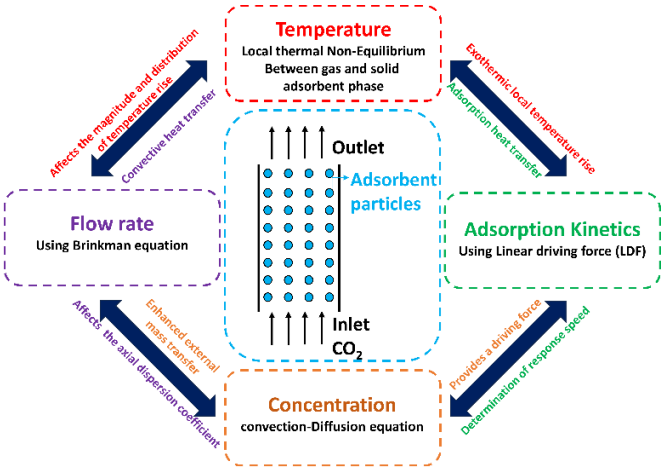

Fig. 1: Schematic of the multi-physics coupling involved in the adsorption process

Structural transformation of two-dimensional oxide thin films supported on Pt(111)/Al_2O_3(0001)

Vipin Kumar Singh[1]*, C. Ruano Merchan[2], J. Ledieu, and V. Fournée[2]

[1]CSIR-Central Glass and Ceramic Research Institute, 196, Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India.

[2]Institut Jean Lamour UMR 7198, Université de Lorraine – CNRS, Nancy, France

svipin65@gmail.com

Two-dimensional oxide quasicrystals have been observed for Ba-Ti-O [1] and Sr-Ti-O [2] ultra-thin films supported on hexagonally close-packed metal substrates. In recent work, a new square approximant with a giant unit cell as well as a hexagonal phase has been reported using an all-thin-film approach where the metal single crystal is replaced by a 10 nm thick Pt-(111) buffer layer grown on an Al_2O_3(0001) substrate by molecular beam epitaxy, whereas the oxide film is grown by pulsed laser deposition [3]. Here, we report the transformation of such Sr-Ti-O quasicrystalline approximant thin films into Sr decorated Ti_2O_3 honeycomb lattices upon annealing under ultra-high vacuum conditions.

The spontaneous formation of a 'labyrinthic' phase as well as a partially ordered $(2\sqrt{3}\times 2\sqrt{3})R30^\circ$ phase will be reported. These results are consistent with a recent proposal based on density functional theory calculations that two-dimensional quasicrystals/approximants can be transformed into Sr-decorated Ti_2O_3 honeycomb lattices through low-energy defects identified as Stone–Wales transformations, typical of hexagonal 2D materials [4]. Besides structural transformation in $SrTiO_3$, we will also discuss interesting structural evolution in $SrRuO_3$ and $DyVO_3$ oxide films upon ultra-high vacuum thermal treatments.

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Anharmonic Chain as a Tool to Understand the Spread of Chaos and Transport Phenomena in Materials

Debabrata Das[1,2], Saurish Chakrabarty[3]*

[1]Beraberi Suryya Narayan Memorial High School (H.S.), Bajemelia, Dist. Hooghly, 712407, India,

[2]Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700009, India

[3]Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata 700131, India
saurish@apccollege.ac.in

The study of chaos in spatially extended systems has been an active area of research in recent decades. Applications of these ideas encompass thermalization phenomena in various condensed matter systems, chaotic effects in quantum circuits, spin chains (both classical and quantum), damage spreading and related systems. After presenting a brief review of such systems, we focus on the Fermi-Pasta-Ulam-Tsingou β (FPUT$-\beta$) chain and study the spread of spatiotemporal chaos, as done for the Heisenberg chain [1]. We find that a perturbation introduced in the system grows exponentially and spreads ballistically. The propagation of the front can be used to calculate the butterfly velocity as well as the light-cone velocity. We hope to get a deeper understanding about the universality of the results obtained in similar studies using spin chains and using quantum systems. Moreover, the results obtained for this system may relate more directly to atomistic condensed matter systems with pairwise interactions.

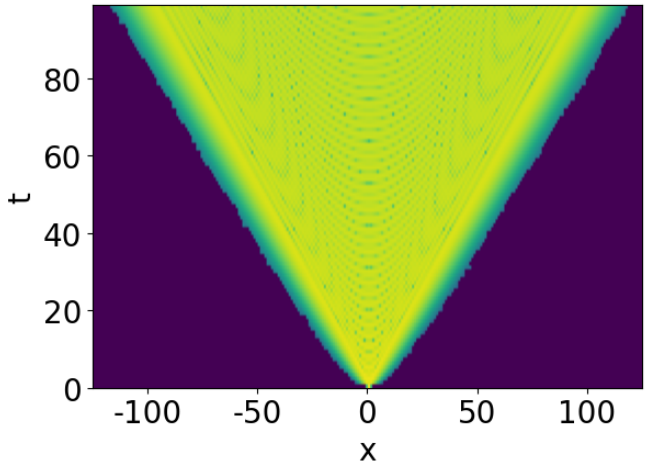

Fig. 1: Light-cone obtained from the decorrelator, D(x,t), of the FPUT$-\beta$ chain

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Machine-Learning Identification and Growth of Ice Phases in Molecular Simulations Using a Variational Autoencoder

Dibyendu Maity[1], Suman Chakrabarty[1]*

[1]S.N, Bose National Center for Basic Sciences, Kolkata-700106

sumanc@bose.res.in

The identification and classification of different phases of ice within molecular simulations remains a challenging problem due to the exceptionally rich phase space of water, encompassing numerous crystalline and amorphous ice polymorphs. Traditional structural order parameters often lack the sensitivity and transferability required to reliably distinguish these phases, particularly in the presence of thermal fluctuations and interfacial disorder.

In this work, we introduce a machine learning–based framework, IceCoder, which combines the Smooth Overlap of Atomic Positions (SOAP) descriptor with a variational autoencoder (VAE) to achieve robust classification of ice phases. High-dimensional local structural information encoded by SOAP descriptors is nonlinearly compressed into a low-dimensional latent space using the VAE, enabling intuitive visualization and clear separation of multiple crystalline ice phases alongside liquid water. The model is trained on an extensive dataset generated from molecular dynamics simulations and demonstrates high accuracy and generalization across diverse thermodynamic conditions.

Beyond phase identification, we show that the learned latent variables provide a physically meaningful, continuous machine-learned order parameter that captures subtle structural transformations along phase-transition pathways. This order parameter can be directly employed to monitor, bias, and control ice nucleation and growth processes in enhanced-sampling simulations, offering a principled route to steer rare-event dynamics beyond the capabilities of conventional handcrafted order parameters.

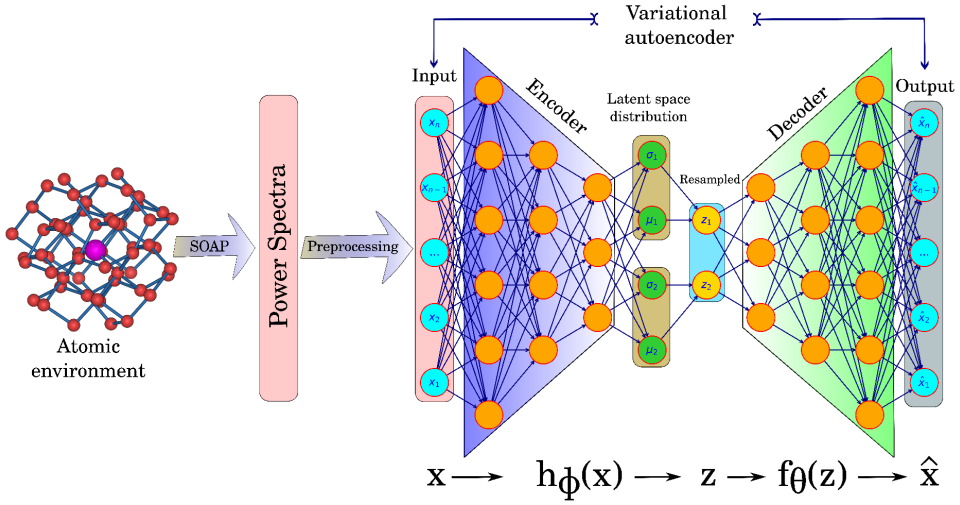

Fig. 1: IceCoder's architecture alongside a schematic of the workflow

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The Schematic Mode Coupling Theory

Kankana Basu[1], **Saurish Chakrabarty**[1]*

[1]Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata 700131, India

saurish@apccollege.ac.in

Glass transition and glassy dynamics have been known since ages. A central goal of some theories of the glass transition was to explain the dynamics of supercooled liquids near the glass transition using their structural information. One of the promising earlier theories along these lines, was the mode coupling theory (MCT). Using structural information, MCT can explain the dramatic slowing down of supercooled liquids approaching the glass transition. However, its prediction deviates from experimental data well above the "glass transition temperature". With a goal of expanding the range of validity of MCT, we focus on the schematic MCT equation which may be thought of as a model describing a damped harmonic oscillator with history dependent damping force [1]. We simulate this system and observe the variation of its relaxation time with a controlling parameter, λ, in the system. We also report the variation of the τ-versus-λ graph with other parameters in the system. We discuss the meanings of our results in the context of MCT.

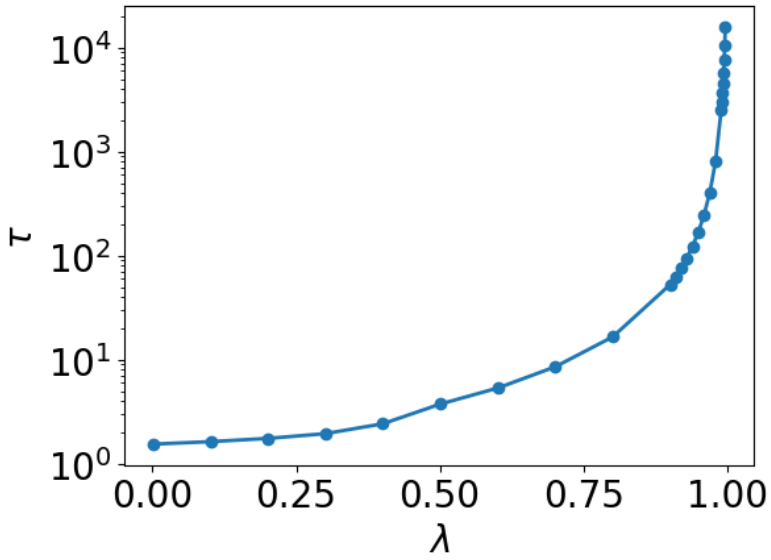

Fig. 1: Variation of the relaxation time, τ, with the parameter, λ

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Unlocking Vanadium Dichalcogenide Monolayers (V_2Se_2 and V_2Te_2) for High-Performing Sodium-Ion Batteries: From Experiment to First-Principles

Mousumi Parvin[1]*, Beena Mol Babu[2], Tata Sanjay Kanna Sharma[2], Jayasmita Jana[2,3], Somnath Chowdhury[2], Seung Hyun Hur[2], Won Mook Choi[2], Sung Gu Kang[2], Bikash Chandra Gupta[1]

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

[2]School of Chemical Engineering, University of Ulsan, 93 Daehakro, Nam-Gu, Ulsan 44610, South Korea.

[3]Department of Chemistry, Manipal University Jaipur, Dehmi Kalan, Jaipur 303007, India

parvinmousu@gmail.com

Developing an efficient anode material is always beneficial for advancing sodium-ion battery (SIB) technology. Experimental studies on vanadium-based dichalcogenides have demonstrated the feasibility of synthesizing layered chalcogenide materials such as V_2Se_2 and V_2Te_2 composed of its two-dimensional (2D) building units. These stacked structures were successfully synthesized using thermal treatment and characterized using X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and field emission scanning electron microscopy (FESEM). Furthermore, Density functional theory calculations were performed to explore the potential of V_2Se_2 and V_2Te_2 monolayers as anode materials. The results confirmed their overall stability, supporting structural robustness during battery operation. Both monolayers exhibit low Na^+ diffusion barriers (0.24–0.28 eV), enabling rapid ion transport, along with a maximum theoretical capacity of 619.17 mAh/g and low open-circuit voltages, highlighting their strong potential as next-generation anode materials for sodium-ion batteries.

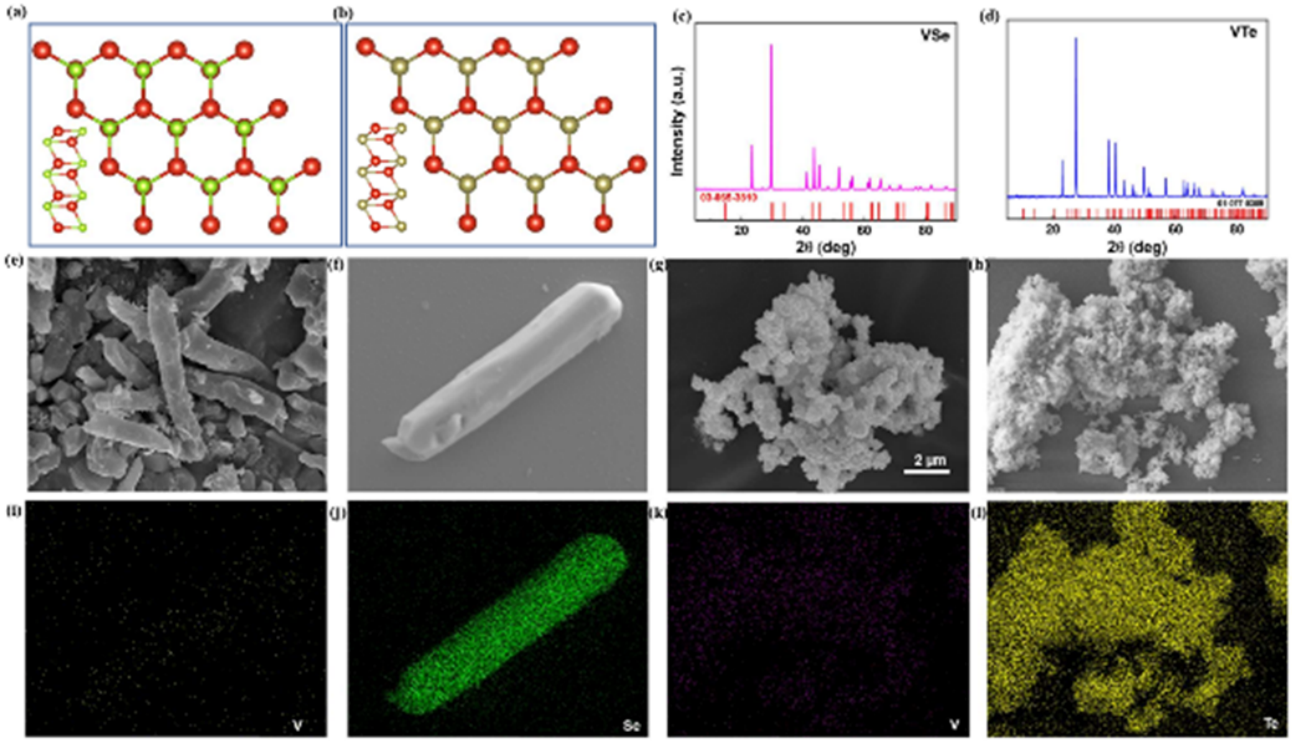

Fig. 1: Optimized structures (top and side view) of (3×3) supercell of (a) V_2Se_2 and (b) V_2Te_2 monolayer. [The red, green, and beige spheres represent V, Se, and Te atoms, respectively.] XRD pattern of (c) VSe and (d) VTe. FESEM Image of VSe and VTe at different magnifications (e, f) and (g, h), respectively. Elemental mapping of (i) V and (j) Se for VSe, and (k) V and (l) Te for VTe.

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A Unified Computational Framework for Two-Dimensional Diffusion-Limited Aggregation via Finite-Size Scaling, Multifractality, and Morphological Analysis

Satish Prajapati[1]*

[1]Department of Ceramic Technology, Government College of Engineering and Ceramic Technology, Kolkata, West Bengal 700010, India

iamsatish.gcect.ac@gmail.com

Diffusion-Limited Aggregation (DLA), the canonical model for non-equilibrium fractal growth, emerges from the simple rule of irreversible attachment by random walkers. Despite four decades of study, a unified computational framework reconciling its stochastic algorithm, universal fractal dimension, multifractal growth measure, and finite-size effects remains essential for applications from materials science to geomorphology. Through large-scale simulations (clusters up to $N = 10^6$ particles) in two dimensions, we perform a tripartite analysis: (1) We establish a definitive finite-size scaling collapse, extracting the universal fractal dimension $D = 1.712 \pm 0.015$ and identifying the crossover to boundary-dominated growth at a scaled mass $x_0 \approx 0.10 \pm 0.02$. (2) We quantify the full multifractal spectrum of the harmonic measure ($\Delta\alpha \approx 1.13$), directly linking the stochastic algorithm to the deterministic Laplacian growth equation $\nabla^2 p = 0$ and explaining the screening effect via an exponential decay $\eta \sim e^{-r/\xi}$ with screening length $\xi = 22.7 \pm 0.8$ lattice units. (3) We provide a complete morphological characterization, revealing power-law branch length distributions ($\tau \approx 2.1$) and angular branching preferences ($\sim 72^\circ$). This work computationally validates DLA as a robust universality class and provides a scalable methodology for analyzing diffusion-controlled pattern formation across disciplines.

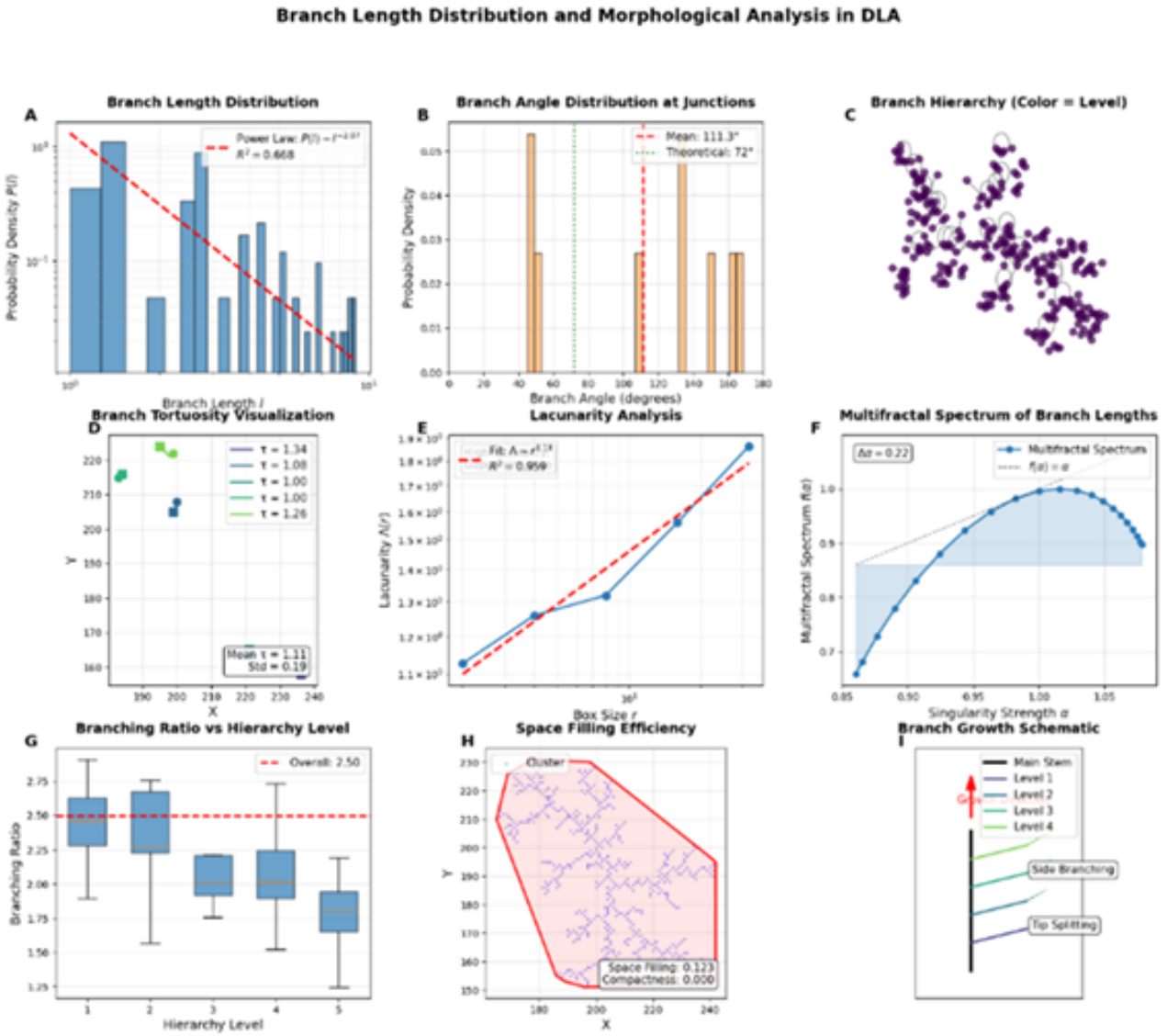

Fig. 1: Branch morphology. (A) Power-law distribution of branch lengths $P(l) \sim l^{-2.1}$. (B) Distribution of branching angles. (C) Hierarchical branch visualization. (D) Branch tortuosity vs. length. (E) Lacunarity $\Lambda(r)$ vs. scale r. (F) Multifractal spectrum of branch lengths. (G) Branching ratio by hierarchy level. (H) Box-counting analysis. (I) Schematic of hierarchical growth

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Local Uncertainty Relations and Planckian Bounds

Saurish Chakrabarty[1]*, Zohar Nussinov[2]

[1]Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata 700131, India.

[2]Department of Physics, Washington University in St. Louis, MO 63130, USA.

saurish@apccollege.ac.in

We discuss bounds on various quantities in thermal quantum many-body systems derived using local uncertainty relations. Such bounds are known in the literature as Planckian bounds.[1] These encompass (non-relativistic) speed limits, minimum relaxation times, bounds on transport coefficients, bounds on chaos and related ideas.[2-4] Similar bounds are derived using other routes in various specific contexts but we use a general approach starting from (local) uncertainty relations and get results which have a wider applicability. We discuss how our results compare to values obtained from experiments and find that in many situations, our bounds are fairly tight.

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Revisiting a Landau-like Theory for Glassy Dynamics

Shagufta Khan[1], Saurish Chakrabarty[1]*

[1] Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata 700131, India

saurish@apccollege.ac.in

Following the work in [1], we study a Landau-like theoretical framework for describing glassy dynamics near a critical point. In glassy systems, relaxation times grow dramatically with decreasing temperature. This growth neither follows a power law (as in critical phenomena), nor the simple Arrhenius law characterized by a temperature independent activation energy (as in phenomena described by simple activated processes). The relaxation time versus temperature data are often well described by phenomenological relations such as the Vogel-Fulcher-Tammann (VFT) law. The work in [1] showed that such behavior can emerge naturally from Landau theory. The novelty of that work was the idea of asymmetric transition rates (for energy increasing and energy lowering processes), borrowed from protein folding literature. We explore the implications of their result from different angles and propose modifications. In particular, we find a new (short) relaxation time-scale which was not discussed earlier. Surprisingly, this time-scale grows as we go away from the transition point.

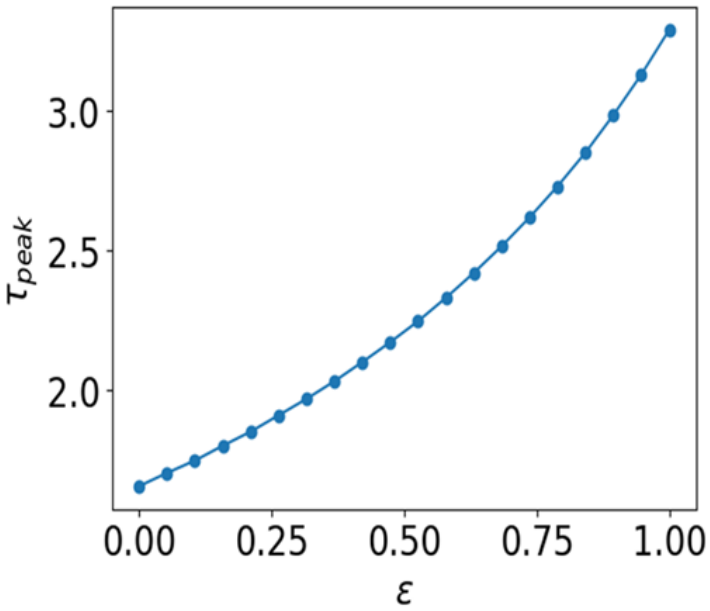

Fig. 1: New time-scale corresponding to the peak in probability distribution of the order parameter. Here, ϵ represents the distance from the transition point.

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Electronic Band Structure of Bulk Materials of Bismuth Antimony Nanowires

Ali Ahmad Ansari[1]*

[1]R.D.S. College, Purnea University, Purnia Bihar, India - 854301

aliahmadkne1@gmail.com

We have developed a model for the miniband gap and the related nonparabolic dispersions at the limiting of bismuth antimony. We have used an interactive one dimensional two band model and developed an analytical approximation for this model. We have studied the band edges and electronic phases as a function of grow the orientation, wire diameter and stoichiometry, including the semimetal phases, the indirect semiconductor phases and the direct semiconductor phases. We have found that bulk materials of bismuth antimony and their alloys have the same symmetry with a rhombohedral lattice structure. There are two atoms per unit cell. The trigonal axis with a threefold symmetry, the binary axis with a twofold symmetry and the bisectrix axis form a natural cartesian coordinate frame. A mirror plane is formed by the trigonal axis and the bisectrix axis which is perpendicular to the binary axis. The band structure does not change notably with temperature.

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Quantum imprisonment and flux induced diffusive modes in a self-similar corral

Sayan Bhattacharya[1]*, Rhiddha Acharjee[2], Atanu Nandy[1]

[1]Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata, West Bengal-700 131, India

[2]Department of Physics, University of Calcutta, 92, Acharya Prafulla Chandra Road, Kolkata, West Bengal-700 009, India

sayanbhatta2002@gmail.com

We have explored the spectral scenarios of a self-similar corral network using the tightbinding formalism. A magnetic flux threading each elemental plaquette can give rise to a resonant band populated by Bloch-like eigenfunctions even in such a scale-invariant fractal entity. Our findings have been corroborated by the evaluation of density of states and inverse participation ratio. The robustness of the diffusive band has been tested in the presence of diagonal disorder. The flux-periodic band spectrum prompts us to study the persistent current offered by such a network. All these spectral issues can be mapped into an effective waveguide model, which helps to study photonic localization as well.

Flat-band, Mobility-edge induced off-diagonal anisotropy in Peano fractal and its optical analogue

Rhiddha Acharjee[1]*, Sayan Bhattacharya[2] , Atanu Nandy[2]

[1]Department of Physics, University of Calcutta, 92, Acharya Prafulla Chandra Road, Kolkata, West Bengal- 700 009, India.

[2]Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata, West Bengal-700 131, India

rhiddhaacharjee777@gmail.com

A tight-binding Peano fractal lattice is reported to exhibit a flat band in the presence of off-diagonal anisotropy. These non-resonant self-localized modes exhibit a cluster-like amplitude distribution leading to the formation of compact localized states. The analysis is substantiated by the calculation of the density of states and transport properties. The spectrum contains critical states at the centre of the band, and they are surrounded by diffusive states. The spectral issue and whether quantum transport indicates a possibility of getting a single particle mobility edge. This is validated through the standard multifractal analysis. The equivalent optical waveguide mode is also discussed using the straightforward analogy between the electronic and optical cases within the tight-binding framework.

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Electrical and thermoelectrical transport in open long-range Kitaev chain

Averi Banerjee[1],Syeda Rafisa Rahaman[2]*, Nilanjan Bondyopadhaya[2]

[1]Department of Basic Science and Humanities, Techno International Newtown, Kolkata 700156, India.[2]Integrated Science Education & Research Centre, Visva-Bharati University, Santiniketan 731235, India.

rahamanrafisa@gmail.com

We investigate electrical, thermal, and thermoelectric transport in a hybrid an N-TS-N junction where the middle topological superconductor (TS) is an LRK/SRK chain, and the leads/baths are made of normal metal (N). Using the quantum Langevin equation and Green's function (LEGF) formalism, we study transport under both voltage and temperature bias and compare the results with the conventional short-range Kitaev chain (SRK). Long-range hopping and pairing interactions significantly modify the spectral and transport properties of the system. In contrast to the SRK chain, the LRK chain exhibits massive Dirac edge modes, absence of gap closing at the topological phase transition, and clustering of delocalized bulk states near the band gap. These features strongly influence current–voltage and current–temperature characteristics. In particular, currents remain suppressed near the transition point and increase rapidly once the bias exceeds the finite gap. Our results demonstrate that electrical and thermal transport measurements can serve as effective probes of long-range interactions and topological phases in superconducting quantum systems.

Keywords:Long-range interaction, Kitaev chain, Transport

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Dy^{3+} – Sb infused Borophosphate Glasses: Prospects for Photonic and Gamma-ray Shielding

Paul Dhinakaran A[1]*, K. Pradheesha[1], P. Vinothkumar[1]

[1]Department of Basic Science and Humanities, Techno International Newtown, Kolkata 700156, India.

[2]Integrated Science Education & Research Centre, Visva-Bharati University, Santiniketan 731235, India.
sagaidhina24@gmail.com

Rare-Earth doped Borophosphate glasses, including the compositions Dy^{3+}–Sb was synthesized using the traditional melt-quench process, and underlying structural, spectroscopic, and gamma (γ)-radiation protection properties were thoroughly assessed. X-ray diffraction and scanning electron microscopy (SEM) were used to confirm the glasses' amorphous nature. Glass transition temperatures ($T_g = 276 - 290$ °C) and higher thermal stability for Dy^{3+} – Sb glass ($\Delta T = 29$ °C, $H = 0.101$, $S = 0.16$) were found by DSC analysis. Characteristic BO_3/BO_4 and PO_4 units were seen in FTIR spectra, indicating that the borophosphate network is intact. Indirect transitions appropriate for optoelectronic devices were found to have optical band gaps of 2.33 eV (Dy^{3+}-Sb). The photoluminescence spectra showed strong emissions at 573 nm (Dy^{3+}). Based on gamma-ray shielding properties, among the glasses under investigation, the Dy^{3+}–Sb BPG glass demonstrated the best attenuation performance, with maximum experimental mass attenuation coefficient and linear attenuation coefficient values of 0.0759 cm^2/g and 0.2629 cm^{-1} at 0.6617 MeV, as well as the lowest HVL (2.64 cm) and MFP (3.80 cm). Radiation Protection Efficiency (RPE) for the Dy^{3+} – Sb glass at increased thicknesses, while its attenuation parameters were 0.2202 cm^{-1} (linear attenuation coefficient) and 0.0756 cm^2 g^{-1} (mass attenuation coefficient) at 0.662 MeV. The transmission factor (TF), which decreased exponentially with increasing thickness. Based on these results, the Dy^{3+}–Sb BPG borophosphate glass is a potential multifunctional material for photonics and gamma radiation protection applications. These finding provides an outstanding gamma shielding efficiency properties.

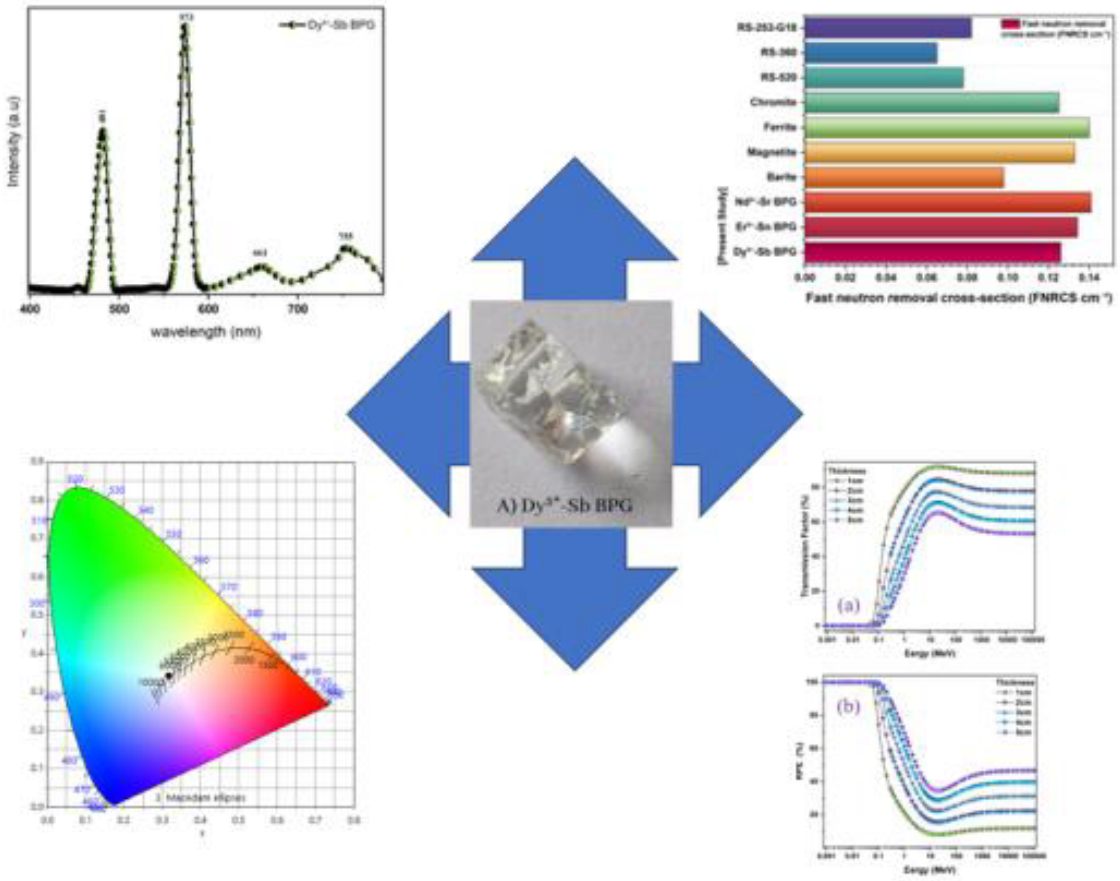

Fig. 1: Dy^{3+}–Sb infused Borophosphate glass

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Optical Band Gap and Dielectric Response of Monoclinic Double Perovskite Sr_2YbNbO_6

Arpita Barua

The lead-free double perovskite Sr_2YbNbO_6 (SYN) was prepared by the conventional solid-state ceramic method. Structural analysis confirms the formation of a monoclinic phase ($P2_1/n$). Microstructural study shows a polycrystalline morphology with an average grain size of $\sim$2.38 μm. Raman spectroscopy identifies 24 vibrational modes, while FTIR spectra reveal the stretching and bending vibrations of YbO_6 and NbO_6 octahedra, confirming the ordered octahedral framework. Optical measurements indicate a band gap of 3.08 eV. The dielectric response was studied over 50 Hz–1 MHz and 303–513 K. The material exhibits polydispersive dielectric relaxation, well described by the Cole–Cole model. The calculated activation energy of 0.52 eV suggests that the conduction process is dominated by p-type small polaron hopping. These results demonstrate the structural stability and dielectric behavior of Sr_2YbNbO_6, highlighting its potential for lead-free dielectric and electronic applications.

$ZnMn_2O_4$, A Bimetallic Oxide as Active Electrode For Supercapacitor Applications

Ratan[5], Akshi Arya[4], Abhay Kaushik[1], Shaifali Tiwari[2], T. Dayananda Sharma[4], Reema Gupta[3], Kajal Jindal[2], Malika Verma[4], Monika Tomar[4]*

[1]Department of Physics, Ramjas College, University of Delhi, Delhi-110007, India.

[2]Department of Physics, Kirori Mal College, University of Delhi, Delhi-110007, India.

[3]Department of Physics, Hindu College, University of Delhi, Delhi-110007, India.

[4]Department of Physics, Miranda House, University of Delhi, Delhi-110007, India.

[5]Electrical Department, Delhi Technological University, Delhi-110042, India

monika.tomar@mirandahouse.ac.in

The rapid population growth and technological advancement fuelled global energy demand. World is on race to develop an efficient, and sustainable energy storage solutions. Amongst the available technologies, supercapacitors have emerged as promising devices, bridging the gap between conventional capacitors and batteries. Supercapacitors exhibit higher energy and power densities, with long cycle life, low maintenance requirements and enhanced safety compared to conventional systems. Transition bi and tri metal oxides, owing to their multiple oxidation states, rich redox chemistry and high theoretical capacitance values have garnered much attention for development of supercapacitor electrodes. In this research, $ZnMn_2O_4$, a bimetallic oxide with a spinel crystal structure, has been synthesized as the active electrode material using a facile co-precipitation method followed by thermal treatment at varying calcination temperatures. The material was thoroughly characterized using a combination of structural and electrochemical techniques, including X-ray diffraction (XRD), UV–Visible (UV–Vis) spectroscopy, Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS). Each technique provided insights into phase composition, crystallinity, band gap, charge storage behaviour and resistance characteristics. The study highlights the effect of calcination temperature on the crystallite size, lattice parameters and electrochemical performance of $ZnMn_2O_4$. Specific capacitance is found to have maximum value of 139.87 F/g at 10 mV/s, revealing pseudocapacitive behaviour and good rate capability. The results demonstrate that $ZnMn_2O_4$ electrodes can significantly enhance supercapacitor performance.

Keywords: Supercapacitor, $ZnMn_2O_4$, Bimetallic Oxide, Pseudocapacitance, Energy Storage

Aging during domain growth of a phase-separating binary fluid confined inside a nanopore

Saikat Basu[1], **Suman Majumder**[2]

[1]Department of Physics, Sonamukhi College, Sonamukhi, Bankura, West Bengal 722207.

[2]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313

saikatjuphy0809@gmail.com

It is well known that hydrodynamics have strong effects on the kinetics of phase separation. Open questions on the manifestation of such effects in confined systems still exist and of great importance. In this particular report, we have undertaken extensive studies of the kinetics of phase ordering in a two-component fluid which is confined inside cylindrical pores having quasi-one-dimensional geometry. Using a thermostat that preserves hydrodynamics, we carry out molecular dynamics (MD) simulations to obtain results for domain growth and aging for varying pore width (where the ratio of pore width to the length of the cylinder is taken 1:10) and temperature. We observe that all systems, irrespective of its size, freeze into a striped morphology where stripes of regions rich in one or the other component of the mixture coexist. Our detailed analysis suggests that the growth of the average domain size, $\ell(t)$, prior to the freezing into stripped patterns, follows the power law, $\ell(t) \sim t^{\alpha}$ which is irrespective of the temperature. Furthermore, this finding is suggesting an inertial hydrodynamic growth, typically applicable for bulk fluids, only in the asymptotic limit. Similarly, the aging dynamics, which is probed by the quantification of two-time order-parameter autocorrelation function, also suggest simple ageing and it exhibits a temperature-independent power-law scaling with an exponent λ, which is much smaller than what is observed in a bulk fluid.

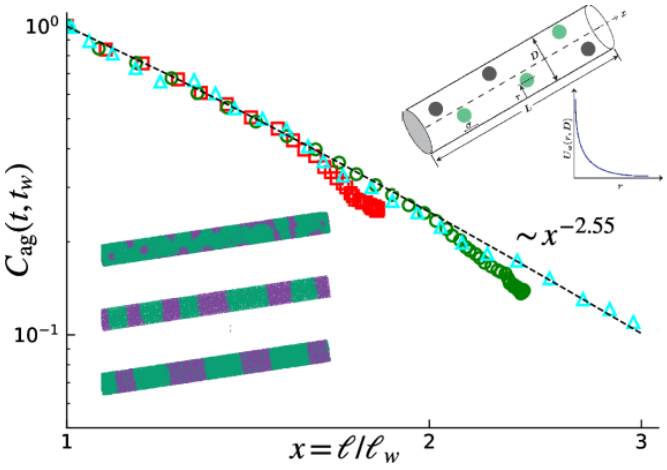

Fig. 1

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Physically consistent enhanced sampling of glass configurations through a DDPM-based framework

Satabdi Roy[1,2], Nagesh B E[3], Jagannath Mondal[3], Indrajit Tah[1,2]*

[1]Specialty Glass Division, CSIR-Central Glass and Ceramic Research Institute Kolkata, 700032, West Bengal, India.

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

[3]Tata Institute of Fundamental Research Hyderabad, Telangana 500046, India
indrajittah.cgcri@csir.res.in

Structural analysis of glass is crucial as the macroscopic properties are strongly governed by its microscopic structure. Glass structures are traditionally generated using molecular dynamics (MD) simulations through the melt-quench technique but this comes with some limitations. Transitions between metastable states in glassy liquids occur on timescales of milliseconds to hours, which remain largely inaccessible to conventional MD simulations.

Generative AI (GenAI) can help enhanced sampling by generating new atomic configurations that traditional MD may take very long time to reach. But achieving efficient enhanced sampling that accelerates configurational exploration while preserving the fundamental physical characteristics of the glass system remains one of the most significant challenges, primarily due to the presence of highly rugged and complex energy landscapes. Therefore, it is truly difficult to generate physically consistent atomic configurations that properly reproduce both local and medium-range structural order of the glass relying solely on brute-force simulation approaches.

Recent advances in generative machine-learning models offer a promising alternative, with approaches such as: Variational Autoencoders (VAE), Generative Adversarial Networks (GAN), Diffusion Models [1, 2] etc. These generative frameworks aim to learn the underlying configurational distribution of glass network which in turn will lead to the generation of statistically consistent structures. In this work, the main objective is to achieve improved configurational sampling by adopting a diffusion model mainly a Denoising Diffusion Probabilistic Model (DDPM) framework. We aim to develop a model capable of generating the structures of entire MD trajectory while maintaining structural consistency with the temporal evolution of the actual system. To achieve this goal, autoencoder-based latent representations have been analyzed on low silica calcium aluminosilicate glass melt which not only can help in dimensionality reduction, but also can capture hidden structural descriptors that are difficult to identify using conventional order parameters. This approach holds potential for generating physically consistent structures and improving configurational sampling.

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