

2nd

International Conference on Recent Developments and Applications in Materials Science and Engineering

RDAMSE 2026

7 – 8th May, 2026



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Editors

Dr. Dipankar Das, Asst. Prof., BSH, SurTech
Dr. Biswajit Das, Asst. Prof., BSH, SurTech

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Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex
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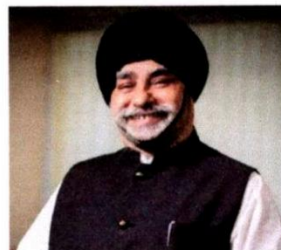
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Messages





Sardar Taranjit Singh,
Chancellor, JIS University
Managing Director, JIS Group

Message

It gives me great pleasure to extend my warm greetings to all participants of the **2nd International Conference on “Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)”**, to be held on 7–8 May 2026.

Following the remarkable success of **RDAMSE 2025**, organized by the Department of Basic Science & Humanities, SurTech, it is encouraging to see this conference grow into a significant international platform in its second edition. **RDAMSE 2026** brings together eminent international speakers from the **USA** and **Japan**, along with distinguished national experts from premier institutions including **IISc, IIT, IEST, IISER, Jadavpur University, IACS, CSIR-CGCRI, DRDO**, and other reputed organizations and industries.

More than an academic gathering, this conference serves as a vibrant forum for the exchange of ideas, innovation, and collaboration. Materials Science and Engineering continues to drive progress in sustainable energy, healthcare, environmental solutions, and advanced technologies, addressing key global challenges.

I am pleased that **RDAMSE 2026** is being organized in association with esteemed partners including the **Indian Photobiology Society, Jadavpur University, Society for Materials Chemistry, Kolkata Chapter, Sripat Singh College**, and **Subhami Biopharma Pvt. Ltd.**, reflecting the collaborative spirit essential for meaningful progress.

At **JIS Group**, we believe innovation emerges through the synergy of academia, industry, and research. I am confident that **RDAMSE 2026** will inspire new ideas, foster impactful collaborations, and contribute significantly to scientific advancement for the betterment of society.

I extend my heartfelt best wishes for the grand success of the conference and wish all participants a highly enriching and memorable experience.

Best Regards,

Sardar Taranjit Singh
Managing Director, JIS Group



Sardar Simarpreet Singh,
Director, JIS Group

Message

It is a matter of immense pride and pleasure to welcome distinguished scientists, academicians, researchers, industry professionals, and students to the **2nd International Conference on "Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)"**, scheduled to be held on 7–8 May 2026.

Following the successful organization of **RDAMSE 2025** by the Department of Basic Science & Humanities, SurTech, I am delighted to witness the continuation of this prestigious event in its second edition. **RDAMSE 2026** brings together eminent international speakers from the USA and Japan, along with distinguished national experts from premier institutions such as **IISc, IIT, IIST, IISER, Jadavpur University, IACS, CSIR-CGCRI, DRDO**, and several reputed institutes and industries, creating an excellent platform for academic interaction, research collaboration, and knowledge exchange.

Organized in association with esteemed partners including the **Society for Material Chemistry, Kolkata Chapter, Indian Photobiology Society, Jadavpur University, Sripat Singh College, Murshidabad** and **Subhami Biopharma Pvt. Ltd.**, the conference strengthens the spirit of collaborative learning and research. Materials Science and Engineering continues to be a transformative discipline, driving advancements in clean energy, sustainability, healthcare, advanced manufacturing, and smart materials.

At **JIS Group**, we strongly believe that education and research are the pillars of societal progress. By fostering collaboration between academia, industry, and research organizations, we aim to translate ideas into impactful innovations. I am confident that **RDAMSE 2026** will strengthen scientific partnerships, inspire meaningful dialogue, and open new avenues for advancement in materials science and engineering.

I extend my sincere appreciation to the organizers, speakers, and participants whose dedication has made this event possible, and I wish **RDAMSE 2026** grand success as a source of inspiration, knowledge, and lasting collaboration for all.

Warm regards,

Sardar Simarpreet Singh
Director, JIS Group



RANI RASHMONI GREEN UNIVERSITY

TARAKESHWAR, HOOGHLY-712410, WEST BENGAL

Prof. Amiya Kumar Panda

Vice-Chancellor

Mob: +91 943347210; Email: vcrrgu18@gmail.com



DATE: April 30, 2026

Message

It gives me immense pleasure to learn that the "Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), Kolkata an AICTE-approved, NBA accredited, NAAC 'A' graded Autonomous Institution under JIS Group", is going to organize the 2nd International Conference on "Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)", scheduled to be held on 7–8 May 2026 in hybrid mode.

I feel honoured to have been invited to attend such a glorious academic seminar.

I'm confident that there will be thoughtful discussions towards achieving the objectives of this conference.

I convey my best wishes to the organizers, dignitaries, and participants, and wish the event a grand success. The exchange of ideas and deliberations will surely benefit all stakeholders.

I also hope this commendable effort motivates researchers to achieve their goals and strive for excellence.

Amiya Kumar Panda
(Amiya Kumar Panda)

Prof. Amiya Kumar Panda
Vice-Chancellor
Rani Rashmoni Green University
Tarakeswar, Hooghly-712410
W.B., India



Present address: Government General Degree College, P.O- Singur, Dist: Hooghly-712409, W.B., India



Dr. Neeraj Saxena
Pro Chancellor, JIS University

MESSAGE

It is a pleasure to note the organization of the **2nd International Conference on Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)** at SurTech, JIS Group, Kolkata .

We are living through an **Age of Reversals**—where knowledge is abundant and instantly accessible, but insight, judgement, and creativity are increasingly valuable. The role of research must therefore shift—from solving given problems to **discovering new ones**, and from incremental outputs to **transformative creation**.

Materials Science lies at the heart of this transition—powering advances in energy, healthcare, sustainability, and next-generation technologies. The future will emerge not from isolated domains, but from **convergence—of materials with AI, biology, and quantum systems**.

RDAMSE 2026 is thus more than a conference—it is a **platform for rethinking research itself**. As we move forward, *the future will reward creators, not repeaters*. This calls for a fundamental shift in how we approach inquiry, learning, and innovation.

I would also encourage researchers to consciously articulate **future challenges and open questions** in their work—not as a formality, but as an **invitation to young minds**. These become the seeds that draw students toward research as a **purposeful and exciting career path**.

I commend the organizing team for this important initiative and wish RDAMSE 2026 great success. May it inspire ideas that go beyond publications—to **solutions that matter and innovations that endure**.

With best wishes,

Dr. Neeraj Saxena
Pro Chancellor, JIS University



JIS INSTITUTE OF ADVANCED STUDIES & RESEARCH, KOLKATA
(An Autonomous Institute under JIS University)



Prof. Ajoy Kumar Ray (Padma Shri)
Director
Former Professor, IIT Kharagpur
Former Director, IIST Shibpur

Message

I am extremely glad to know that Sur Tech is going to organize the International Conference on Advanced Materials during May 7th and 8th at its Dumdum campus. The rapid technological transformation in this field stands at the forefront of innovation across the globe.

The quest of identifying novel materials—whether nanostructured systems, smart materials, or sustainable composites—is shaping industries across the globe in application areas ranging from energy and healthcare to electronics and sustainability. The recent advances in Material Science and Engineering are also addressing some of the most pressing global challenges, including climate change, resource scarcity, and clean energy transitions.

I am sure that the conference will serve as a platform for the dissemination and exchange of ideas, fostering collaboration amongst institutions in India. I congratulate the organizers and wish the conference all the success.



INDIAN PHOTOBIOLOGY SOCIETY

(Regd. No. : S/10422)

(Affiliated to the Association Internationale de Photobiologie)

Department of Chemistry, Jadavpur University, Kolkata 700 032

President: Prof. Ashok Kumar Mishra

Secretary: Prof. Chittaranjan Sinha

www.ipbsindia.in/ <indianphotobiology@gmail.com>

Prof. Ashok Kumar Mishra, FNASc
President, Indian Photobiology Society
Emeritus Professor, Department of Chemistry
IIT Madras, Chennai 600036

Message from the President, Indian Photobiology Society

It is with great pleasure that I extend my warm greetings to the organizers, participants, student and scholar delegates, and distinguished guests of the 2nd International Conference on *Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)*, scheduled to be held during 7–8 May 2026.

The successful continuation of this conference series reflects the unwavering dedication of the Department of Basic Science & Humanities, Sur Tech, toward advancing scientific research and fostering academic excellence. I would also like to emphasize that India, despite its vast human resource potential, must strive more actively to strengthen its global scientific impact. It is a collective responsibility of our academic and research community to uphold and advance India's rich scientific heritage while contributing meaningfully to the global knowledge economy.

In today's rapidly evolving scientific landscape, the convergence of materials science with fields such as photobiology, environmental science, and energy research has become increasingly significant. Conferences like RDAMSE 2026 provide an invaluable platform for researchers, academicians, and industry experts to exchange ideas, explore emerging technologies, and address contemporary challenges. This edition, being organized in collaboration with the Indian Photobiology Society, further strengthens our shared vision of promoting interdisciplinary dialogue and innovation. The focus on sustainable solutions aligned with global priorities such as clean water, affordable and clean energy, and climate action is both timely and essential.

The presence of eminent international and national experts from leading institutions adds immense value to this conference, ensuring rich discussions and meaningful collaborations. I am confident that the interactions and knowledge-sharing during this event will inspire innovative research directions and contribute to the development of sustainable and impactful scientific solutions.

As President of the Indian Photobiology Society, I am delighted that we are a part of this diverse and distinguished academic initiative. I extend my best wishes for the grand success of RDAMSE 2026 and encourage all participants to actively engage in the sessions and make the most of this opportunity for learning and collaboration.

With warm regards and Best Wishes,

President
Indian Photobiology Society



SRIPAT SINGH COLLEGE

[NAAC ACCREDITED]

P.O. Jiaganj, Dist. Murshidabad, West Bengal, PIN 742 123
e-mail: sscollege2009@gmail.com

Sripat Singh College Joins Hands with RDAMSE 2026 for Academic Collaboration

It is a privilege for Sripat Singh College, Murshidabad, to collaborate with the Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), an Autonomous Institution under JIS Group, Kolkata, for the 2nd International Conference on *Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)*, scheduled to be held on 7–8 May 2026.

Following the successful organization of RDAMSE 2025, this second edition of the conference continues to strengthen its global academic presence by bringing together eminent international speakers from countries such as the USA and Japan, along with distinguished national experts from premier institutions including IISc, IITs, IEST, IISER, Jadavpur University, IACS, CSIR laboratories, and other reputed organizations and industries.

This prestigious international conference, organized in association with the Indian Photobiology Society, Jadavpur University, aims to provide a multidisciplinary platform for discussions on cutting-edge innovations, recent advancements, and emerging challenges in materials science and engineering. The conference is also aligned with key Sustainable Development Goals (SDGs 6, 7, and 13), emphasizing sustainability, clean energy, and environmental responsibility.

Sripat Singh College is proud to be an integral part of this academic initiative, fostering knowledge exchange, research collaboration, and innovation-driven discussions. We look forward to engaging with leading scientists, academicians, industry experts, and young researchers to contribute meaningfully to the advancement of materials science and engineering.

We extend our best wishes for the grand success of RDAMSE 2026.

Dr. Kamal Krishna Sarkar

Principal
Sripat Singh College
Jiaganj, Murshidabad



From the Desk of Dr. Subhalakshmi Ghosh

Founder & Director, Subhami Biopharma (OPC) Pvt Ltd

I am delighted to convey my heartfelt congratulation to the Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), JIS Group, Kolkata, India, for organising the 2nd International Conference on “Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)”, scheduled on 7 - 8 May 2026.

This conference would promote the integration and exchange of innovative ideas, emerging developments, and contemporary challenges in the multidisciplinary platforms of Material Science and Engineering through effective collaboration between industry and academia.

I extend my sincere appreciation to the organizing team, members of the advisory board, eminent speakers, sponsors, faculties and student participants for their dedication and involvement for this event. I firmly believe that, the participants will be immensely benefitted from the opportunity to share ideas, learn from the experts, and will gain insights about cutting edge advancements in Material Science research that would be instrumental in localizing global knowledge to create a societal solution that would be relevant and sustainable.

I extend my best wishes for the successful execution of this conference and absolutely looking forward to its translational outcomes in near future.

Dr. Subhalakshmi Ghosh

Founder & Director

Subhami Biopharma (OPC) Pvt Ltd

Subhami Biopharma (OPC) Pvt Ltd

Registered Address: 5, 1st Road, Eastern Park, Santoshpur, Kolkata - 700075
Office Address: Kolkata Biotech Park, EN-24, Sector V, Salt Lake, Kolkata - 700091
subhami.biopharma@gmail.com | info@subhamibiopharma.com |
www.subhamibiopharma.com | +91- 8584853334 | +91- 9830248534



Dr. Srabanti Ghosh

Convener

Society for Material Chemistry (SMC) Kolkata Chapter

Message from Convener, Society for Material Chemistry (SMC) Kolkata Chapter

It is indeed a privilege for me to convey my heartfelt greetings to all distinguished scientists, academicians, researchers, industry leaders, professionals, and students assembled for the **2nd International Conference on “Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)”**, scheduled to be held on **7–8 May 2026**. This prestigious gathering reflects SurTech’s continuing commitment to academic excellence, research advancement, and global scientific engagement.

Following the successful organization of **RDAMSE 2025** by the Department of Basic Science & Humanities, SurTech, I am delighted to witness the continuation of this esteemed conference in its second edition. **RDAMSE 2026** brings together eminent international speakers from the **USA and Japan**, along with distinguished national experts from premier institutions such as **IISc, IIT, IEST, IISER, University of Calcutta, Jadavpur University, Rani Rashmoni Green University, IACS, CSIR-CGCRI, and DRDO**, as well as several reputed academic institutions and industries, creating a vibrant platform for scholarly interaction, interdisciplinary dialogue, and collaborative research.

I am pleased to note that the conference is being organized in association with esteemed partners including the **Society for Materials Chemistry, Kolkata Chapter**, the **Indian Photobiology Society, Jadavpur University Campus, Sripat Singh College**, and **Subhami Biopharma Pvt. Ltd.**, which reflects the strong spirit of partnership between academia, research organizations, and industry.

As Materials Science and Engineering continues to shape the future through innovations in sustainable energy, healthcare, advanced manufacturing, smart materials, and environmental technologies, I am confident that **RDAMSE 2026** will serve as a catalyst for new ideas, meaningful collaborations, and impactful scientific progress. I extend my sincere appreciation to the organizers, management, speakers, collaborators, and participants whose dedication and efforts have made this conference possible. I wish **RDAMSE 2026** every success and hope that it leaves a lasting impact on the scientific community through knowledge sharing, innovation, and enduring collaborations.

Warm regards,

Srabanti Ghosh

Convener

Society for Material Chemistry (SMC) Kolkata Chapter



Prof. (Dr.) Saradindu Panda

Principal –

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex
(SurTech), (Autonomous Institution), Dum Dum, Kolkata

Message from the Principal

It gives me immense pleasure to extend my warm greetings on the occasion of the publication of the Book of Abstracts for the 2nd International Conference on Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026), scheduled to be held on 7–8 May 2026 at Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, Kolkata.

At RDAMSE 2026, researchers, academicians, industry experts, and students can share ideas, present cutting-edge research, and collaborate in the dynamically evolving field of materials science and engineering. The abstracts in this issue show the diversity, breadth, and quality of global research contributions.

The Department of Basic Science & Humanities, organizing committee, reviewers, writers, and stakeholders who made this publication possible deserve my gratitude.

I'm pleased to note that the conference is being organized with esteemed partners like the Society for Materials Chemistry, Kolkata Chapter, the Indian Photobiology Society, Jadavpur university campus, Sripat Singh College, Murshidabad, and Subhami Biopharma Pvt. Ltd., Kolkata, demonstrating the strong spirit of partnership between academia, research.

The conference promotes intellectual rigor and scholarly excellence, and this Book of Abstracts shows that. RDAMSE 2026 brings together renowned international speakers from the US and Japan and national experts from top institutions like IISc, IIT, IEST, IISER, University of Calcutta, Jadavpur University, Rani Rashmoni Green University, IACS, CSIR-CGCRI, and DRDO, as well as several reputable academic institutions and industries, for meaningful interaction and knowledge exchange.

I believe RDAMSE 2026 will deepen academic discourse and encourage new research and technology advances.

I wish the conference great success and hope that all participants have a fruitful and enriching experience.

With best wishes,

Prof. (Dr.) Saradindu Panda

Principal –

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex



Dr. Soumen Basu

Registrar

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex
(SurTech), (Autonomous Institution), Dum Dum, Kolkata

Message

It is a privilege to extend my heartfelt greetings to all scientists, academicians, researchers, industry leaders, professionals, and students attending the 2nd International Conference on “Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026)”, scheduled for 7–8 May 2026. This event reflects SurTech’s commitment to academic excellence, research advancement, and global engagement.

Following the success of RDAMSE 2025, the second edition brings together eminent international and national experts from leading institutions and industries, providing a vibrant platform for knowledge promotion, interdisciplinary dialogue, and collaboration.

I am pleased to note that the conference is organized in association with esteemed academic, research, and industry partners, strengthening the bond between industry institute linkage.

Heartily congratulate all the organizers and wish RDAMSE 2026 for great success, it’s fosters innovation, meaningful collaborations, and impactful scientific progress.

Dr. Soumen Basu

Registrar

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex



Dr. Dipankar Das

Convenor, RDAMSE 2026 and Head of Department
Department Basic Science & Humanities
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex

Message from Convener

It is my great pleasure, as the Convener, to welcome you to the International Conference on Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026). I am honored to bring together a distinguished community of academicians, researchers, and industry professionals who share a common vision of advancing the frontiers of materials science.

Following the successful organization of RDAMSE 2025 by the Department of Basic Science & Humanities, SurTech, I am delighted to witness the continuation of this esteemed conference in its second edition. RDAMSE 2026 brings together eminent international speakers from the USA and Japan, along with distinguished national experts from premier institutions such as IISc, IIT, IEST, IISER, University of Calcutta, Jadavpur University, Rani Rashmoni Green University, IACS, CSIR-CGCRI, and DRDO, as well as several reputed academic institutions and industries. This convergence creates a vibrant platform for scholarly interaction, interdisciplinary dialogue, and collaborative research.

I am also pleased to note that the conference is being organized in association with esteemed partners including the Society for Materials Chemistry, Kolkata Chapter; the Indian Photobiology Society, Jadavpur University Campus; Sripat Singh College; and Subhami Biopharma Pvt. Ltd. These collaborations reflect a strong and meaningful partnership between academia, research organizations, and industry.

Materials science continues to play a transformative role in shaping modern society, with far-reaching impacts on energy, healthcare, manufacturing, and environmental sustainability. RDAMSE 2026 provides an excellent platform to exchange ideas, present pioneering research, and explore innovative solutions to some of the most pressing global challenges. It also offers a valuable opportunity to build meaningful collaborations that can drive future scientific and technological breakthroughs.

As the Convener of this conference, I encourage all participants to actively engage in the sessions, interact with fellow delegates, and make the most of the knowledge-sharing opportunities available. At DSCSITSC, we remain committed to fostering an environment that promotes both intellectual growth and practical innovation.

The themes of this conference are highly relevant to current and future industrial needs, encompassing areas such as advanced materials, nanotechnology, and sustainable energy solutions. The insights gained here will undoubtedly contribute to the continued evolution of this dynamic field.

I extend my sincere appreciation, as Convener, to all participants, speakers, and organizers for their valuable contributions to RDAMSE 2026. I am confident that this conference will be both enriching and inspiring, and I wish you a productive and memorable experience.

Thank you and best wishes for a successful conference.

Dr. Dipankar Das

Convenor, RDAMSE 2026 and Head of Department
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex



Dr. Biswajit Das

Co-Convenor, RDMSE 2026

Department of Basic Science & Humanities

**Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex
(SurTech), (Autonomous Institution), Dum Dum, Kolkata**

Message from Co-Convenor

It is my great pleasure, as the Co-Convenor, to welcome you to the 2nd International Conference on Recent Developments and Applications in Materials Science and Engineering (RDAMSE 2026).

Following the successful completion of RDMSE 2025, we are proud to present the second edition of this conference with the same spirit and motivation, while significantly expanding its scale and impact. This year, RDMSE 2026 has witnessed remarkable growth in terms of participation and academic engagement, with more than 110 participants, over 20 invited speakers, and more than 15 keynote speakers from across India and abroad.

We sincerely acknowledge and thank our esteemed associating partners and sponsors for their valuable support in making this conference a success. I would also like to express my heartfelt gratitude to our Honorable MD Sir, Director Sir of JIS Group, and the Principal of SurTech for their continuous support, encouragement, and inspiration.

RDAMSE 2026 aims to provide a vibrant platform for knowledge exchange, collaboration, and innovation in the field of materials science and engineering. I hope all participants will benefit from the enriching discussions and interactions throughout the conference.

Wishing everyone a successful and memorable conference.

Dr. Biswajit Das

Co-Convenor, RDMSE 2026

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex



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Plenary Lectures





A Cursory Glance into the Domain of Colloid and Interface Science with Special Reference to Nanocrystalline Materials

Prof (Dr.) Amiya Kumar Panda
Vice-Chancellor

Rani Rashmoni Green University, Tarakeswar-71240, Hooghly,
West Bengal, India



ABSTRACT

In the proposed lecture, the main focus will be on the introduction of the colloid and interface science, its need on the various branches of science. It will follow the journey through the development of colloidal science around the world and in India. The academic lineage will be drawn with the legendary colloidal scientists in India. Brief introduction on the nanomaterial synthesis and associated problems will be discussed. Finally, presentation will be made on the simple synthesis and characterization of nanoparticles by a one pot approach. Synthesis and characterization of nanocolloidal dispersions of AgX in aqueous surfactant media will be presented.

BIOGRAPHY

Dr. Amiya Kumar Panda is currently serving as the Vice-Chancellor of Rani Rashmoni Green University and is the former Vice-Chancellor of Sadhu Ram Chand Murmu University of Jhargram. He is on lien from the Department of Chemistry, Vidyasagar University, Midnapore, West Bengal, India. Dr. Panda obtained his M.Sc. and Ph.D. degrees from Tripura University, India, and has made significant contributions in the fields of nanoparticles, lipid monolayer and bilayer systems, nanostructured lipid carriers, micelles, and microemulsions. He has actively contributed to the scientific community, including serving as the Working President of the 5th Asian Conference on Colloid and Interface Science held in India in 2013.

Dr. Panda has received numerous prestigious awards and fellowships, including the BOYSCAST Fellowship (DST, Govt. of India), Indian Science Congress Association Young Scientist Award, Endeavour Award (Govt. of Australia), Best Teacher Award from the Chemical Research Society of India, Siksha Ratna (Govt. of West Bengal), and several international visiting fellowships in Australia and Japan. He is also an Endeavour Ambassador and a recipient of the Bronze Medal from the Chemical Research Society of India. With an impressive academic record, Dr. Panda has published over 130 research papers and successfully guided 21 Ph.D. scholars, reflecting his strong commitment to research, teaching, and academic leadership./

**Reversible porphyrin assemblies via coordination interactions and dynamic covalent bonds****Prof. (Dr.) Joe Otsuki**

**Department of Materials and Applied Chemistry,
College of Science and Technology, Nihon University, Tokyo, Japan**

**ABSTRACT**

Porphyrins play essential roles in biological systems, including oxygen transport, light harvesting, electron transfer, and catalysis. These functions arise from their incorporation into well-defined supramolecular architectures. Such structural organization is directly relevant to applications in energy conversion, environmental remediation, and healthcare. Therefore, understanding how porphyrin molecules assemble, how their structure governs their properties, and how these assemblies can be utilized is of considerable importance.

In this lecture, I will present our recent studies on the design, synthesis, structural characterization, and functional properties of porphyrin assemblies. Axial coordination of pyridyl ligands to the central metal ion of a porphyrin is a simple and effective strategy for constructing organized architectures. We have employed this approach to develop energy-harvesting assemblies of chlorophylls and porphyrins [1–3]. Another strategy involves introducing chelating ligands, such as bipyridine or terpyridine, onto the porphyrin framework. These functionalized porphyrins assemble upon metal-ion coordination [4–6]. By tuning the spacer units between the porphyrin core and the chelating sites, we can control the size of the resulting cavities as shown in Figure 1. These cavity-containing assemblies function as selective host systems. In addition, dynamic covalent bonds, such as imine linkages, provide another powerful means of constructing complex architectures. Using this approach, we have developed porphyrin-based cages linked by imine bonds, which are capable of encapsulating fullerene guests such as C₆₀ and C₇₀.

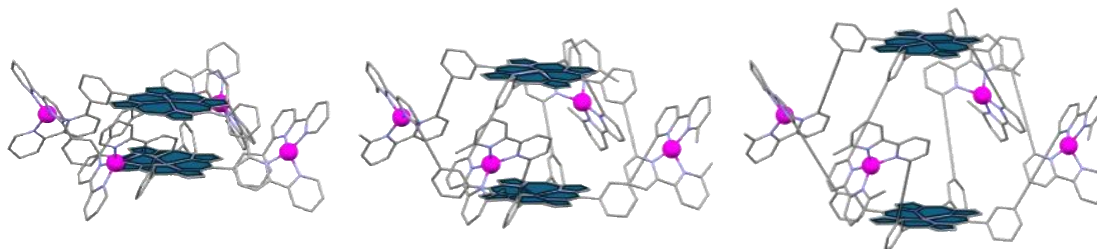


Figure 1. Porphyrin assemblies from our laboratory [4].



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BIOGRAPHY

Prof. (Dr.) Joe Otsuki is a distinguished academic and researcher in the field of materials and applied chemistry, currently serving as a Professor in the Department of Materials and Applied Chemistry, College of Science and Technology, Nihon University, Tokyo, Japan. He obtained his Doctor of Engineering degree in Chemistry from the University of Tokyo in 1991. He began his academic career as a Research Associate at the Institute of Industrial Science, University of Tokyo (1991–1999), during which he also served as a post-doctoral fellow at Université Louis Pasteur, France (1993–1994). He later joined Nihon University as an Assistant Professor (1999–2004), was promoted to Associate Professor (2004–2010), and has been serving as a Professor since 2010.

Prof. Otsuki has received numerous prestigious recognitions for his contributions to research and academia. He is a recipient of the Sir J. C. Bose Endowment Award from the Indian Photobiology Society (2024) and has been listed among the World's Top 2% Scientists by Stanford/Elsevier (2023–2025). He has also been recognized as a Top Peer Reviewer in both Chemistry and Cross-Field categories by Publons (2019), received the Solar Energy Journal Best Paper Award (Elsevier, 2019), and multiple Peer Review Awards (Publons, 2018). Additionally, he has been honored with the Lecture Award by Institut Kimia Malaysia and the Chemical Society of Vietnam (2017), and recognized as an Outstanding Reviewer for Materials Chemistry Frontiers by the Royal Society of Chemistry (2016). His career reflects a strong commitment to excellence in research, innovation, and global scientific collaboration.



Role of Sensors and AI in Material Science

Padma Shri Prof (Dr) Ajoy Kumar Ray
Director,

JIS Institute of Advanced Studies & Research, India



ABSTRACT

The rapid evolution of materials science is increasingly driven by the integration of advanced sensing technologies and artificial intelligence (AI), enabling a transformative shift in the way materials are designed, characterized, and deployed. Sensors play a pivotal role in real-time monitoring of physical, chemical, and environmental parameters, providing high-resolution data essential for understanding material behavior under diverse conditions. From nanoscale sensing to smart embedded systems, modern sensors facilitate precise measurement of properties such as temperature, strain, humidity, and chemical composition, thereby enhancing the reliability and functionality of advanced materials.

Simultaneously, the incorporation of AI and machine learning techniques has revolutionized data analysis and predictive modeling in materials science. AI-driven approaches enable the rapid screening of materials, optimization of synthesis processes, and accurate prediction of material properties, significantly reducing experimental time and cost. The synergy between sensor-generated big data and AI algorithms allows for the development of intelligent materials and systems capable of self-diagnosis, adaptive response, and autonomous decision-making.

This integration is particularly impactful in emerging domains such as smart manufacturing, energy storage systems, environmental monitoring, healthcare diagnostics, and sustainable material development. AI-assisted sensor networks are paving the way for the realization of Industry 4.0, where materials and devices are interconnected, responsive, and efficient.

In conclusion, the convergence of sensor technology and artificial intelligence is redefining the landscape of materials science, fostering innovation, enhancing performance, and contributing to the development of next-generation smart and sustainable materials for a technologically advanced society.

BIOGRAPHY

Professor Ajoy Kumar Ray is a distinguished academic and researcher currently serving as the Director of JIS Institute of Advanced Studies & Research. With a career spanning over four decades, he has significantly contributed to engineering and technology education, leading initiatives that foster innovation and excellence.



Before his current role, Professor Ray served as the Vice Chancellor of Bengal Engineering and Science University (BESU), Shibpur, from 2009. He had previously led the School of Medical Science and Technology at IIT Kharagpur and was a Professor in the Department of Electronics and Electrical Communication Engineering there. A graduate of Bengal Engineering College, Shibpur, he earned his master's and doctoral degrees from IIT Kharagpur, where he began teaching in 1980.

A notable milestone in his career was receiving the Padma Shri in 2017, India's prestigious civilian award, for his instrumental role in transforming BESU into the Indian Institute of Engineering Science and Technology (IIST). Professor Ray's research includes 17 projects funded by various global organizations, and he has co-invented six U.S. patents with Intel and filed three more with Texas Instruments. He has published over 90 research papers and authored five books, making significant contributions to image processing, video coding, and medical diagnostics, particularly in areas like brain activity monitoring and breast cancer detection.

Professor Ray's research focuses on advanced algorithms for medical image analysis, signal processing, and diagnostics. He has improved image compression and video coding, enhanced data transmission, and applied artificial neural networks (ANN) and convolutional neural networks (CNN) for medical applications. His work has advanced digital pathology and EEG signal analysis, contributing to better healthcare technologies.

Beyond research, Professor Ray has shaped India's technical education landscape, participating in national committees and fostering industry-academic collaborations. His leadership and contributions have earned him international respect in the engineering community.





Keynote Lectures





Nanomaterials from Geopolymer through Scalable Synthesis

Prof (Dr.) Don Seo

School of Molecular Sciences (
formerly Department of Chemistry and Biochemistry)
Arizona State University (ASU)



ABSTRACT

Aluminosilicate geopolymer is one of the few inorganic materials that can be produced efficiently on a scale of millions of tons, offering a unique solution to the “tyranny of scale” often faced in solving humanity’s sustainability problems. While traditionally recognized as “green cement” or low-temperature ceramics, recent innovations in geopolymer synthesis have enabled unforeseen levels of control over nanoscopic morphologies and porosity. This presentation will illustrate how top-down synthetic strategies can transform these scalable materials into functional nanoaggregates and highly crystalline hierarchical zeolites with performances far superior to other material classes.

We will highlight advances relevant to critical sustainability applications, demonstrating how geopolymer nanomaterials can serve as excellent arsenic absorbents for groundwater purification and as highly effective biodiesel catalysts. The talk will also detail nanozeolites that exhibit exceptional CO₂ capacity, sorption kinetics, and selectivity for cost-effective gas separation, alongside silver-ion exchanged variants that demonstrate superb antibacterial efficacy against antibiotics-resistant MRSA bacteria. Furthermore, we will discuss the development of high-structure nanoaggregates with controlled zeolicity for energy-saving polymer nanocomposite applications.

BIOGRAPHY

Dong-Kyun (Don) Seo is a Professor of School of Molecular Sciences (formerly Department of Chemistry and Biochemistry) at Arizona State University (ASU). He received his B.S. degree (1990) in Chemistry at Seoul National University in South Korea and his Ph.D. (1997) in Theoretical Chemistry at North Carolina State University. He joined the ASU Chemistry Department Faculty in 2001. He was a recipient of NSF Career Award and Camille Dreyfus Teacher-Scholar Award. He served as an Invited Professor at Université de Nantes – Jean Rouxel Institute of Materials in Nantes and École Polytechnique de l’Université de Nantes in France. His current research interests



are centered on the synthetic development of high-surface area materials and their sustainability-related applications. He has founded or co-founded a few companies and is credited for attracting investments for large-scale production and applications of functional porous aluminosilicate materials.



Harnessing Interfacial Assembly to Unleash the Luminescence Potential of Lanthanide Complexes

Prof (Dr.) Miki Hasegawa

Professor, Department of Chemistry and Biological Science,

College of Science and Engineering, Aoyama Gakuin University, Japan

Email: hasemiki@chem.aoyama.ac.jp



ABSTRACT

Lanthanide coordination complexes possess intrinsically sharp ff emissions and long excited-state lifetimes, yet their luminescence performance is highly sensitive to the surrounding coordination and interfacial environments [1,2]. Recent studies have demonstrated that interfacial assembly—ranging from thin-film formation to mechanically induced cleavage at well-defined layers—provides powerful means to enhance or activate the photonic functions of discrete lanthanide complexes. This presentation highlights how controlling interfacial structures enables systematic modulation of luminescence efficiency, stability, and responsiveness.

Thin-film formation of lanthanide complexes offers a versatile platform for improving emission properties through controlled molecular packing and interface-driven stabilization[3,4]. Film fabrication suppresses vibrational quenching, enhances antenna efficiency, and enables integration into device-compatible architectures. These interfacial effects reveal that even subtle changes in packing density or orientation can significantly influence radiative and nonradiative pathways.

In parallel, lamellar-cleavage-induced triboluminescence in chiral lanthanide complexes demonstrates how mechanical stimuli at anisotropic interfaces can trigger bright emission[5]. The phenomenon arises from cleavage along crystallographically defined planes, which generates charge separation and subsequent radiative recombination. This interface-specific response underscores the critical role of layered packing motifs and interlayer interactions in governing excited-state dynamics.

Together, these findings establish interfacial complexation engineering as a unifying strategy for unlocking the latent luminescence potential of lanthanide complexes. By designing and manipulating thin-film interfaces and cleavage-responsive layered structures, we can create next-generation photonic materials with enhanced emission[6], mechanical responsiveness, and device applicability..

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BIOGRAPHY

Prof (Dr.) Miki Hasegawa is a distinguished scientist and Professor in the Department of Chemistry and Biological Science, College of Science and Engineering at Aoyama Gakuin University (AGU), Japan. She received her Ph.D. in 1998 from AGU under the supervision of Prof. T. Hoshi, specializing in molecular spectroscopy and photochemistry, and subsequently continued her research as a research professor. In 2002, she began leading her own research group at AGU as a lecturer, later serving as Associate Professor (2008–2011) before being promoted to full Professor in 2011. Since 2018, she has also been serving as the Director of the Mirai (Future) Molecular Materials Design Institute at AGU. Her research focuses on the photochemistry of coordination compounds and rare earth chemistry, with particular emphasis on lanthanide luminescence, polarized emission, and triboluminescence across molecular and soft-crystalline systems.

Prof. Hasegawa has made significant contributions to the scientific community, with over 150 peer-reviewed publications, including 13 review articles, as well as several books and book chapters. Her work has been published in leading journals such as Coordination Chemistry Reviews, Journal of Photochemistry and Photobiology C, and ACS Applied Materials & Interfaces, earning multiple cover features and recognitions. She has received prestigious awards including the Incentive Award for Young Researcher (Adachi Award, 2011) and the Rare Earth Society of Japan Award (Shiokawa Award, 2023). An active global academic leader, she has delivered more than 80 plenary, keynote, and invited lectures worldwide and serves as Associate Editor of the Journal of Photochemistry and Photobiology A, as well as an editorial board member of Scientific Reports and Pure and Applied Chemistry. She also holds several prominent professional roles, including Executive Board Member and Titular Member of IUPAC Division II (2026–2027), and has contributed extensively to international collaborations and advisory roles across leading research institutions and scientific bodies.



Metal–Organic Frameworks: A Story of Materials for Hydrogen Storage, Carbon Capture, and Water Harvesting

Prof (Dr.) Rahul Banerjee
Department of Chemical Sciences,

Indian Institute of Science Education and Research (IISER) Kolkata,

Mohanpur Campus, Mohanpur 741 246



ABSTRACT

Covalent Organic Frameworks (COFs) represent a novel class of highly porous, crystalline polymers with uniformly ordered pore channels. Despite their extensive use for storing various molecular species such as gases, nanoparticles, enzymes, and drugs, the potential of their ordered pore channels for molecular separation still needs to be utilized. In this context, we have successfully addressed the chemical stability issue by synthesizing β -ketamine-based frameworks. for hydrogen storage and CO₂ capture. We have also developed a simple, scalable, and innovative methodology that allows for the synthesis of COFs by merely mixing and heating the reactants. These COFs show high capacity for the storage of hydrogen and CO₂. This method enables the processing of COFs into self-standing Covalent Organic Framework Membranes (COMs). These self-standing membranes are flexible, continuous, free from internal defects or cracks, and demonstrate long-term durability. They maintain structural integrity in water, organic solvents, and mineral acids (3 N HCl). We have applied these COMs in separation applications, such as wastewater treatment and recovering valuable Active Pharmaceutical Ingredients (APIs) from organic solvents. Our findings highlight that COFs have significant potential to address some of the world's most challenging separation problems, including wastewater treatment and drug recovery in the pharmaceutical industry. Covalent Organic Nanotubes (CONTs) are an emerging subclass of one-dimensional crystalline materials that harness the principles of reticular chemistry to create structurally ordered and functionally tunable architectures. Unlike traditional carbon nanotubes formed via top-down methods, CONTs are constructed through bottom-up molecular assembly using reversible Schiff-base condensation reactions, allowing for error correction and crystallinity control. In this work, we demonstrate the rational design and synthesis of CONTs with dual pore architectures—featuring axial (front) and radial (side) channels. These structures exhibit exceptional thermal and chemical stability and can be further tuned to form advanced architectures such as toroids and vesicles through supramolecular assembly.

BIOGRAPHY

Organized by: Department of Basic Science & Humanities,
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), (Autonomous), Kolkata



Prof. Rahul Banerjee received his PhD degree from the University of Hyderabad, Hyderabad, in 2006. After a postdoctoral work at UCLA (2006-2008), he joined CSIR-National Chemical Laboratory, Pune, India, in 2008 as a Scientist. Prof. Rahul Banerjee is currently a Professor at the Indian Institute of Science Education and Research (IISER) in Kolkata. His research interests include the study of structural chemistry with the flavor of chemical synthesis to design new porous materials. Rahul Banerjee's research group is working with TATA Steel to develop a process to make porous covalent organic frameworks with exceptional chemical stability for CO₂ capture. This concept is being considered globally as a breakthrough in porous material research. Prof. Rahul Banerjee has published over 190 publications and 24 patent applications from CSIR-National Chemical Laboratory and Indian Institute of Science Education and Research (IISER) Kolkata on various porous framework materials since 2010. His current h-index is 96. Prof. Banerjee is an editorial board member and associate editor of the Journal of the American Chemical Society.



Multifunctional Stimuli-Responsive Chemogenetic Crystalline Platform: Structural Modalities, Photosalient Behavior, Catalytic C–C Coupling, and Selective Ion Sensing

Dr. Koushik Saha, and Prof (Dr.) Chittaranjan Sinha

Department of Chemistry, Jadavpur University,
Kolkata-700 032, India



ABSTRACT

Smart materials are next-gen objectives towards fulfilment of Sustainable Development Goals (SDGs). The progress of multifunctional crystalline materials, those could integrate mechanical responsiveness, catalytic efficiency, and sensing ability, have made a significant advancement in this direction. Herein, we report a chemogenetically engineered crystalline platform that exhibits stimuli-responsive photosalient behavior alongside catalytic and sensing functionalities. In this talk, we report a 0D Zn(II) complex, which exhibits “photosalient effect” under UV-light with manifestation of rapid bending, delamination, cracking, hopping, and popping. A stereo selective [2+2] photo-dimerization along with single-crystal-to-single-crystal (SCSC) structural transformation is surprising function of the material. Polyvinyl alcohol blended film of the material displays light-induced bending, walking and swimming. In addition, a selective sensing is noted to Fe³⁺ in aqueous solution which has been released upon photo-irradiation; and possibly opens an avenue for targeted iron delivery in required cellular system.

The integration of photomechanical actuation, catalytic reactivity, and ion recognition within a single crystalline architecture highlights the versatility of this system. This work provides a new strategy for designing multifunctional smart materials with potential applications in adaptive devices, sustainable catalysis, and chemical sensing.

**BIOGRAPHY**

Professor & Former Head, Department of Chemistry and Ex-Dean, Faculty of Science, Jadavpur University, Kolkata-700 032, India. Education from Calcutta University and Ph. D. degree from Indian Association for the Cultivation of Science, Kolkata (Jadavpur University), Joined as Lecturer in Chemistry, Burdwan University, 1992; with brief stay in Vidyasagar University (1994) returned to Burdwan University and now in Jadavpur University since 2004. Published more than 490 original research articles in the national and international journals having h-index 52, citation 10,350+; awarded 56 Ph. D. degree and supervised more than 23 research projects from UGC, DST (New Delhi), State DST (Kolkata), CSIR, AICTE. Awarded Best Chemistry Teacher Award (2012) by Confederation of Indian Industries (CII) and AICTE. Elected Fellow of West Bengal Academy of Science & Technology (2018); Elected Fellow of Energy Science (2023); Elected Fellow of Royal Society of Chemistry (FRSC) (2023). Visited Taiwan, Japan, Singapore, Italy and received Centenary Lecture Award from Tokyo Institute of Science, Japan (2005). Organised large number of national and international conferences. Served as Editor, Inorganic & Analytical Chemistry Section of Journal of Indian Chemical Society (2010-2016); Chemistry-An Indian Journal (2010-); Sr-Editor, Journal of Spectroscopy & Dynamics (2014-); Associate Editor, Current Organocatalysis, Bentham Science (2018-); Associate Editor, Current Microwave Synthesis, Bentham Science (2018-). Honorary Secretary: Indian Chemical Society (2016-2022). Secretary, Indian Photobiology Society (2023-). He has been enlisted in top 2% Indian Scientists in the list of Stanford University in 2020-2025.



Nanoscale Materials Design for Energy Sustainability

Prof (Dr.) K.K. Chattopadhyay

Thin Film and Nanoscience Laboratory, Department of Physics
School of Materials Science and Nanotechnology,

Jadavpur University, Kolkata – 700 032



ABSTRACT

To overcome the limitations of fossil fuels and mitigate their adverse environmental impact, the widespread adoption of alternative energy sources is urgently needed. Advances in nanotechnology at both the materials and device levels, are demonstrating bright prospects in this research domain. In particular, harvesting wasted mechanical energy to develop self-powered devices has emerged as a promising field within green energy research. Concurrently, there is significant recent momentum in developing efficient neuromorphic devices capable of mimicking biological synaptic computations. Perovskite materials have shown great promise for applications across diverse fields, including photovoltaics, luminescence, piezophotonics, and neuromorphic computing. This lecture will discuss some concepts of nanoscale materials design which include hierarchical growth of 2D-2D assembly, edge-oriented growth for harnessing edge states for energy storage applications etc. Also, band engineering and novel doping approaches will be presented. Some self-powered sensors and self-charging storage devices will also be discussed [1-7]. Mechanistic understanding using nanoscale physics and chemistry will be presented.

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BIOGRAPHY

Professor Dr. K.K. Chattopadhyay is at present a Professor in the Department of Physics, Jadavpur University, Kolkata. He has served as Head of the Department of Physics and Director of the School of Materials Science and Nanotechnology. His current field of research interest includes semiconductor nanostructures, carbon-based nanomaterials, perovskite nanostructures and their applications. He is also extensively involved in ab-initio calculations using Density Functional Theory.

Prof. Chattopadhyay has published more than 490 research papers in various international journals of repute and more than 350 papers in the proceedings of national / international conferences. His current 'h-index' is 69 and has over Eighteen Thousand citations. He has supervised 60 students to their Ph.D. degrees. He is the author of five books and several book chapters in the areas of physics and nanotechnology and has 4 patents. He is the recipient of various awards like MRSI Medal; Dr. Meghnad Saha Gold Medal; Dr. J.N. Mukherjee memorial award from the Indian Chemical Society; Shishka Ratna Award from the Govt. of West Bengal etc. Due to his contribution in the field of physical science and nanotechnology he was elected as Fellow of the West Bengal Academy of Science and Technology and Fellow of the National Academy of Sciences (NASI), India. He was listed among the World's top 2% scientists list published by the Stanford University in consecutive years since 2021 – 2025 and top 0.05% scientists in the world since 2024 by Scholar GPS.

Prof. Chattopadhyay was a visiting professor at many foreign universities and institutes including the NIMS Japan, the Ulsters University, UK, the Hanyang University, South Korea etc. He is the Vice President of MRSI, Kolkata Chapter and life member of many academic bodies. He was an Editor of Springer journal 'Journal of Materials Science: Materials in Electronics' and an editorial board member of Indian Journal of Physics. He is in the panel list of expert committees for research project review of European Union and Singapore Science Academy.



Materials Science And Engineering: A New Paradigm

Prof (Dr.) N. R. Bandyopadhyay

Former Professor & Head

School of Materials Science and Engineering

Indian Institute of Engineering Science and Technology, Shibpur

(formerly Bengal Engineering and Science University, Shibpur)

Howrah 711103, INDIA



ABSTRACT

We are currently at the early but secure and irreversible stages of a remarkable and far reaching materials revolution. Materials scientists and engineers are now able to intervene at the electronic, atomic and molecular structure of matter, in order to both synthesize and process new materials. These breakthroughs in materials science and engineering are having two consequences. Firstly, the new insight has permeated traditional and conventional materials leading to marked improvement in processing technologies. Secondly, the transformation underway have spawned proliferating clusters of high performance, knowledge based new and advanced materials, high temperature super conducting materials, advanced composite, engineering polymers etc.

The development of materials for the 21st Century has to follow from clear vision/composite functionality, i.e. the combination of service performance, processing advantage and ecological sustainability should be the prime considerations. Service requirement specificity is one of the key factors playing an important role in materials activity and therefore in this article we take a stock of such developing materials.

The materials technology can influence a lot by way of being re-described as a powerful tool to secure a balance between the present and future, between consumption and conservation. It is the challenge to this generation to create a new relationship between human kind and its materials, linking the brilliance of nature and life with its wisdom and technology so that the creative powers of man are continued to be nurtured in a meaningful way during 21st century too.

**BIOGRAPHY**

Born in Calcutta in 1955, Dr. Bandyopadhyay had his graduation in Metallurgy from Bengal Engineering College, Shibpur, Masters in Metallurgical Engineering from Jadavpur University and further Ph.D. (Metallurgical Engineering) from Calcutta University. He spent more than 15 years in industry prior to taking up research and academic pursuit with Indian Institute of Engineering Science and Technology, Shibpur (erstwhile B.E. College, Shibpur 1856) where he is presently Hony Adjunct Professor after superannuating on 31st January 2020 as Professor & Head of School of Materials Science & Engineering, IEST, Shibpur.

He teaches the subjects like Introduction to Materials, Metallic Materials, Materials Characterization, Nano-crystalline & Nano-composite materials and energy materials at post graduate level. He supervised forty four (44) M.Tech theses and under his able guidance twenty five (25) PhD theses have been awarded degree, two (2) under evaluation for award.

Prof. Bandyopadhyay has more than hundred (100) research publications in Indian and foreign journals and four (4) book chapters, in his field interest viz high strength steel and engineered materials. In recognition to his contribution in the field of advanced steels, he was entrusted by Ministry of Steel, Government of India with a “National Project on Capacity Augmentation” in collaboration with Tata Steel. He also visited Universities of USA, Australia, Germany and Poland with short tenured research and academic assignments

During last five years he worked in the area of Silicon Nanostructures and Advance Nano composite. Extensive efforts are being given in this emerging field, which culminated to the initiation a project on ‘Luminescent silicon nanostructures’ under DST-NSTI program of Department of Science and Technology, Govt. of India and Indo-US Science and Technology Forum (IUSSTF). He also represented Indian scientists’ delegation to Australia for development of collaborative programmers with leading Australian Universities on “Nano-composite for Clean Energy” under IASRF of DST, GoI.

He is the recipient of Eminent Material Scientist award in 2004 for his contribution for the cause of materials science and engineering from The Institution of Engineers (I) besides Metallurgical & Materials Engineering Division Medal for best research publications in the year 2000, 2001 and 2006.

Dr. Bandyopadhyay is the Fellow of The Institution of Engineers (India) and former Chairman of its Committee for Advancement of Technology and Engineering (CATE) and Metallurgical and Materials Engineering Division Board (MMDB). He is also the Editor-In-Chief of IEI-Springer Series D Journal dedicated for Metallurgical and Materials Engineering. Presently he is also the Council Member, Materials Research Society of India (MRSI) and Fellow West Bengal Academy of Science and Technology (WAST).



Recent progress in 2D Memristors

Prof (Dr.) Santanu Mahapatra

Nano Scale Device Research Laboratory

Department of Electronic Systems Engineering

Indian Institute of Science Bangalore

Bangalore 560012 INDIA



ABSTRACT

Non-volatile resistive switching devices, referred to as memristors, are becoming increasingly significant for in-memory computing, which enables the data-intensive computations necessary for deep neural networks. Memristors are simple structures that consist of a metal-insulator-metal (MIM) matrix, with the insulator serving as the active layer. Upon the application of electrical field, these devices can shift from a high resistive state (HRS) to a low resistive state (LRS), emulating the function of biological synapses. Following Hewlett-Packard's (HP) announcement of the development of a memristor in 2008, transition metal oxides, such as titanium oxide, have been employed as active layers. Notwithstanding the significant advancements made in recent years, oxide-based memristors have not satisfied the critical performance metrics. Consequently, new active layer materials are being explored globally to enhance memristive device performance. In this talk we focus on the recent advancement of memristor technology utilizing 2D semiconductor as active layer. We discuss the remarkable resistive switching exhibited at the mono-atomic-layer limit, and at the system level, how deep learning algorithms have been directly implemented on wafer-scale two-dimensional memristor arrays.

BIOGRAPHY

Prof. Santanu Mahapatra received his Ph.D. degree from Swiss Federal Institute of Technology Lausanne (EPFL) in 2005. For his Ph.D. dissertation he worked on the modeling of Single Electron Transistor (SET) and its co-simulation and co-design with CMOS. He joined Department of Electronic Systems Engineering (formerly CEDT), at Indian Institute of Science (IISc), Bangalore, India, as an assistant professor in August 2005 and promoted to associate professor and then full professor rank in September 2010 and December 2015 respectively. He founded Nano Scale



Device Research Laboratory in 2006, where his research team engaged in modeling of carrier transports in nano materials at circuit, device and atomistic level. His research interests include two-dimensional channel transistors, energy efficient electronic switches and energy-storage at nanoscale. He is the author of the book Hybrid CMOS Single Electron Transistor Device and Circuit Design. He received IBM Faculty award in 2007, Microsoft Research India Outstanding Faculty Award in 2007 and the associateship of Indian Academy of Sciences in 2009. He is also the recipient of Ramanna Fellowship (2012 to 2015) in the discipline of electrical sciences from Department of Science and Technology, Government of India for his contribution in compact modeling.



Self-Assembled Nanostructures from Stimuli-Responsive Copolymers in Relevance to Drug Delivery: Stabilizing by Cross-linking, Probing by Energy Transfer Phenomenon

Prof (Dr.) Dibakar Dhara

Professor, Department of Chemistry,

Indian Institute of Technology Kharagpur, West Bengal 721302, India

Email: dibakar@chem.iitkgp.ac.in



ABSTRACT

The ability to regulate and probe the formation of nanostructures through self-assembly of amphiphilic block copolymers is of immense significance in the field of biology and medicine. In this presentation we show few examples of such nanostructure formation. We demonstrate the usefulness of energy transfer phenomenon (NSET and FRET) in establishing their structure. We also demonstrate effect of cross-linking in stabilizing the structures against dilution. These nanostructures were shown to be effective in delivering drugs in cancer cells in vitro. In this lecture I will present the details of the copolymers, their characterization, solution behaviour and potential application in drug delivery.

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BIOGRAPHY

Prof. Dibakar Dhara is a Professor in the Department of Chemistry at the Indian Institute of Technology Kharagpur, India. He completed his B.Sc. (Hons.) and M.Sc. from Jadavpur University, Kolkata (1990–1995), followed by a Ph.D. from the Indian Institute of Chemical Technology, Hyderabad (1995–1999). He pursued postdoctoral research at the University of Florida, Gainesville (1999–2001), and subsequently worked as a Lead Scientist at GE Global Research, Bangalore (2001–2007), before joining IIT Kharagpur as a faculty member in 2007. His current research focuses on the design and synthesis of advanced smart architectural polymers—including block, graft, bottle-brush, star, and nanogel systems—as well as polymer-coated nanoparticles for applications in targeted drug delivery and catalysis, employing modern organic transformations and controlled radical polymerization techniques.

Prof. Dhara has made significant contributions to both academia and industry, holding 25 patent families across multiple international jurisdictions and publishing over 85 research articles. Notably, he played a key role in inventing and commercializing GE Plastics' first blood-compatible polycarbonate material, earning the “Excellent Award” in 2006, along with multiple management awards for outstanding R&D contributions. He actively contributes to the scientific community as an Associate Editor for Polymer Chemistry, Frontiers in Chemistry and serves on the editorial boards of Journal of Macromolecular Science Part A and Scientific Reports. In addition to his research, he is deeply involved in education, having developed several widely accessed NPTEL and SWAYAM courses on polymer science, polymer chemistry, and chemical thermodynamics, reflecting his commitment to advancing both research and teaching in chemical sciences.



Conjugated Polymer based nanohybrids in photoelectrocatalysis for sustainable fuels and chemicals

Dr. Srabanti Ghosh

Principal Scientist , Energy Materials & Devices Division (EMDD),

CSIR - Central Glass and Ceramic Research Institute,

Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, India

Academy of Scientific & Innovative Research (AcSIR),

Ghaziabad, 201002, India Kolkata, India



ABSTRACT

Photocatalytic water splitting is a solar-powered method for producing hydrogen from water.¹ Although it holds significant promise, its large-scale implementation is limited by challenges such as the low efficiency of semiconductor nanostructures, primarily caused by rapid charge recombination and slow reaction kinetics. Constructing semiconductor heterojunctions has emerged as an effective strategy to address these issues, leading to enhanced efficiency and stability. Conjugated polymer nanostructures (CPNs) exhibit a unique ability to integrate with other nanomaterials, forming hybrid heterostructures.^{2,3} For instance, polypyrrole (PPy) nanofibers modified with Bi₂WO₆ have demonstrated substantial improvements in both conductivity and catalytic activity for water splitting. Notably, femtosecond transient absorption spectroscopy studies indicate that combining metal oxide and polymer nanostructures significantly promotes charge separation and transfer.³ More recently, gold-based photocatalysts developed through an in situ dopamine polymerization-guided assembly approach have shown high efficiency in hydrogen generation via water splitting.⁴ In addition, the development of an indigenous prototype device incorporating a photocatalyst layer within a photochemical reactor highlights progress toward practical application. A deeper understanding of the photoelectrochemical behavior of advanced semiconductor heterostructures along with their underlying mechanisms and associated challenges is essential for enabling scalable solar fuel production technologies.

Keywords: Conjugated polymer nanostructures, Heterostructures, Surface engineering, S-scheme heterojunction, Photocatalytic water splitting



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BIOGRAPHY

Dr. Srabanti Ghosh is presently working as a Principal Scientist at CSIR - Central Glass and Ceramic Research Institute, Kolkata. She received her PhD degree from UGC-DAE CSR, Kolkata Centre, and Jadavpur University. She is a recipient of Marie Curie Fellowship at the University of Paris SUD, France. She worked as GOT ENERGY TALENT Marie Curie Fellow at UNIVERSIDAD DE ALCALA, Spain. Her main research interests include materials at the nanoscale, applications in photocatalysis, sensor and therapeutics. She co-authored 126 publications (including *Nature Materials*, *Nature Sustainability*, *Small* etc.), 4 patents, edited 7 books, and h-index of 49 with Citation: 7591. She mentored master students, Ph. D. - 03 completed, and Ph. D.- 06 (ongoing), involved in CSIR, DST, ICMR funded projects on energy conversion, water splitting and biomaterials for therapeutic applications. She has been conferred with several prestigious awards, including the MRSI Young Scientists award, top 5% of highly cited authors in the RSC Materials portfolio, Young Investigator Award in Gordon Radiation Chemistry, USA, and Top 2% Most Influential Indian Scientists, Sandford University, 2019-2024. She received Society of Materials Chemistry (SMC) Bronze Medal -2024, BARC, Mumbai, and “MRSI Medal for 2024” by the Materials Research Society of India (MRSI). Recently, she received CRS Silver Medal for excellent achievements in Research and Innovation, the society Chirantan Rasayan Sanstha® (CRS), 2025.



Dirac Materials: Past and Present

Prof. (Dr.) Debnarayan Jana

Department of Physics

University of Calcutta



ABSTRACT

The physics of two dimensional (2D) materials is always intriguing in their own right. Dirac materials are a class of complex and functional nanomaterials offering great potential in the development of new electronic components. In this talk, we would like to present some theoretical calculations of electronic properties of graphene, S-graphene, phagraphene, and 8-16-4 Graphyne systems. A tight binding (TB) model along with density functional theory (DFT) will be used to unravel the characteristic features of Dirac points in these systems. Further, we will discuss an analytical scheme to address the emergence and robustness of Dirac fermions in phagraphene network. All these theoretical results in non-honeycomb structure may shed light on device fabrication in nano opto-electronic technology and materials characterization techniques in 2d carbon allotropes.

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BIOGRAPHY

Dr. Debnarayan Jana is a Professor in the Department of Physics at the University of Calcutta, Kolkata, India. He completed his M.Sc. (1990) from the University of Calcutta with 2nd rank, followed by Post-M.Sc. studies at Saha Institute of Nuclear Physics (1991), also securing 2nd rank, and obtained his Ph.D. in 1997 from Raman Research Institute, Bengaluru, in association with Jawaharlal Nehru University, New Delhi. He began his academic career as a lecturer at Narendrapur Ramakrishna Mission Residential College and joined the University of Calcutta in 2000, where he was promoted to Professor in 2011. He also served as a Visiting Fellow at CCMS, National Taiwan University (2003–2004) and was elected Fellow of the West Bengal Academy of Science and Technology (2015).

Dr. Jana's research spans both theoretical and experimental condensed matter physics. He has supervised 22 Ph.D. scholars and mentored several postdoctoral fellows, including UGC D.S. Kothari and National fellows. With over 235 publications in peer-reviewed journals, his work has gained significant recognition, including a highly cited review article in Reports on Progress in Physics. He has authored 15 books in physics and has over 5,800 citations with an h-index of 41. His contributions to teaching and research have been honored with the prestigious INSA Teachers Award (2020). He has been consistently listed among the World's Top 2% Scientists (2022–2025) and was also recognized among Asia's top scientists in 2023. An active contributor to the scientific community, he served as Guest Editor for Journal of Physics: Condensed Matter (IOP, 2023), reflecting his strong commitment to academic excellence and scientific advancement



Possibilities of Deep Decarbonization through Solid Oxide Cell Technology - A Short Review in Indian Perspective

Dr. Jayanta Mukhopadhyay

Senior Principal Scientist and Head of Energy Materials & Devices Division,
CSIR-Central Glass & Ceramic Research Institute
(CGCRI), Kolkata,
West Bengal,
India



ABSTRACT

India has declared the goal to achieve Net Zero emissions by 2070. As India's growth story unfolds, its demand for energy and resources is set to rise. Energy use has doubled in the last 20 years and is likely to grow by at least another 25% by 2030. As per the report of National Green Hydrogen, published by Ministry of New and Renewable Energy (MNRE), India currently imports over 40% of its primary energy requirements, worth over USD 90 billion every year. Major sectors like mobility and industrial production are significantly dependent on imported fossil fuels. This necessitates a shift towards technologies that enable enhanced share of renewable sources in the energy mix, and progressively reduce the reliance on fossil fuels. Innovation will be supported with an aim to increase the affordability of Green Hydrogen production, storage, transportation, utilization enhancing the efficiency, safety and reliability of the relevant systems and processes. R&D projects will be goaloriented, time bound, and suitably scaled up to achieve quantifiable returns. Blue Sky Projects having a long term (0-7 years in the first phase field trials and 8-12 years down the line for commercialization) horizon is planned with a focus on establishing global IP and competitive advantage for the Indian industry which will aim to develop capabilities of the Indian R&D sector within an array of subjects like 18 development of 3rd generation electrocatalysts, reversible Solid Oxide Electrolysers (SOECs) and Solid Oxide Fuel Cells (SOFCs), seawater electrolysis, thermo-catalytic pyrolysis, plasma pyrolysis, salt cavern surveys, high entropy alloys for reversible hydrogen storage etc.

Solid oxide cell technology has the potential to deep decarbonize the eco-system by suitably converting the commercial grade H₂ for the usage along with methane, reformat gases, syn gases, bio gases including the flare gases from petroleum industries. Solid oxide cells (SOCs) play a major role in strategic visions to achieve decarbonization and climate-neutrality. With its multifuel capability, this technology has received rapidly growing amount of attention from researchers worldwide. Due to the great flexibility of SOCs with respect to the fuels that can be used, not only hydrogen, but also biogas, natural gas, diesel reformates and many other conventional and alternative fuels can be used. This makes it possible to couple SOCs with diverse sustainable fuel sources to generate



electricity or to generate valuable fuels such as syngas when utilizing renewable electricity. The steel sector is one of the most carbon-intensive industries, and the sustainable strategies to reduce CO₂ emission on integrated mill plants are being discussed globally. By renewable H₂ utilization on blast furnace (BF), it is expected to achieve both sustainable operation and CO₂ emission reduction. It is evaluated that the application of the solid oxide electrolysis cell (SOEC) process as a source of H₂ for use as an alternative to CO as the reductant in a BF. The techno-economic analysis is suggestive to the maximum H₂ injection for the technical aspect and demonstration of the process economic viability considering the effects on the price of the SOEC system. It is further understood that the net reduction of global warming potentials and carbon intensity shows that the coke replacement ratio ranges from 0.255 ~ 0.334 kg. Coke/ kg H₂ depending on injection conditions and that 25 kg H₂/ tHM was an acceptable maximum injection rate within the stable range of BF operating indexes. H₂ production cost to be US\$ 8.84 ~ 8.88 / kg H₂ in the present (2021-2022), but it is expected to be decreased to US\$ 1.41 ~ 4.04/ kg H₂ by 2050. Economic parity with the existing BF process will be reached between the years 2036 and 2045, depending on the maturity of the SOEC process. Injection of 25 kg H₂/ tHM can reduce CO₂ emission by 0.26 ~ 0.32 tCO₂-eq./ tHM. It is expected that this priming sustainable strategy to reduce CO₂ emission from integrated mill plants will widen applications of H₂ utilization in BFs if the economic efficiency of SOEC systems can be increased.

In this presentation, a short review of the existing knowledge about solid oxide fuel cell (SOFC) and solid oxide electrolysis (SOE) systems and how to safely operate them over the long-term, placing a special focus on realworld operating environments will be discussed in perspective of Indian Scenario and also to that of the role of the CSIR-CGCRI as a potential stakeholder for the development of this particular technology in Nation.

BIOGRAPHY

Dr. Jayanta Mukhopadhyay has joined CSIR-Central Glass & Ceramic Research Institute (CGCRI), Kolkata in 2006 and is presently working as a Senior Principal Scientist and Head of Energy Materials & Devices Division. He is currently also the Professor in the Academy of Scientific and Innovative Research (AcSIR). Prior to joining at CSIR-CGCRI, Kolkata, Dr. Mukhopadhyay served International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Hyderabad from 2003 – 2006 as the capacity of a Research Scientist. Dr. Mukhopadhyay obtained his B. Sc. (Chemistry Hons) from the University of Calcutta in 1997 and was awarded with National Scholarship from Ministry of “Human Resources and Development” (MHRD) during his graduation. He obtained his B. Tech (Chemical Technology) in 2000 and M. Tech. (Ceramic Engineering) in 2002 from the University of Calcutta. He was the recipient of Gold Medal both in B. Tech and M. Tech. from the University. Dr. Mukhopadhyay secured all India rank 52 in Engineering Science in Graduate Aptitude Test (GATE) in Engineering in 2002. He obtained his PhD in Engineering from Jadavpur University in field of Metallurgy and Materials Engineering.

Dr. Mukhopadhyay is one of the key members for the development of Solid Oxide Fuel Cell (SOFC) Technology at



CSIR-CGCRI, Kolkata who has demonstrated indigenously made 1 kW SOFC stack with H₂ and O₂/air and also with Reformed Natural Gas (NG) and O₂/air successfully for the first time in India. He is one of the leading researchers from CSIR-CGCRI, Kolkata for the “SolidOxide Fuel Cell and Electrolyzer Cell Consortium Project” (Project targeted value: 70.00 Crores) that is framed out with ARCI, Hyderabad and industries like HPCL for effective commercialization of the Fuel Cell and Electrolyser Cell Technologies in National perspective sponsored by MoP&NG. He is the Nodal Scientist for CSIR H₂T Mission project on Solid Oxide Electrolyser Technology and also leads Next Generation thin cell based Reversible Solid Oxide Cell based technology for circular economy enabler under DST-AHFC proposition. He is also the lead for the CSIR-CIMFR sponsored project for evaluating coal gasified syn gas in kW scale SOFC. At present, he owns the ECF near 250 Lakhs in the various fields of SOC research projects. He has been selected as the member of CSIR National Strategic Sector Member from CSIR-CGCRI out of the total 9 members from the country under National Hydrogen Strategic Mission.

Dr. Mukhopadhyay has published 60 research articles in various reputed SCI Journals and delivered 40 invited talks in different National and International events. He has guided 15 numbers of M. Tech & M. Sc students and 08 (02 numbers completed and 06 numbers ongoing) numbers of PhD students on various fields of SOFC and SOEC research activity. Dr. Mukhopadhyay has been conferred with Dr. Anil Kaviraj Johnson Memorial Award 2025 on 27th Nov 2025 from Indian Ceramics Society on the occasion of technology development on Solid Oxide Cell and also was conferred with Best technology award under Platinum Jubilee Award on 22nd May by the selection committee.



Quantum well ,Wire and Dot

Prof. (Dr.) Debashis De

Department of Computer Science & Engineering

Maulana Abul Kalam Azad University of Technology,

West Bengal, India



ABSTRACT

Quantum wells, wires, and dots are semiconductor nanostructures that utilize quantum confinement to restrict electron movement in one, two, or three dimensions, respectively, resulting in discrete energy levels. These structures alter density of states, enabling high-performance optoelectronics (lasers, LEDs) and quantum computing components.

Quantum Wells (2D): Created by confining electrons within a thin, low-bandgap semiconductor layer (e.g., GaAs) sandwiched between higher-bandgap layers. This reduces motion to two dimensions, creating 2D electron gas (2DEG) with high mobility.

Quantum Wires (1D): Formed by restricting electrons in two dimensions (e.g., using lithography or chemical vapor deposition). Electrons are free to move only along the wire length. They exhibit size-dependent conductivity and potential applications in nanoelectronics.

Quantum Dots (0D): Known as "artificial atoms," these particles are confined in all three dimensions to a scale of few nanometers. They exhibit discrete, atom-like energy levels. Their properties depend on size, allowing for tuning of their optical properties.

These nanostructures are used in lasers, photovoltaics, and electronics due to their unique properties arising from reduced dimensionality

BIOGRAPHY

Dr. Debashis De, PhD, is a Professor in the Department of Computer Science and Engineering at Maulana Abul Kalam Azad University of Technology, West Bengal, India. He earned his M.Tech from the University of Calcutta (2002) and his PhD in Engineering from Jadavpur University (2005). A Senior Member of IEEE, Fellow of IETE, Fellow of the Institute of Engineers, and Life Member of CSI, ACM, IET, and Chartered Engineer. He has received



prestigious awards such as the Boyscast Fellowship (India) to work at Heriot-Watt University, Scotland, Edinburgh, Endeavour Fellowship (Australia) from deputy Prime minister of Australia for his Postdoc at the University of Western Australia, Perth, and URSI Young Scientist Award (2005) from president of India APJ KALAM at New Delhi and 2011 at Istanbul, TURKEY. He was honored with the JC Bose Research Award, IETE New Delhi (2016). Shiksha-Ratna Award (2019) by the Govt of West Bengal and the IETE Chartered Engineer for his contributions. He is an IBM-certified Quantum Systems Engineer.

He served as the AICTE Doctoral Fellow (ADF) coordinator of University 2000 -2025. He served as Vice Chairman of the BOS of all Computer Science and Engineering. Courses of West Bengal under the State Technical University. He is currently serving as a five-member expert committee of West Bengal DSTBT, Govt of West Bengal, for AI-related projects in West Bengal. He served as HOD CSE and IT, Director, School of Computational Science, and IQAC director of the university. He delivered 1000+ talks in various conferences and workshops in India and abroad. He has been serving as International Research Expert of NRDIO - National Research Development and Innovation Office (NKFIH), Budapest, Hungary since 2024. He served as Vice Chair of the Dew Computing Special Technical Committee, IEEE USA 2021-2025. He is a member of IEEE Consumer Communications Networks and Connectivity (CCN), IEEE, USA. With over 400+ journal papers, 200+ conference papers, 20 books, 6 patents, 2 copyrights, he has led research projects funded by AICTE, UGC, DST, DST-FIST, World Bank, TEQIP I and TEQIP II coordinator, AMAZON WEB Services, and MeitY with a total budget of Twenty (20) crore. He received the Ten Best Paper Award at the International Conference. He has held leadership roles as Chairman of CSI and IETE Kolkata and EC Member of IEEE Kolkata. He served as a governing council member of IETE, New Delhi. His h-index is 52 with 12600 citations, and he ranks among the top 2% of global scientists, Stanford, USA, and is ranked 122 in India by Research.com. He guided 27 PhD students, 200+ B.TECH, M.TECH students. He is serving as president of the Institute Innovation Cell (IIC), MHRD of the University. He established the Centre of Mobile Cloud Computing. Currently, he serves as Associate Editor for several reputed journals, including IEEE Access, Springer MST, Wiley IJCS, IETE J Research, and IET Quantum Communication. He is Editor-in-Chief of Frontiers of Internet of Things. His research focuses on Edge Intelligence, Federated learning, Sustainable computing, Internet of Things, and Quantum Computing.



Emergent Critical Fluctuations and non-gaussian Statistics Beyond Ginzburg–Landau Theory

Dr. Mintu Mondal

Associate Professor, School of Physical Sciences,

Indian Association for the Cultivation of Science,

Kolkata, India



ABSTRACT

Second-order phase transitions are surprisingly common in nature—they occur when a ferromagnet loses its magnetization, when a material enters the superconducting state, or even when microbial populations collapse under environmental stress. Despite arising in seemingly unrelated systems, these transitions are governed by a shared underlying mechanism, typically captured by the Ginzburg-Landau theory. This theoretical framework models how a system's internal state evolves as it nears the critical point. A central concept in this framework is the order parameter, a quantity that measures the degree of order in the system - such as magnetization in a ferromagnet or the amplitude of superconductor and charge density wave. As a system approaches the critical point, fluctuations in the order parameter become increasingly important, influencing their thermodynamic properties such as conductivity, heat capacity, and magnetization. However, directly observing these fluctuations—particularly in real, solid-state systems—has remained a significant experimental challenge.

In this talk, I will present our recent results on the quasi-one-dimensional material $(\text{TaSe}_4)_2\text{I}$, which undergoes a charge density wave (CDW) transition at about 263 K. Using phase sensitive low-frequency resistance noise spectroscopy, we demonstrate that fluctuations of the CDW order parameter persist over an unusually wide temperature range and become sufficiently slow (~ 10 Seconds) to influence the system's properties even in the thermodynamic limit. As the system approaches the critical temperature, we observe two hallmark features of critical phenomena: (1) the fluctuations become stronger and slower—a behavior known as critical slowing down and (2) near the critical point, statistical nature of fluctuations deviates from the usual expectations of mean-field theory and shows non-Gaussian behaviours. These features are manifestation of critical opalescence, a well-known concept associated with second-order phase transition.

Our results provide direct experimental evidence of fluctuation-dominated critical dynamics in a solid-state electronic system, offering new insight into how second-order phase transitions unfold beyond mean-field theory.



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BIOGRAPHY

Dr. Mintu Mondal is an experimental condensed matter physicist and Associate Professor at the Indian Association for the Cultivation of Science. His research focuses on low-dimensional quantum materials, including superconductors, topological systems, van der Waals magnets, and correlated electron materials. He completed his Ph.D. at Tata Institute of Fundamental Research and pursued postdoctoral research at ETH Zurich and Johns Hopkins University.

At IACS, he leads the Spectroscopy of Quantum Materials laboratory, developing advanced techniques such as low-frequency noise spectroscopy to investigate critical phenomena and phase transitions in quantum materials. He has published widely in leading journals including Physical Review Letters.



Solar cell: Overview and Recent Trends

**Dr. Madhupriya Samanta¹, Joy Chakraborty¹, Akhilesh Pandey²,
Mahadeva Bhat²**

1Centre for Millimeter wave Semiconductor Devices and Systems (SSPL),
DRDO, Kolkata, India

2Solid State Physics Laboratory,
DRDO, Delhi, India

Presenting author: Dr. Madhupriya Samanta, Scientist C



ABSTRACT

Solar cell has emerged as a powerful device for harvesting renewable energy. It is expected to become a prominent sustainable energy source due to the availability of unlimited solar energy for meeting the energy requirements in future. The applications include terrestrial, power source in unmanned systems and also in Space Satellites. Solar cells can be classified into three main generations evolving from high-cost, high efficiency Crystalline Silicon (CSi) solar cell to low-cost, flexible thin film based and further towards high efficiency emerging technologies like organic, perovskite and multi-junction solar cells. Each generation has its own merits and demerits. Recently third generation of solar cells is gaining immense importance in the field of renewable energy. Multi-junction solar cells are one class of third generation solar cells aiming to achieve high efficiency. Multi-junction tandem solar cells utilize a stack of integrated photovoltaic sub cells with varying bandgap energies, enabling each sub-cell to selectively absorb distinct spectral regions of sunlight. This integration facilitates efficient charge carrier transport and minimizes the optical losses, thereby enhancing the overall performance and scalability of such architecture. In multi-junction structure, the key feature is to obtain high crystal quality, the lattice matching and bandgap matching conditions in between the sub-cells. In recent years, new materials and new structures are continuously evolving in order to achieve lowcost, lightweight, flexible and transparent solar cell.

The multi-junction solar cell consists of double junction, triple junction or more. Materials for double / triple junction solar cells can be either perovskite or III-V compound semiconductor based. Single junction Perovskite cell integrated with either perovskite or C-Si makes their tandem cells highly efficient. Hybrid metal halide perovskite solar cells have recently emerged as highly promising candidates for multi-junction tandem applications, due to their rapid advancements in power conversion efficiency (PCE), which has reached 26%. III-V based double/triple junction solar cells have also achieved their potential application as space solar cell due to high PCE as well as superior resistance towards various radiations in space.



BIOGRAPHY

Dr. Madhupriya Samanta is presently working as Scientist-‘C’ in Centre for Millimeter wave Semiconductor Device and Systems (Solid State Physics Laboratory), DRDO, Ministry of Defence, Govt of India, Kolkata. She has completed M. Tech in Materials Science and Nanotechnology in 2015 from Jadavpur University, Kolkata. She received gold medal in M.Tech program from Jadavpur University in 2015 and was awarded DST INSPIRE fellowship for doctoral program. She obtained her PhD degree from the Department of Electronics & Telecommunication Engineering of Jadavpur University in 2022. Her research area includes synthesis, characterization of organic semiconductor and its hybrid with 2D layered materials e.g. Graphene, MoS₂ etc. and their applications in the field of energy storage, conversion and harvesting.

She has published more than thirty International peer-reviewed journals with total 960 citations and presented in fifteen National/International conferences. She is a life member of Electron Microscopic Society of India (EMSI). She joined DRDO in 2024. Currently, she is working in design, simulation and fabrication of multiple semiconductor devices including W band IMPATT diodes, Triple Junction based Space Solar cells.



Revitalizing Lead Acid Battery Technology Through Advanced Materials Engineering: Recent Developments and Emerging Applications

Dr. Avik Ghosal

Senior Manager – Process & Product Development,

Exide Industries Ltd



ABSTRACT

Lead-acid batteries remain one of the most widely deployed electrochemical energy storage technologies due to their cost effectiveness, high recyclability, and established manufacturing infrastructure. Despite competition from lithium-ion systems, recent advances in material science and engineering have significantly improved the performance, durability, and application scope of lead-acid batteries. This presentation reviews key developments in electrode materials, including advanced carbon and nanostructured additives, optimized grid alloys, and electrolyte engineering strategies aimed at mitigating sulfation, corrosion, and water loss. Progress in lead-carbon battery designs has enabled improved charge acceptance and high-rate partial-state-of-charge cycling performance. Furthermore, smart manufacturing practices and integration with battery management systems have enhanced reliability and lifecycle predictability. These developments demonstrate that lead-acid battery technology, supported by modern material science innovations, continues to play a strategic role in sustainable and affordable energy storage solutions.

BIOGRAPHY

Dr. Avik Ghosal is a Senior Manager – Process & Product Development (Industrial Batteries) at Exide Industries Ltd., Kolkata, with over 24 years of extensive experience in the lead-acid battery industry. He holds a B.Tech in Chemical Engineering and a B.Sc. (Hons.) in Chemistry from the University of Calcutta. His expertise lies at the intersection of materials science, electrochemistry, and manufacturing technology, with significant contributions to R&D, quality systems, and large-scale production operations. He has been instrumental in advancing grid alloy optimization, integrating carbon additives for enhanced cycle life, and improving paste rheology for better battery performance. His work focuses on both negative and positive plate material engineering, curing and formation



processes, and optimizing parameters such as charge acceptance, high-rate partial state of charge (HRPSoC) behavior, and durability.

Mr. Ghosal has played a key role in the development of a wide range of lead-acid battery technologies, including tubular, industrial, inverter, motive power, and EV-supporting batteries. His strategic approach to process control and product innovation has enabled the successful translation of advanced material concepts into robust and scalable manufacturing solutions. He continues to contribute to the development of next-generation energy storage systems for applications in electric vehicles, renewable energy, and industrial sectors.





Special Lectures





Recent Developments in Scholarly Publishing: Editor's Perspective

Dr. Raja Chakraborty & Dr. Anurag Mukherjee

Wiley,

India

ABSTRACT

This Wiley stands as one of the leading scientific publishers, with a legacy spanning over 200 years and a global mission to enable discovery, power education, and shape the workforce. Renowned for its high-quality journals across fundamental and interdisciplinary research domains, Wiley consistently delivers publications with well-deserved recognition.

Wiley's journal portfolio represents one of the most diverse and strategically curated collections in scholarly publishing, encompassing research across fundamental science, chemistry, physics, materials science, engineering, polymer science, and biomedical disciplines. The portfolio spans studies ranging from molecular-level design and synthesis to device physics, biointerfaces, data-driven materials discovery, theory-computation-robotics approaches, and translational applications. By emphasizing this breadth, Wiley aims not only to provide appropriate publication pathways for high-quality research but also to actively promote cross-disciplinary exchange and long-term scientific innovation.

This talk will introduce Wiley's portfolio with that interdisciplinary scope in mind and take a closer look at how Wiley engages with researchers in India. From an editor's vantage point, we will share practical advice on communicating research clearly and choosing the right publication strategy. Given how quickly generative AI is reshaping academic writing, the talk will also address what the responsible and ethical use of these tools looks like in peer-reviewed publishing. The session will close with a look at peer review itself, the major open access models, and what recent ONOS developments mean for researchers in India.



Recent Developments in Scholarly Publishing: Editor's Perspective

Dr. Anurag Mukherjee

Deputy Editor, Wiley,

India



BIOGRAPHY

Dr. Anurag Mukherjee received his PhD in polymer and supramolecular materials from the Indian Association for the Cultivation of Science (IACS), India. He subsequently carried out postdoctoral research at the University of Münster, Germany, and Brandeis University, USA. In 2025, he joined Wiley as a Deputy Editor, overseeing the Wiley Advanced Science along with Polymer and Macromolecular journal portfolio (Macromolecular Rapid Communications, Macromolecular Bioscience, Macromolecular Chemistry and Physics, Journal of Applied Polymer Science etc.). In this role, he manages editorial responsibilities and publishing development across materials science, physical science and polymer research.

Recent Developments in Scholarly Publishing: Editor's Perspective

Dr. Raja Chakraborty

Assistant Editor, Wiley,

India



BIOGRAPHY

Dr. Raja Chakraborty earned his Ph.D. from the Indian Association for the Cultivation of Science, Kolkata, in 2023, specializing in experimental condensed matter physics. He joined Wiley as an Assistant Editor in January 2024 and currently manages several of Wiley's popular titles, including Angewandte Chemie, Advanced Functional Materials, Advanced Energy Materials and ChemistrySelect.



Invited Lectures





Thin and Thick Film Ceramic Sensor: an Overview of Development and Applications

Dr. Debdulal Saha

Senior Principal Scientist

Functional Materials and Devices Division,

CSIR-Central Glass & Ceramic Research Institute,

196, Raja S.C. Mullick Road, Jadavpur, Kolkata-700 032, India



ABSTRACT

We have developed capacitive moisture sensor devices based on nanoporous γ -alumina sensor elements. Moisture absorbed within the pores enhances the dielectric constant, thereby increasing the capacitance at higher levels of moisture uptake. Thin films of γ -alumina were fabricated via sol-gel and screen-printing techniques [1], and integrated with appropriate electronic circuitry to construct trace moisture meters. The developed porous dielectric films enable detection of moisture in the range of 2–100 ppm. For low-level moisture detection in transformer oil, a ceramic-based moisture sensor with adequate sensitivity in the 2–100 ppm range has also been demonstrated [2].

In addition to moisture sensing, we have extended our research towards ceramic gas sensors for toxic gas detection. Formalin (HCHO), a highly flammable compound widely used in manufacturing and food industries, poses severe health hazards including carcinogenicity, respiratory complications, and damage to ocular, lymphatic, and hematopoietic systems. We investigated semiconducting copper ferrite (CuFe_2O_4) inverse spinel nanoparticle-based gas sensors for the detection of formalin adulteration in fish [3]. The nanoparticles were synthesized via a simple sol-gel route and comprehensively characterized using XRD, XPS, FESEM, TEM, EDS, UV–Vis spectroscopy, laser diffraction particle size analysis, I–V measurements, infrared imaging, and non-contact optical profilometry. The fabricated sensor demonstrated high p-type sensitivity towards trace levels of formalin gas (5–30 ppm), with a rapid response time (~ 2.7 s), fast recovery (~ 34 s), and excellent selectivity against interfering gases such as acetone, ethanol, and saturated moisture at a moderate operating temperature (260 °C).

Keywords: Porosity effect, Moisture sensor, thin film, Dielectric layer and Capacitive sensor, Formalin gas sensor

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BIOGRAPHY

Dr. Debdulal Saha is a Scientist-F in the Functional Materials and Devices Division at CSIR–Central Glass and Ceramic Research Institute (CGCRI), Kolkata. He completed his B.Tech. in Chemical Technology (2001) and M.Tech. in Ceramic Engineering (2003) from the University of Calcutta, followed by a Ph.D. in Material Science from Jadavpur University in 2010, where his research focused on the development of trace moisture sensors using micro/nanoporous ceramic materials. With over 23 years of experience, Dr. Saha has developed significant expertise in the design and development of humidity, moisture, and gas sensors. His contributions include the successful development and deployment of high-temperature humidity sensors for BARC, wireless moisture detection systems for NTPC units, and advanced moisture meters for industrial applications such as transformer oil monitoring.

Dr. Saha has been actively involved in research and development, having contributed to more than a dozen major projects sponsored by government agencies and industry, with several successfully completed and ongoing initiatives. He has supervised doctoral research, with two Ph.D. scholars awarded and one ongoing, and has published over 55 research papers in reputed international journals. He also holds three Indian patents and has delivered more than 25 invited lectures. His work reflects a strong commitment to advancing sensor technology and functional materials for critical industrial and scientific applications..



Strategic Opportunities and Innovation of Ultra High Temperature Ceramic Research: CSIR-CGCRI Case Studies

Dr. Shirshendu Chakraborty

Scientist E, Advanced Ceramics & Composites Division

CSIR-Central Glass & Ceramic Research Institute, Kolkata- 32



ABSTRACT

A special class of structural ceramics known as advanced ultra high temperature ceramics (UHTCs) has superior high temperature thermo-mechanical and tribological qualities. These special qualities make UHTCs the preferred material for a variety of industrial, defense, and aerospace industries, including automotive, refractory and energy under challenging circumstances. [1-2] Ultra high temperature ceramics are typically defined as borides, carbides, and nitrides of group IVB and VB transition metals with high melting temperatures ($>2500^{\circ}\text{C}$) and outstanding thermo-mechanical characteristics. The last 20 years have seen the beginning of UHTC research. However, there are many opportunities to progress UHTC materials toward net-shape development in terms of scale-up processing, functionally graded design, and optimal selection. The primary obstacles are the production of net-shaped components, high purity raw materials and their processing, and property evolution and testing. [3-4]

For the past two decades, CSIR-CGCRI, which specializes in non-oxide ceramic processing, has been concentrating on UHTC components with a focus on special applications for the defense, civilian, and strategic sectors. Some of the examples like ZrB₂ based composites for aerospace, RBSN/BN based EM window and leading edge, LaB₆ based emitter for electric propulsion thruster, Cf-SiC clutch plate & jet vane for missiles and SiC Foam for aerospace thermal insulation. An overview of research on non-oxide-based UHTCs, a few case studies of technological and component advancements, and the challenges encountered in this field at CSIR-CGCRI will be covered here.

Keywords: Non-oxide ceramics; Mechanical Properties; Tribology.

Acknowledgments

The author is thankful to DRDO for financial support. Thanks are also due to all ACC Departmental staff members.

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BIOGRAPHY

Dr. Shirshendu Chakraborty is a Scientist-E in the Advanced Ceramics and Composites Division at CSIR–Central Glass and Ceramic Research Institute (CGCRI), Kolkata, and also serves as an Associate Professor at the Academy of Scientific and Innovative Research (AcSIR). He obtained his M.Tech. from the Indian Institute of Technology (IIT BHU), Varanasi, and completed his Ph.D. from Jadavpur University. With over 20 years of research experience, his work focuses on non-oxide ceramics, ultra-high temperature ceramics, refractories, and nanomaterial synthesis. Dr. Chakraborty has successfully handled 18 government- and industry-sponsored research projects as Principal Investigator, with a total funding value of approximately ₹52.68 crore.

He has made significant contributions to the field through 43 publications in SCI-indexed journals, 76 conference papers, 17 invited lectures, and holds 5 Indian patents. In addition to his research, he has actively contributed to academia and professional bodies, serving as a guest faculty at Nirma University, a visiting researcher at the Slovak Academy of Sciences, Bratislava, and an external examiner at institutions such as IIT BHU and Rajasthan Technical University. He is also associated with the Indian Institute of Ceramics as a paper setter and tabulator and is currently serving as its Secretary (2025–2026). His work reflects a strong commitment to advancing ceramic materials research and fostering academic and industrial collaboration.



Toward Cleaner Air: Theoretical Design of Cu(I)-Anchored Heterocycles for Efficient CO, CO₂, and CH₄ Capture

Abhishek Bag, **Dr. Gourisankar Roymahapatra^{1*}**
Associate Professor, Department of Applied Sciences,

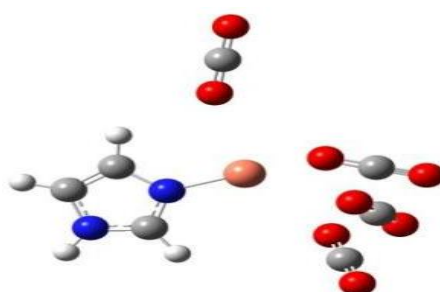
Haldia Institute of Technology,

Haldia-721657, West Bengal, India



ABSTRACT

This work delivers a detailed DFT-based exploration of Cu(I)-decorated five-membered aromatic heterocycles—imidazole, pyrazole, thiazole, oxazole, isoxazole, and isothiazole—as efficient molecular platforms for greenhouse gas capture (CO, CO₂, CH₄). Using B3LYP/6-31+G(d,p), we examine optimized geometries, electronic structures, and adsorption energetics, supported by CDFT descriptors, NBO analysis, NICS, PDOS, ELF, NCI, ADMP simulations, and Gibbs free energy calculations. The studied systems typically bind up to four gas molecules, with adsorption strengths consistently following CO > CO₂ > CH₄. CO exhibits strong chemisorption driven by notable charge transfer and π -back donation from Cu, while CO₂ and CH₄ interactions are comparatively weaker. Aromatic integrity remains largely intact upon adsorption, and dynamic simulations confirm robust stability. Thermodynamic results indicate spontaneous CO capture, favorable CO₂ uptake, and limited CH₄ adsorption at ambient conditions. Notably, Cu(I)-imidazole and Cu(I)-oxazole systems stand out as highly effective, offering valuable design insights for advanced gas-capture materials.



Imidazole- Cu(I)@4CO₂

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**BIOGRAPHY**

Dr. Gourisankar Roymahapatra, FICS, FIC, FRESI, MRSC is currently working as an Associate Professor of Chemistry at the School of Applied Science and Humanities, Haldia Institute of Technology (HIT) Haldia, India. He completed his Ph.D. from Jadavpur University, Kolkata (2014) with N-Heterocyclic Carbene Chemistry as a major field. His area of research interest includes NHC complexes, organometallics, and catalysis, antibiotics, anti-carcinogenic, gas adsorption, super alkali, computational chemistry and DFT.

Before joining to Global Institute of Science and Technology (GIST Haldia), as a Lecturer in Chemistry in the year 2011, he worked at MCC PTA Chem. Corp. Pvt. Ltd India (MCPI), Haldia, (2003 ~ 2011) as a Senior Chemist. He joined HIT Haldia in 2015 as an Assistant Professor of Chemistry.

For his contribution in research, he got the 'Distinguished Young Scientist Award in Chemistry -2014' from world science congress, Kolkata; 'Indian Chemical Society Research Excellent Award 2021', 'A. P. C. Ray memorial Lecture Award – 2024' by Dr. C. V. Ramn University. Chattisgarh, "Bangya Ratna Award- 2025' by Kolkata Literary and Cultural Society.

Dr. Roymahapatra is a Life Fellow of the Indian Chemical Society (FICS), Institutes of Chemistry (India) (FIC), The Renewable Energy Society of India (FRESI), Life member of Chemical Research Society of India (CRSI), Association of Chemistry Teachers (ACT), Member of Royal Society of Chemistry (MRSC). He is the Vice-president of Haldia Vigyan Parishad (2018-2026) and Treasurer of Indian Photobiology Society (2023-2027).

Dr. Roymahapatra has published 153 international articles, 27 book chapters, 01 book, 01 DST-SERB project, and having 11 joint patents in his name. Dr. Roymahapatra edited the 'Chemical Warta' - a chemistry newsletter and 'Education in Chemical Science and Technology' – a book series, published by the Indian Chemical Society. He also edited the Acharya PC Ray special issue published by ES Material and Manufacturing, March-2023; and the contributor of ACS Axial on Acharya PC Ray, published in August 2023, Acharya PC Ray special issue published by ES Chemistry and Sustainability, December-2025. Currently he is the executive editor of ES Chemistry and Sustainability and Associate Editor of ES Energy & Environment published from USA.

Dr. Gourisankar Roymahapatra, FICS, FIC, FRESI, MRSC, is an Associate Professor of Chemistry at the School of Applied Science and Humanities, Haldia Institute of Technology (HIT), Haldia, India. He earned his Ph.D. from Jadavpur University, Kolkata in 2014 with specialization in N-Heterocyclic Carbene (NHC) Chemistry. His research interests Organometallic chemistry, catalysis, drug design, gas adsorption, super alkali, green energy, and computational chemistry with DFT. Before entering academia, he worked as a Senior Chemist at MCC PTA Chem. Corp. Pvt. Ltd. (MCPI), Haldia (2003–2011). He later served as a Lecturer at Global Institute of Science and Technology, Haldia, and joined HIT in 2015 as an Assistant Professor. He also served as Guest Lecturer at Midnapore



College, Raja NL Khan Women's College and Netaji Open University. Dr. Roymahapatra has received several honors, including the Distinguished Young Scientist Award in Chemistry (2014), Indian Chemical Society Research Excellence Award (2021), A.P.C. Ray Memorial Lecture Award (2024), Meghnad Saha Award (2025), and Bengal Excellence Award (2025). He has published over 150 international research articles, 27 book chapters, one book, and holds 11 joint patents..



Integration of Advanced Materials Manufacturing Processes for Next Generation Polymeric Biomimetic Scaffold

Prosenjit Saha*

Associate Professor , Centre for Interdisciplinary Sciences,

JIS Institute of Advanced Studies & Research (JISIASR),

JIS School of Medical Science and Research Campus, 51,

South Nayabaz, GIP Colony, Santragachi, Howrah 711112, West Bengal, India



ABSTRACT

The development of advanced biomaterials integrating structural functionality with therapeutic performance is the key to next-generation biomedical applications. 3D printing of hydrogel systems, and electrospinning have emerged as promising techniques due to their ability to create highly controlled and biomimetic structures. These techniques enable precise tuning of material properties, including porosity, mechanical strength, and surface characteristics, which are essential for supporting biological interactions and improving therapeutic outcomes. Hydrogels, with their high-water content and soft, tissue-like nature, provide a favorable environment for cell survival and the incorporation of bioactive molecules. Their physicochemical properties can be tailored to achieve controlled and sustained release of therapeutic agents, making them highly suitable for localized treatment applications. On the other hand, electrospun scaffolds offer a nanofibrous architecture that closely resembles the natural extracellular matrix, thereby facilitating cell attachment, proliferation, and differentiation. The interconnected porous network of these scaffolds further enhances nutrient diffusion and waste removal, which are critical for tissue growth. Advances in 3D printing have further expanded the potential of these materials by enabling the fabrication of complex, customizable structures with high precision. This allows for better control over scaffold geometry and spatial distribution of functional components, improving their applicability in patient-specific treatments. Such integrated platforms hold great promise for advancing regenerative medicine, enabling controlled therapeutic delivery, and addressing critical challenges in clinical and translational research.

Keywords: 3D Bio-Printing, Electrospinning, Polymer Scaffold, Drug Delivery, Wound Healing

**BIOGRAPHY**

Dr. Saha received his PhD degree from Indian Institute of Technology -Kharagpur, in the year 2013 for his significant contribution in the field of natural biopolymer and their engineering applications. Immediately after completion of his PhD degree, he joined a technical textile industry as Head-R&D, to continue his career there for about one year. After that, he has decided to shift into academia and went to South Korea for advanced postdoctoral research on 3D printing and organ printing using common biopolymers such as cellulose, chitosan, lignin, etc. He returned back to India on availing a very prestigious Inspire Faculty award conferred by Department of Science and Technology, Govt. Of India. In India, he joined at IEST-Shibpur, as an Assistant Professor in 2015. In IEST-Shibpur, he continued his academic career till 2019. During this period he was awarded with several research grant from different funding agencies of Govt. of India to establish a state-of-the art research infrastructure in the field of Polymer Science and Materials fabrication. Presently, he has been working as an Associate Professor, at JIS Institute of Advanced Studies and Research-Kolkata. Till date Dr. Saha has published more than 50 international research articles, 3 reference books. Dr. Saha has successfully guided that two PhD scholars got awarded with the doctoral degree. He has brought research funding of about INR 2.5 Crores so far as principal investigator. His research expertise includes, 3D bioprinting, biopolymer design and synthesis, processing of natural fiber based fire retardant composites, organ printing and tissue engineering to name a few..



Characteristic Features of Green Synthesized Silver Nanoparticles from Aloe Vera Plant Extract and Biological Activity Analysis

Dr. Sucheta Banerjee

Assistant Professor, Department of Chemistry,

Sir Parashurambhau College,

(Empowered Autonomous), Pune – 411030, Maharashtra, India



ABSTRACT

From In this study, green synthesis of silver nanoparticles (Ag NPs) at different temperatures is done in cost-effective and environment-friendly procedure. Synthesis temperature has played an important role in the synthesis of NPs where presence of Aloe vera leaf extract acts as reducing agent for silver. Change in the reaction system from colorless to yellow and finally to grey black confirms the formation of Ag NPs. These NPs are characterized by Scanning Electron Microscopy (SEM), UV-Visible spectroscopy and X-ray diffraction (XRD). With increasing temperature, the size of the nanoparticles increases. As a result of it, more surface area is exposed for the study of antibacterial activity against gram-negative and gram-positive bacterial species. X-ray diffraction results show the crystalline nature of AgNPs with a face-centered cubic structure (FCC). UV-visible spectroscopy confirms the presence of surface-plasmon bands in silver nanoparticles. It has been found that the silver nanoparticles with higher size show the maximum antioxidant properties with FeCl₃ method. It is observed that size of the silver nanoparticle and also silver concentration has an influential role in inhibiting bacteria. Along with this, the antioxidant activity is also checked using Ascorbic acid as standard.

Keywords: Nanoparticle, bacteria, surface-area, green, anti-oxidant

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BIOGRAPHY

Dr. Dr. Sucheta Banerjee is born and raised in Kolkata. After completing her school education from Kolkata, she joined to Presidency College from where she has obtained her B.Sc degree in Chemistry Honours under University of Calcutta on 2012. During the break after graduation studies, she has worked as summer student in the group of biophysical chemistry with Prof. Samita Basu in Saha Institute of Nuclear Physics. With AIR- 59 rank in IIT-JAM exam of 2012, she joined IIT Kharagpur for post-graduation. She worked with Prof. Sabyashachi Mishra for her MSc project on Computational Chemistry in Kharagpur. In addition to this, she held UGC-NET AIR 63 and GATE AIR 299 during her M.Sc period. Then she joined to the ultrafast dynamics lab of Chemistry Department, IIT Bombay as UGC PhD scholar in the group of Prof. Anindya Datta. She has published total 6 research articles in international journals like ChemPhysChem, Nanoscale, Physical Chemistry Chemical Physics, Chemical Communications etc. She has done teaching assistantship in IIT Bombay and IIT Dharwad for B.Tech 1st year and M.Sc 1st year students. She has attended several conferences and workshops in Bombay, Hyderabad, Bangalore, Kolkata throughout her PhD time. On 2019, after five years of PhD, she joined to Sir Parashurambhau College, Pune (affiliated to SPPU) as UGC Assistant Professor, level 10 in the department of Chemistry. She defended her PhD thesis on 2019 while working in the college. Her area of research involves synthesis and spectroscopic studies of molecules as well as exotic nanostructures using steady state and time resolved fluorescence with ultrafast transient absorption techniques time regime upto femtosecond timescale. Total 13 MSc Chemistry students from S.P College and 2 Biochemistry students from Fergusson College has completed their MSc Projects under her guidance. She has promoted to Level 11, Assistant Professor in 2023. In the S.P. college, she is teaching chemistry to UG as well as PG students for almost seven years. She plays an important role in several college activities as department exam coordinator, ABC ID coordinator for Science, NAAC criteria related committee member etc.



An Insight into Non-Destructive Testing: Characterization & Properties Evaluation for different Materials or Samples

Dr. Soumya Mukherjee¹

¹Department of Metallurgical Engineering,

Kazi Nazrul University,

Asansol-713340, India



ABSTRACT

With evolution of modern engineering and scientific principles, testing of materials characterization have undergone tectonic changes. Initial testing of materials are destructive, but for last few decades non-destructive testing is playing a critical role and becomes prominent. Initially, NDT is meant mainly for mere quality inspection, but with rise in industrial competition, ISO standards for every specification of products, NDT becomes a pertinent for every industrial sector. NDT based testing, characterization help in smart, fast inspection without deterioration of sample. It is primarily important for aerospace, automobile, marine engineering, power sector(oil, gas, nuclear etc) and even in medical instrumentation. Principles of NDT is found to have scientific essence comprising, chemistry, physics of materials, instrumentation, IT and software. Different NDT testing techniques are on use in different industrial sectors. With most popular ones are Liquid penetration test(LPT), Ultrasonic pulse test(UT), Magnetic particle testing(MPT), Eddy current test (ET), Radiography, Leak proof test and others. In brief, NDT improves overall quality, reliability of products, predicts damage, fracture, failure of materials in critical services. Catastrophic failures in past lead to disastrous events in history which got prevented by substantial amount with applications, evolution of different NDT techniques. Modern NDT techniques equipped with advance electronics aids in 3D scan of defects which may predict failure behaviour of materials with higher accuracy. NDT also provides pathways for corrosion/degradation studies, mechanical property evaluation of different materials without hampering sample integrity or sample loss in standard corrosion or property evaluation testings.

Keywords: Non-destructive technique, Pulse echo test, LPT, radiography, leak proof test etc

BIOGRAPHY

Dr. Soumya Mukherjee, joined the Department of Metallurgical Engineering of School of Mines and Metallurgy, Kazi Nazrul University, Asansol, India in 10th December, 2018 as an Assistant Professor. He obtained his PhD (Engineering) from Jadavpur University in 2015. He did his doctoral thesis work in the Department of Metallurgical & Materials Engineering. He has done his Master of Engineering in Industrial Metallurgy in 2010 with Gold Medal

Organized by: Department of Basic Science & Humanities,

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), (Autonomous), Kolkata



standing 1st from the Department of Metallurgical Engineering, Jadavpur University. He obtained Bachelor's Degree in Ceramic Technology from Government College of Engineering & Ceramic Technology (WBUT, India) with Bronze Medal in 2008 and subsequently did Mechanical Engineering from Institutions of Engineers (India) (Mechanical Engineering) in 2015. In 2017 he got Chartered Engineering Certificate from Institute of Engineers (India). He had worked with Amity University Kolkata as an Assistant Professor in the Department of Mechanical & Automation Engineering from 24th August, 2015 to 7th December, 2018. Prior to Amity University Kolkata Dr. Mukherjee served at Shroff S. R. Rotary Institute of Chemical Technology (Ankleshwar, Gujarat) as Assistant Professor in the Department of Chemical Technology (Ceramic & Glass) from 15th January 2015 to 21st August 2015.

His domain of research interests include composite and nano-composite materials, advanced ceramics, nanomaterials, multiferroics, electronic materials, refractory materials, waste recycling and engineering, characterization techniques, mechanical properties of metals and manufacturing science and engineering (Welding, Casting, Advance Machining etc).

At present his teaching interest includes Characterization techniques, Physics of Materials, Industrial Management, Fuel, Furnaces & Refractories, Nanomaterials, Mechanical Engineering, Metal working, Transport phenomena, NDT testing of materials, Advance Ceramics and others.

He has published about 95 peer-reviewed research papers in international/National peer-reviewed journals, 42 Full papers in International/National conference proceedings, 6 Book Chapters, presented 77 papers International Conference and 60 National conference papers till date. He also obtained 1 Indian patent Patent File Number: 556821 entitled Development of a Medicated Hemostatic Film, Granted on 24/12/2024. Till now he has attended 30 Faculty Development Programmes organized by NITTTR, Jadavpur University, NIT's, (Andhra Pradesh, MANIT Bhopal) MAKAUT, IIITDM Kaanchedpuram, Ministry of Education (1 Month Orientation Programme) and UGC-HRDC. He has supervised twelve M.Tech Thesis and one PhD in collaborative mode with 3 newly added PhD candidates under his supervision. In addition he has supervised 22 UG projects, 5 Diploma projects too and act as visiting faculty to University of Calcutta for 2023, 205 session for Nanotechnology course. He is also the reviewer and Editorial board member of several International peer-reviewed journals at present. He has membership with several professional bodies like Institutions of engineers (India), Indian Institute of Metals, Indian Institute of Ceramics, International Association of Advanced Materials, Institute of Science, Education and Culture, (ISEC), Powder Metallurgy Associations of India (PMAI) and others. He has received INSA Visiting Scientist Programme 2021 followed by INSA Visiting Scientist Programme 2023 followed by recipient of DST-TARE fellowship from SERB, Govt of India for the duration 2024-2027. He is the principal investigator of a project based on metamaterial composites by UGC DAE CSR Indore along with Co-PI of another project sponsored by UGC DAE CSR Indore. He have completed 26 minor projects with several laboratories in collaborative mode.



When Solvents Become Catalysts: Engineering Reactivity in Water, Ionic Liquids, and Interfacial Media

Dr. Arpan Manna

Assistant Professor, Department of Chemistry,

Tarakeswar Degree College,

Tarakeswar, Hooghly



ABSTRACT

Solvents are traditionally regarded as passive media; however, emerging evidence demonstrates that they can actively influence and even catalyze chemical transformations. This lecture highlights how structured solvents such as water, ionic liquids, and heterogeneous/interfacial systems can dramatically alter reaction kinetics, selectivity, and mechanistic pathways.

Emphasis will be placed on water-promoted organic reactions and the remarkable rate acceleration observed in Diels–Alder reactions under heterogeneous and supersaturated conditions. The role of hydrogen bonding networks, hydrophobic effects, and solvent organization in modulating transition states will be discussed. In addition, ionic liquids are shown to function as tunable reaction environments, where ion pairing, viscosity, and microheterogeneity govern reactivity and energy landscapes.

Insights from time-resolved spectroscopic studies on excited-state intramolecular proton transfer (ESIPT) and photoinduced electron transfer processes will further illustrate how solvent dynamics influence molecular behavior at ultrafast timescales. Special attention will be given to interfacial phenomena, where unique physicochemical environments lead to unconventional kinetic regimes.

Overall, this talk aims to establish a unifying perspective in which solvents are redefined as active participants in chemical processes, offering new opportunities for green chemistry, sustainable synthesis, and the design of advanced functional materials.

BIOGRAPHY

Dr. Arpan Manna is an Assistant Professor of Chemistry at Tarakeswar Degree College, West Bengal since July, 2021, and former Head of the Department of Chemistry at Adamas University, Kolkata (2016–2021). He obtained his Ph.D. from Savitribai Phule Pune University (CSIR-NCL) and completed postdoctoral research at Pusan National University, South Korea. His research focuses on solvent-mediated reaction dynamics, particularly in water, ionic liquids, and interfacial systems. A SERB-DST Early Career Research awardee, he has published in leading journals



and contributes to advancing green and sustainable chemistry.



From Arsenic Mobilization to Sustainable Remediation: Development of Microbial Biofilter and Biofertilizer for Groundwater Safety and Agricultural Enhancement

Dr. Abhishek Basu¹

Assistant Professor ¹Department of Molecular Biology and Biotechnology,

Sripat Singh College, Jiaganj,

West Bengal, India



ABSTRACT

Arsenic contamination in groundwater of the Bengal Delta Plain (BDP) poses a significant environmental and public health challenge, driven by complex hydrogeochemical and microbial processes. This study combines field-based investigation of arsenic mobilization with the development of microbial technologies for its remediation and sustainable agricultural application. Groundwater analysis from shallow aquifers of Chakdah block (Nadia District, West Bengal) revealed arsenic concentrations ranging from 0.069 to 0.178 mg L⁻¹ (mean: 0.119 mg L⁻¹), exceeding permissible limits. A depth-dependent distribution indicated higher arsenic levels in shallow aquifers under reducing conditions. Arsenic release is primarily governed by microbial-mediated reductive dissolution of iron oxyhydroxides, followed by transformation into the more mobile and toxic arsenite [As (III)]. Elevated bicarbonate levels and the presence of total and fecal coliforms across sites suggest active biogeochemical cycling and anthropogenic influence. Sanitary risk assessment categorized most water sources as high to very high risk, underscoring the urgency for effective mitigation strategies. An arsenic-hypertolerant, plant growth-promoting bacterium was isolated from the same region and identified as *Enterobacter sichuanensis* strain WCHECL1597 through biochemical and molecular characterization. The strain exhibited high arsenic tolerance (up to 1000 ppm sodium arsenite) and efficient biotransformation capability, converting arsenite to arsenate. Under optimized conditions (37°C, pH 7.0), it achieved over 90% arsenic removal within 24 hours. A biofilter system was developed using immobilized bacterial biomass combined with a β -cyclodextrin-embedded iron oxide composite. This hybrid design integrates microbial transformation with enhanced adsorption, achieving up to 90% arsenic removal from contaminated water within a pH range of 7.0–8.5. The system offers a low-cost, eco-friendly, and scalable solution suitable for rural water treatment. Additionally, the strain was formulated as a biofertilizer due to its plant growth-promoting traits, including nitrogen fixation, phosphate and potassium solubilization, and production of indole-3-acetic acid, siderophores, acetoin, and ammonia. Pot and field studies demonstrated significant improvements in plant growth parameters, including biomass, chlorophyll content, root development, and yield in chilli plants. This integrated approach highlights the link between arsenic mobilization mechanisms and microbial remediation strategies. The dual



application of *Enterobacter sichuanensis* WCHECL1597 as a biofilter and biofertilizer provides a sustainable solution for improving groundwater quality while enhancing agricultural productivity in arsenic-affected regions.

Keywords: Groundwater, Arsenic, Coliform, Sanitary Risk, Anthropogenic Factors, Arsenic hyper-tolerant bacteria; Bioremediation; Biofilter; Plant growth promoting bacteria; Biofertilizer

BIOGRAPHY

Dr. Abhishek Basu is an Assistant Professor (former Head) and Ph.D. Supervisor in the Department of Molecular Biology and Biotechnology, Sripat Singh College, Jiaganj. He completed his graduation from Presidency College, Kolkata, post-graduation from Rajabazar Science College, and earned his Ph.D. in Biochemistry from CSIR-Indian Institute of Chemical Biology. His research interests span structural biology, microbial biotechnology, and environmental bioremediation, particularly arsenic contamination and mitigation strategies. Dr. Basu qualified CSIR-NET, UGC-NET, GATE, and SET. He has completed two research projects funded by DST & BT, Government of West Bengal, and has applied for a patent. Dr. Basu has published over 30 research articles and book chapters with reputed international publishers (Springer Nature, Elsevier, Wiley Periodicals, BioMed Central, and Taylor & Francis) and has served as editor of several books. He is a recipient of multiple research awards, has delivered invited lectures, organized many international seminars and workshops, guided Ph.D. and PG dissertations. In addition to his academic contributions, he plays a significant role in institutional development through various administrative and academic committees, fostering research, innovation, and student development.



Scaling Approach for the Pre-assumption of Optical Properties of the Thin Film Developed by Competitive Growth Models

Dr. Diptonil Banerjee

Associate Professor, Thin Film and Nanotechnology Laboratory,
Department of Applied Science, Teerthanker Mahaveer University,
Moradabad 244001, UP, India



ABSTRACT

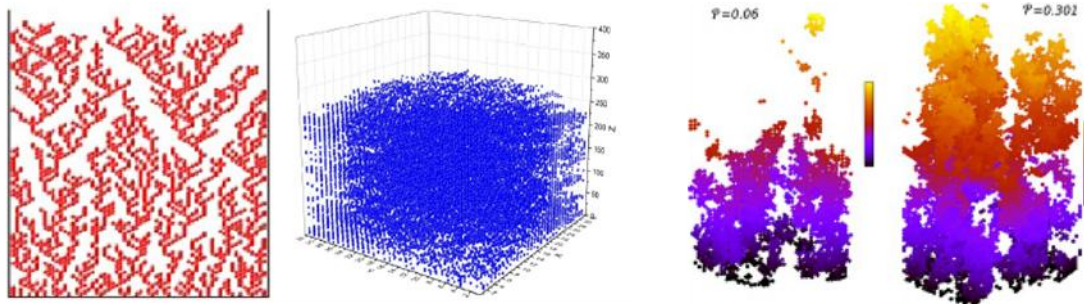
In the era of microchips and nanotechnology the coating is one of most widely technique that makes the system durable, efficient as well as versatile. The coating though can be achieved by both the physical as well as chemical approach in microchip industry mainly physical processes are explored that includes sputtering, evaporation and other molecular beam epitaxial method.

In view of this, the talk will explore different growth mechanism that can be solely responsible for the growth or can develop the thin film through a collective or competitive growth model. In doing this the growth mechanism like random deposition, random deposition with surface relaxation or ballistic deposition along with their widely accepted values of scaling exponent will be discussed.

How the correlation impacts the morphology and the interface width as well as the porosity of the film will be explored as well.

Not only that efforts will be there in explaining that this simple approach can well-explain the quantum confinement effect and can successfully predicts the optical band gap of few well-studied materials also.

The work that will be shared has the possibilities to open up an ample of opportunities for the researchers in field of materials scientist to pre-assume the properties (both optical and electronic) of material in thin form.



Keyword: Thin film, Competitive growth, scaling, correlation, porosity, roughness

**Reference:**

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BIOGRAPHY

Dr. Diptonil Banerjee is currently working as an associate professor in the department of physics, faculty of engineering, Teerthanker Mahaveer University since 2020. Dr. Banerjee, completed both his graduation and Masters in Physics from University of Calcutta in the year of 2005 and 2007 respectively.

He did his PhD from Jadavpur University on Materials Science and Nanotechnology in the year of 2012. Presently Dr. Banerjee is working on mainly carbon-based nanotechnology and related applications. He has also started working on some oxide-based nanostructures as well. He is entrusted by the Department of Science and Technology (Gov't of India) with few projects of considerable budget.

Also, he is belonging to the editorial board members of different journals. He is also reviewer of good many numbers of quality journals. Currently he has published around 120 research articles in different national and international journal of repute along with good many numbers of book chapters and authored a couple of books in the related field of nanoscience and technology entitled “Nano Science - Concepts and Fundamentals” and “Nanomaterial Induced Removal of Textile Dyes from Wastewater” from Bentham publisher. He is the owner of 2 patent and more than 50 conference articles.

He has supervised over 25 PG projects in both M.Sc. and M-Tech in the fields of physics and material Science and presently 5 scholars are pursuing PhD under his supervision along with 2 others already completed. In this journey he received the award of best supervisor of his college in consecutive 3 years. He has delivered numbers of invited talks in different national and international seminars/conference.

Presently Dr. Banerjee is having h index 26 and i10 index 53 with cumulative citation around 2150. Presently the main focus of his research is the indigenous development of electron gun for X-ray generator and electron microscope, a project he has received from DST Gov't of India under Device Development Scheme along with IIT Delhi and INST Mohali.



From Semiconductor Design to Reactor Engineering: Reliable Solar Hydrogen Production

Dr. Debabrata Sarkar

Associate Research Professor , Applied NanoPhysics Laboratory,

Department of Physics and Nanotechnology,

SRM Institute of Science and Technology,

Kattankulathur, 603203, Tamil Nadu, India.com



ABSTRACT

The dual challenge of environmental pollution and sustainable energy demand necessitates integrated technological solutions that can simultaneously address water purification and clean fuel generation. Solar-driven semiconductor photocatalysis has emerged as a promising pathway for pollutant degradation and green hydrogen (H₂) production. However, despite significant progress in material development, the reproducibility, accuracy, and scalability of photocatalytic H₂ generation remain critical bottlenecks.

Surface defects and oxygen vacancies play a pivotal role in tuning the electronic structure of oxide semiconductors, creating active sites and promoting charge carrier separation. Phase engineering, particularly in heterojunction systems, further facilitates interfacial charge transfer through favorable band alignment. Coupled with rational heterojunction design, these strategies significantly enhance light absorption, charge dynamics, and photocatalytic efficiency. Nanostructured systems, developed through controlled synthesis approaches, provide an effective platform to systematically correlate defect density, phase composition, and interfacial energetics with photocatalytic performance.

Equally critical is the design of experimental systems used to evaluate hydrogen evolution. Reactor configuration, gas-tight operation, elimination of leakage, calibration of analytical systems, and careful implementation of control experiments directly influence the accuracy of H₂ measurements. Variations in reactor geometry, light distribution, and mass transport can lead to significant discrepancies in reported performance if not properly optimized. Establishing standardized and scalable experimental setups is therefore essential for obtaining reproducible and error-free hydrogen generation data.

The convergence of defect and phase engineering in semiconductor materials with rigorously designed reactor systems enables more accurate assessment of photocatalytic activity and provides a pathway toward scalable solar-



to-hydrogen conversion technologies. These insights contribute to advancing next-generation photocatalysts for sustainable water purification and clean energy production.

BIOGRAPHY

Dr. Debabrata Sarkar is an Associate Professor in the Department of Physics and Nanotechnology at SRM Institute of Science and Technology, Chennai, India. He leads the Applied NanoPhysics Laboratory, where his research focuses on the design and development of advanced semiconductor nanomaterials for energy and environmental applications, particularly green hydrogen production, photocatalytic water splitting, and air filtration technologies.

Dr. Sarkar obtained his M.Sc. degree in Physics from Jadavpur University, Kolkata, and completed his Ph.D. in Materials Science and Nanotechnology from the same institution. He further pursued postdoctoral research at the Hebrew University nano centre, Israel, gaining international research experience in nanostructured materials.

With over a decade of academic and research experience, Dr. Sarkar has established expertise in semiconductor nanomaterials, band structure engineering, heterojunction photocatalysts, and electrospun nanofiber systems. His research contributions include the development of novel materials for solar energy conversion, environmental remediation, and high-efficiency particulate filtration.

Dr. Sarkar has significant experience in leading externally funded government research projects. He has served as Principal Investigator on projects supported by DST, ANRF. He is currently leading two active funded research projects focused on sustainable materials and environmental technologies, demonstrating his ability to secure competitive funding and manage independent research programs.

At SRM IST, Dr. Sarkar actively contributes to teaching and mentoring undergraduate, postgraduate, and doctoral students. He is an active member of departmental academic committees and has played a key role in new curriculum and syllabus development, including the introduction of updated courses aligned with emerging areas in nanotechnology and energy materials. His current research vision is centered on developing scalable nanomaterial-based solutions for clean energy production and environmental sustainability, with a strong emphasis on translational research and industry collaboration.



Synthesis, Characterization and Applications of doped Carbon Dots

Dr. Dipsikha Bhattacharya¹, Poushali De²
Assistant Professor , ¹Department of Chemistry,

School of Basic and Applied Sciences, Adamas University, Kolkata, India

²La Martiniere for Girls, Kolkata, Dr. U. N. Bhramachari Street,
Kolkata, India



ABSTRACT

From the last two decades, Carbon dots (CDs) have recently gained substantial attention as a fluorescent material due to their strong attributes including excellent photoluminescence properties, versatile surface functionalization efficiency, superior aqueous solubility, and low intrinsic toxicity. Compared to the traditional organic dye and inorganic semiconductor quantum dots, CDs have shown many advantages because of their good solubility in water, simple preparation techniques, high fluorescence intensity, good stability and good biological compatibility and hence it can be widely used in medicine, biology, energy, the sensors, photoelectric conversion and photoelectric catalysis.¹⁻² Among many synthesis techniques, doping with nonmetal heteroatoms into the carbon core is one of the most promising method to prepare CDs with enhanced fluorescence properties because these heteroatoms can change the electronic structure of the carbon core as well as incorporate multiple surface states, which in turn alter the properties from the undoped ones.³ Especially, the use of hetero atom doped CDs in the fluorescence detection of metal ions has become one of the most important applications where the highly photostable CDs can guarantee the stability of fluorescence signal to ensure the accurate detection of the analytes. Among many heavy metals, for our work, we have selected iron (Fe³⁺) as one of the most common metal pollutants detected in environmental water bodies as a trace amount of iron (Fe³⁺) plays an important role in the human body.⁴⁻⁵ Additionally, the accumulation of Fe³⁺ ions in the environment will cause a great threat to living organisms. In our work, cyan color emitting doped CDs were prepared using sulfanilic acid with excitation dependent emission properties and based on its luminescence properties, it has been used to detect the presence of Fe³⁺ ions by detecting changes in their fluorescence intensity.

MATERIALS AND METHODS

Sulfanilic acid, Ethanol, n-Hexane were purchased from SRL, India. 0.4 gm of Sulfanilic acid was dissolved in 1:1 ethanol and water mixture and it was completely dissolved in the reaction mixture after stirring the reaction mixture



at 1000 rpm for 30 minutes and then the liquid was transferred to a Teflon-lined stainless-steel autoclave and kept in the oven at 180°C for 16 hours. The obtained as prepared brown colored liquid was transferred into a beaker and checked under UV lamp where a fluorescence glow was observed. These as prepared CDs were purified using the column chromatography technique using hexane and ethanol. After the purification, the solution containing carbon dots was dried in a rotatory evaporator.

RESULTS AND DISCUSSION

CDs were synthesized by the high temperature and high-pressure carbonization of Sulfanilic acid. The broad nature of the peaks in the XRD pattern indicates that the S, N doped CDs exhibit amorphous carbon nature. From the TEM images of S, N doped CDs, these CDs exhibited almost spherical shape with good dispersibility. The particle size of CDs was statistically analyzed, and its size is mainly distributed at about 5-7 nm. We used FTIR to characterize the structure and surface groups of nitrogen and sulfur co-doped CQDs. The peaks at 1020, 1109, 1220, 1420 and 1630 cm^{-1} strongly indicate the presence of C-S, SO_3^- , C-O, C-N and C=C stretching vibrations of aromatic compounds. The presence of O-H and N-H stretching vibration peaks between 3000–3600 cm^{-1} indicated the presence of amino and hydroxyl groups on the surface of the CDs. From the UV-Visible and fluorescence spectra of the purified CDs, a broad peak at 302 nm along with a sharp peak at 355 nm with a narrow full width at 434 nm confirmed the characteristic of C=N bonds in aromatic rings and the presence of intrinsic surface states. The fluorescence emission peak at 502 nm exhibited the excitation independent nature. The fluorescence intensity of doped CDs was monitored through fluorescence spectra and it was decreased monotonically as the Fe(III) concentration increased⁵ which might be due to the strong coordination of Fe(III) to the oxygen-rich or amine groups on the surface of doped C-dots

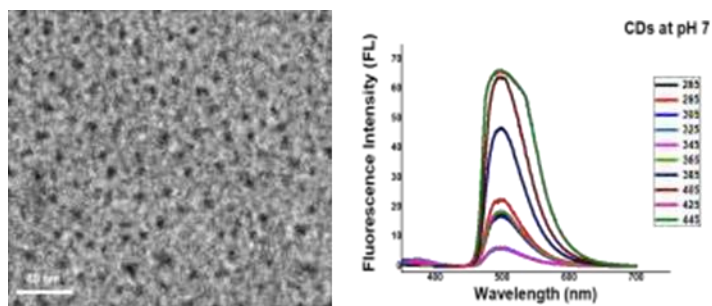


Figure 1. TEM and Fluorescence spectra of purified S, N doped CDs

CONCLUSION

The study successfully demonstrates a simple and efficient method for synthesizing nitrogen and sulfur co-doped carbon dots using sulfanilic acid. These CDs exhibit strong fluorescence, excellent stability, and high selectivity toward Fe^{3+} ions. The sensing mechanism is based on photoinduced electron transfer, leading to fluorescence



quenching upon interaction with Fe³⁺. The CDs show a low detection limit and a wide detection range, making them suitable for real-world applications, especially in environmental monitoring.

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BIOGRAPHY

Dr. Dipsikha Bhattacharya is an academician and researcher in the field of nanoscience and nanotechnology, currently serving as an Associate Professor at the Department of Chemistry, School of Basic and Applied Science, Adamas University, India from October 2022 onwards. She completed her Ph.D. (Science) from the Indian Institute of Technology, Kharagpur, and holds both M.Sc. and B.Sc. degrees in Chemistry from Jadavpur University. She completed two national post-doctoral fellowships from CSIR-Indian Institute of Toxicology Research and CSIR-Central Glass and Ceramic Research Institute and her research focuses on the design and synthesis of advanced nanomaterials with interdisciplinary applications. Her key areas include the development of nanosensors for ultrasensitive detection of metal and biomolecules, multifunctional nanoparticles for targeted drug delivery applications, nanogel-based scaffolds with multifunctional therapeutic properties for wound healing in Wistar rat models, and carbon dot–silica matrices for multicolour light-emitting devices. She is experienced in a wide range of analytical and characterization techniques including FT-IR, ATR-IR, XRD, HPLC, DLS, UV-Vis spectroscopy, fluorimetry, and zeta potential analysis, with working knowledge of NMR, TEM, SEM, and XPS. She has received several prestigious fellowships and recognitions, including the DST Nano Mission Postdoctoral Fellowship (2013–2015), CSIR Senior Research Associateship (2016–2017), and the ISER Certificate of Excellence (Toronto, 2019)..



Naphthalimide-based reversible colorimetric and luminescent sensor for detecting trace water in organic solvents

Sk Sujauddin and Dr. Mijanur R. Molla
Assistant Professor, Department of Chemistry,

University of Calcutta,

92, A. P. C Road, Rajabazar, Kolkata,

West Bengal 700009, India



ABSTRACT

A naphthalimide-based colorimetric and luminescent organic sensor (NMI-S2) has been developed for rapid and reversible detection of trace water in organic solvents such as THF, DMSO, and deuterated NMR media. Unlike conventional techniques like Karl Fischer titration or gas chromatography that require costly instruments, toxic reagents, and lengthy procedures, NMI-S2 enables low-cost, fast, and visual moisture quantification using simple color change or smartphone-assisted analysis. Structurally, NMI-S2 contains amine and amide groups capable of hydrogen bonding, a tri-alkoxy benzene unit that enhances hydrophobic interactions, and a naphthalimide π -chromophore responsible for π - π stacking. These features promote self-assembly and supramolecular responsiveness. In dry THF, the probe exists in a monomeric form with absorption bands at 300–350 nm (π - π^*) and 365–480 nm (ICT). Upon addition of fluoride ions, hypochromic and bathochromic shifts occur along with a new band near 500 nm, signifying supramolecular polymerization. At higher fluoride concentrations, deprotonation of the C4 amine enhances charge transfer, leading to a visible color change from greenish yellow to red. Exposure to trace water reverses this process through reprotonation, regenerating the monomeric state and original color.

This reversible fluoride–water-mediated polymerization–depolymerization process underlies the sensor's high sensitivity and reproducibility. With its color chart calibration and smartphone compatibility, NMI-S2 offers a practical, on-site alternative for trace moisture detection in chemical, pharmaceutical, and environmental samples.

Keywords: Supramolecular polymerization; Naphthalimide sensor; Colorimetric detection; Moisture sensing.

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Dr. Mijanur Rahaman Molla is an Assistant Professor in the Department of Chemistry at the University of Calcutta, Kolkata, India. He obtained his M.Sc. degree in Chemistry from the University of Calcutta in 2008 and pursued his Ph.D. at the Indian Association for the Cultivation of Science (IACS), Kolkata, under the supervision of Dr. Suhrit Ghosh, completing it in 2013. Following his doctoral studies, he undertook postdoctoral research at the University of Massachusetts, Amherst, USA, working on biologically relevant polymer assemblies in the group of Prof. Thayumanavan. He was subsequently awarded the prestigious Alexander von Humboldt Fellowship and conducted further postdoctoral research with Prof. Pavel Levkin at the Karlsruhe Institute of Technology, Germany. Since December 2016, he has been serving as a faculty member at the University of Calcutta.

Dr. Molla's research contributions have been widely recognized through several prestigious awards and fellowships, including the Early Career Research Award from DST-SERB (2019), the S. S. Bhatnagar Young Scientist Award from the Indian Chemical Society (2020), and the JMS-PAC Early Career Research Award from Taylor & Francis (2023). He was elected as an Associate of the West Bengal Academy of Science and Technology in 2023. Earlier, he also received the Sir P. C. Ray Research Award from the University of Calcutta (2014) and the Alexander von Humboldt Postdoctoral Award (2016). His work reflects a strong commitment to advanced research in chemistry, particularly in polymer science and functional materials.



Earth-Abundant Kesterite-Type Chalcogenides for Bifunctional Energy Applications

Dr. Samrat Sarkar¹, and Prof. K. K. Chattopadhyay²

Assistant Professor, ¹Department of Physics,

S.U. College, Hilsa, Nalanda, Patliputra University, Patna, India

²Thinfilm and Nanoscience Laboratory, Department of Physics,

Jadavpur University, Kolkata, India

³School of Materials Science and Nanotechnology, Jadavpur University, Kolkata, India



ABSTRACT

The transition toward sustainable energy technologies demands electrode materials that exhibit high performance while composed of earth-abundant, low-toxicity elements. Here we report the development of Mn- and Ni-substituted kesterites, i.e., Cu_2MSnS_4 ($\text{M} = \text{Mn}, \text{Ni}$), synthesized via scalable hydrothermal routes that enable precise control over morphology, composition, and hierarchical architectures. In one work, $\text{Cu}_2\text{MnSnS}_4$ (CMTS) nanospheres with spherulitic morphology are used as a pseudocapacitive electrode material for supercapacitor applications. It exhibits a high specific capacitance of 524 F g^{-1} at 2 A g^{-1} , along with excellent cycling stability. The hierarchical morphology facilitates efficient ion diffusion and provides abundant electroactive sites. Additionally, CMTS demonstrated promising oxygen evolution reaction (OER) activity in alkaline media, delivering a low overpotential of 353 mV at 10 mA cm^{-2} , a Tafel slope of 92 mV dec^{-1} , and a charge-transfer resistance of 30 ohm, with sustained performance over 3000 cycles. These results highlight the synergistic roles of multi-metallic active centres, sulfur defects, and nanostructure engineering in enhancing electrochemical performance. In another work, $\text{Cu}_2\text{NiSnS}_4$ (CNTS) is engineered into flower-like microarchitectures using a structure-directing strategy, enabling enhanced electrolyte accessibility and charge transport. The CNTS electrodes, directly grown on nickel foam, delivered a high specific capacitance of 508 F g^{-1} at 2 A g^{-1} . A solid-state asymmetric supercapacitor assembled using CNTS and activated carbon achieved a gravimetric capacitance of 105.7 F g^{-1} , with a maximum energy density of 30.88 Wh kg^{-1} and a power density of 2.42 kW kg^{-1} . The device also demonstrated excellent cycling stability, retaining 95.7 % of its initial capacitance after 2000 cycles.

Overall, this study establishes Mn- and Ni-substituted kesterite sulfides as promising, earth-abundant, and low-toxicity materials for integrated energy storage and electrocatalytic systems for next-generation sustainable technologies.



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BIOGRAPHY

Dr. Samrat Sarkar is an Assistant Professor in the Department of Physics at S.U. College, Patliputra University, Patna. He completed his postdoctoral research at the Institute for Sustainable Energy, Shanghai University, China, in 2021. He earned his Ph.D. from the School of Materials Science and Nanotechnology, Jadavpur University, India, in 2018, and his M.Sc. in Physics from Banaras Hindu University, India, in 2011.

Dr. Sarkar has authored 26 research publications in the field of materials science and has presented his work at several national and international conferences. Currently, he is the Co-Principal Investigator in a UGC-DAE Collaborative Research Scheme.

His research focuses on the design, synthesis, and application of nanostructured materials for advanced energy storage and conversion technologies, including supercapacitors, batteries, and electrocatalysis..



Silver Nanoparticle Conjugated Stearic Acid Nanoparticles Induce Selective ROS Amplification and Actin Cytoskeletal Destabilization: Integrated Experimental and MD Simulation Insights

Dr. Debabrata Ghosh Dastidar^{1, *}, Dipanwita Mukhopadhyay¹, Arunima Das¹,
Santanu Paul², Amlan Das³

Associate Professor, 1Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Panihati, Kolkata 700114

2Indian Institute of Science Education and Research (IISER)Tirupati,

Andhra Pradesh - 517619.

3The Assam Royal Global University, Betkuchi, Guwahati, Assam 781035



ABSTRACT

Silver nanoparticles (AgNPs) exhibit strong anticancer potential but suffer from aggregation and non-specific toxicity, motivating the development of stabilized delivery platforms. In this study, AgNPs synthesized through an ethanol-based method were encapsulated within stearic acid solid lipid nanocarriers (SLN), yielding an optimized AgNP@SLN formulation with a particle size of 424 nm and a PDI of 0.139. UV–Vis spectroscopy confirmed a surface plasmon resonance at 447 nm, while TEM imaging demonstrated a uniform core–shell morphology; FTIR analysis further validated matrix encapsulation through characteristic molecular interactions. AgNP@SLN exhibited markedly higher cytotoxicity against human NSCLC cell lines (H1299 and A549), reducing IC₅₀ values by ~1.5-fold compared to free AgNPs, while maintaining minimal toxicity in WI-38 normal fibroblasts. Mechanistic studies revealed pronounced, dose-dependent ROS generation supported by NAC rescue experiments, accompanied by significant actin cytoskeletal disruption and an 83% reduction in colony formation at 25 µg/mL. To complement experimental observations, an in silico model of a 2.5 nm AgNP core coated with Tween-20 (final diameter ~5 nm) was constructed to examine nano–bio interface interactions. Docking analyses demonstrated preferential binding toward actin, which was further validated through 100 ns molecular dynamics simulations revealing stable association, local residue perturbations, and restricted protein mobility. MM-GBSA binding free energy and PCA further supported the nanoparticle-induced structural constraints on actin. Together, these integrated experimental and computational findings indicate that stearic acid-based AgNP@SLN enhances nanosilver stability while promoting selective, ROS-mediated cytoskeletal disruption in NSCLC cells, providing mechanistic insight relevant to the design of next-generation metal-based nanocarriers.



Keywords: Silver nanoparticles, Stearic acid, Solid lipid nanocarriers, Lung cancer cells, ROS-mediated cytotoxicity, In vitro studies.

BIOGRAPHY

Dr. Debabrata Ghosh Dastidar is an Associate Professor at Guru Nanak Institute of Pharmaceutical Science and Technology, Kolkata, with core expertise in nanomedicine and advanced drug delivery. His research spans the design and development of solid lipid nanoparticles, polymeric and lipid–polymer hybrid nanocarriers, and metal nanoparticles including silver, gold, and copper systems.

He has made significant contributions in emerging nanomaterials such as carbon quantum dots and functionalised nanostructures for diagnostic and therapeutic applications. His work integrates synthesis, physicochemical characterisation, and biological evaluation with advanced computational approaches including molecular docking, molecular dynamics, and MM-GBSA analysis to understand nano–bio interactions.

His research portfolio reflects strong contributions to cancer nanotechnology, antimicrobial systems, and targeted delivery platforms, supported by a substantial body of peer-reviewed publications, patents, and national collaborations. Dr. Dastidar has supervised over 150 postgraduate theses and continues to contribute actively to translational nanoscience, focusing on improving selectivity, efficacy, and clinical relevance of next-generation nanotherapeutics.



Defect Luminescence of Semiconductor Nanocrystals- A Single Particle Spectroscopic Perspective

Dr. Arunasish Layek¹, Subhasree Banerjee² and Arindam Chowdhury³
Associate Professor, 1Department of Chemistry, Adamas University,

Barasat-Barrackpore Road, Kolkata 700126, India

2Department of Chemistry, Panchmura Mahavidyalaya, Panchmura,

Bankura-722156, India

3Department of Chemistry, Indian Institute of Technology Bombay,

Mumbai 400076, India



ABSTRACT

The particle size dependent optical properties of semiconductor are largely a result of internal structure of the NCs. However, for small NCs (<10 nm in size), surface states become very important as the size of a structure reduces; the ratio of the number of surface to bulk atoms, which increases with reducing particle size.¹ Therefore surface property plays a critical role in determining the optical properties of the NCs. The atoms on the surface of crystal are incompletely coordinated within the crystal lattice. These surface atoms give rise to energetically different electronic levels from those of the bulk levels.^{1,2} These surface states can act as traps for charge carriers and are often responsible for a large Stokes shifted broad defect luminescence and hence comprehensive understanding of the surface mediated photophysical dynamics is very important.²

To address this issue, optical spectroscopy has prevailed as one of the most important and versatile tools available to the experimentalist. While ensemble-averaged results are important, however, they often devoid of detailed information because of averaging effect which can obscure the discrete behaviour of individual particles. Single molecule fluorescence microscopy has emerged as one the most versatile tool to the scientists. Observations at single particle level removes the usual ensemble average, allowing the exploration of hidden heterogeneity in condensed phases as well as direct observation of complex photophysics without synchronization.

Here, we explore the luminescence properties of chemically grown ZnCdS and CdS nanocrystals systems which display broad visible luminescence. However, it is difficult to characterize the linewidths of the defect luminescence using ensemble photoluminescence (PL) measurements. Conversely, if photophysical properties of NCs can be probed at single-particle level, it is possible to decouple such homogeneous broadening effects arising from particle-



size distributions. Herein, we demonstrate that the defect PL, irrespective of their transition energies, almost all single-particle emission profiles are found to have large spectral line-width (FWHM~400 meV). We also observe a small variation in the transition energies of individual NCs and this may be assigned to the particle size distribution as revealed by transmission electron microscopy image (data not shown). To further confirm our findings, we also recorded single particle PL spectroscopy of CdS NCs. This study conclusively establishes that defect luminescence semiconductor NCs are inherently broad due to distribution of multiple defects.

MATERIALS AND METHODS

The synthesis of ZnCdS was carried out following the procedure reported elsewhere.³ CdS NCs were prepared by reverse micelle microemulsion method as prescribed in the literatures with few modifications.⁴ Single particle fluorescence microscopic experiments (detail procedures are given reference 5) were performed by appropriate dilution of the colloidal NCs solution and thereafter drop casting on a freshly cleaned fused silica coverslip. For the excitation of ZnCdS we have used 457 nm Ar ion laser while 405 nm diode laser was used for CdS sample. All the experiments were performed at room temperature.

RESULTS AND DISCUSSION

The absorption and PL spectrum of ZnCdS solution recorded at room temperature is shown in Figure 1 (a). The absorption spectrum shows sharp excitonic feature at 460 nm. The ensemble PL spectrum shows a narrow band edge luminescence at 480 nm along with a broad defect luminescence band centered around 630 nm. The single particle spectrum of individual NCs shown in Figure 1 (b) are distinctly broad in nature. The line width of single particle spectrum is very large >400 meV as observed in ensemble spectrum. The observed large spectral width of defect luminescence is due to the presence homogeneously distributed large number of closely spaced defect states within individual NCs. It is worth mentioning that slight variation in the PL emission maxima of individual NCs may be assigned to effect of size distribution. The single particle spectroscopic study further corroborates our proposition that large spectral line-widths of defect luminescence in semiconductor NCs originates primarily from the multiple low lying defect distribution while size distribution may also contribute to a small extent.

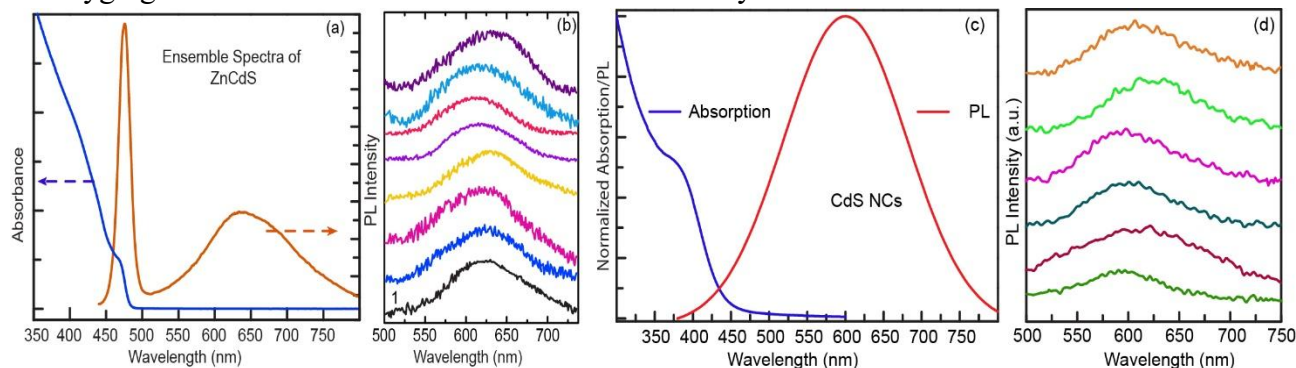


Figure 1. (a) Ensemble absorption and PL spectrum of ZnCdS NCs. The ensemble PL spectrum displays sharp excitonic emission along with a large Stokes shifted broad defect luminescence. (b) Representative PL spectra of



individual ZnCdS NCs. (c) Ensemble absorption and PL spectrum of CdS NCs. The ensemble PL spectrum shows only a large Stokes shifted broad defect luminescence. (d) Representative PL spectra of individual CdS NCs. The single particle defect PL spectra shown in (b) and (d) clearly indicate that defect luminescence of single NCs are inherently broad.

CONCLUSION

Single particle PL spectroscopy study reveals that the large spectral line-width of the defect luminescence of semiconductor NCs is primarily due to presence of multiple closely spaced defects within individual NCs. The small variation in the single PL maxima for individual NCs may be assigned to the sample size inhomogeneity. Therefore, our proposition is quite general that defect luminescence of semiconductor NCs is inherently broad and is independent of materials and synthesis processes.

ACKNOWLEDGMENT

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BIOGRAPHY

Dr. Arunasish Layek is an Associate Professor in the Department of Chemistry at Adamas University, Kolkata, with extensive research experience in nanoscience and photophysics. He completed his Ph.D. in Chemistry from the Indian Institute of Technology (IIT) Bombay, focusing on semiconductor nanocrystals and their photoluminescence behavior, and holds both M.Sc. and B.Sc. degrees in Chemistry from IIT Bombay and the University of Calcutta, respectively. He has pursued postdoctoral research at the University of Waterloo, Canada, and KU Leuven, Belgium, contributing significantly to advanced spectroscopy, nanomaterials, and catalysis research. Dr. Layek has led a SERB-funded research project and has received several recognitions, including the Star Faculty Award (2025) and Early Career Research Grant. With numerous publications in reputed international journals and active participation in global conferences, his research primarily focuses on nanomaterials, quantum dots, and their optical and catalytic properties.

**Piezocatalysis: Mechanical Energy Driven ROS generation for Environmental Remediation****Dr. Subhajit Saha**

Assistant Professor , Department of Renewable Energy Engineering,

Maulana Abul Kalam Azad University of Technology, West Bengal,

Haringhata-741249, India

**ABSTRACT**

Piezocatalysis is a technique that relies on the conversion of mechanical energy to trigger chemical reactions that can be utilized to catalyze the degradation of pollutants in water. In Piezocatalysis technology the strained state of a piezoelectric material is utilized for surface electrochemical reactions under dark conditions. When the piezoelectric crystals are subjected to mechanical stress in water, they can produce reactive oxygen species (ROS) which in turn exhibit series of applications ranging from the water splitting to degradation of organic dyes. While the current generation decontamination technologies such as photocatalysis, is plagued by some major drawbacks like slow reaction rate and conditional usage; piezocatalysis offers some key advantages. Especially, operability under dark conditions as well as availability of abundant low-frequency vibration energy as a source of mechanical energy resource establishes piezocatalysis as a highly promising technology over its peers. Moreover, the built-in electric field in the piezocatalysts is highly beneficial for hindering the electron-hole recombination which further ensures high reaction rate. The built-in-field mediated band bending in the piezoelectric crystals are also responsible for the swift reaction performance. Development of highly efficient piezocatalytic technology that can harness natural driving forces will pave the way for its practical application in the field of environmental remediation.

BIOGRAPHY

Dr. Subhajit Saha has received his M. Tech. and Ph.D. (Engineering) from School of Materials Science and Nanotechnology, Jadavpur University, India. After that he carried out his postdoctoral research from Indian Association for the Cultivation of Science, Kolkata and National Tsing Hua University, Taiwan. Dr. Saha has also worked as a Senior UPE Fellow in Nanoscience and Technology program under UGC-UPE scheme at Jadavpur University. Currently, he is working as an Assistant Professor and Head at Department of Renewable Energy Engineering, Maulana Abul Kalam Azad University of Technology, West Bengal. He is also serving as a Visiting Faculty of Department of Industrial Chemistry & Applied Chemistry, Ramakrishna Mission Vidyamandira, Belur Math, Howrah. His research interest includes Energy-efficient lighting, Self-powered nanosensors and Environmental remediation.



Sustainable Bioethanol Production from Valorised Waste Biomass: Novel Catalytic Approach

Dr. Susmita Singh

Associate Professor, Department of Chemistry,

Amity Institute of Applied Sciences, Amity University,

Kolkata, Major Arterial Road, Action Area II, Newtown, Kadampukur,

West Bengal 700135, India



ABSTRACT

The increasing depletion of conventional fossil-based energy resources, coupled with escalating environmental concerns, necessitates the development of sustainable and renewable energy alternatives. Bioethanol derived from waste biomass offers an efficient route to reduce dependence on crude oil and address environmental pollution and climate change. This study presents a novel catalytic waste-to-energy strategy utilizing cellulosic biomass obtained from discarded fruit and vegetable peels as a renewable feedstock for ethanol production. Bifunctional catalysts were synthesized through various preparative routes and characterized using X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, and scanning electron microscopy (SEM) to investigate their structural and morphological properties. The catalytic efficiency was evaluated by quantifying ethanol production using high-performance liquid chromatography (HPLC). The results reveal excellent catalytic activity and conversion efficiency, demonstrating the feasibility of transforming low-value organic waste into high-value bioethanol. This approach underscores the potential of waste valorisation in promoting sustainable energy generation, advancing circular economy principles, and contributing to environmentally friendly solutions for climate change mitigation.

Keywords

Bioethanol; Chemocatalytic approach; Green Chemistry; Sustainable Energy; Waste-Valorisation.

BIOGRAPHY

Dr. Susmita Singh is an Associate Professor in the Department of Chemistry at Amity Institute of Applied Sciences, Amity University Kolkata, India. She has done her M.Sc. in Inorganic Chemistry from Banaras Hindu University (BHU) and obtained Ph.D. in Chemistry from IEST Shibpur. She has completed her postdoctoral research at the University of Calcutta under the prestigious D. S. Kothari Postdoctoral Fellowship. With over a decade of academic



and research experience, she has established herself in the field of sustainable energy materials and electrocatalysis. Her research focuses on biomass valorisation and waste-to-energy conversion, with emphasis on catalytic strategies for sustainable biofuel production. She has made significant contributions to the development of advanced functional nanomaterials and electrocatalysts for Direct Alcohol Fuel Cells (DAFCs), particularly targeting alcohol oxidation and the Oxygen Reduction Reaction (ORR).

Dr. Singh has published over 25 research articles in reputed international journals such as Journal of Electroanalytical Chemistry, Materials Chemistry and Physics, and Ionics, along with several book chapters with leading publishers including CRC Press and Taylor & Francis.

She is currently serving as Principal Investigator on funded projects from UGC-DAE CSR Collaborative Research Scheme (3 years) and has also successfully led a DST Women Scientist Scheme-A project (3 years) in the same capacity. She holds two granted patents in advanced functional materials.

Dr. Singh has been recognized with several honors, including the Young Scientist Award (Bose Institute), Best Paper Award (ACMS 2026), Best Oral Presentation (ICRETBS 2025), gold medal award (VIT). She is also an active reviewer for journals such as Scientific Reports (Springer Nature), Journal of Energy Engineering etc. and is a life member of the Indian Photobiology Society, Indian Institute of Chemical Engineers.

Her research aims to advance next-generation energy technologies through the rational design of catalytic materials and sustainable chemical processes.



Opportunities with Atomic layers for Quantum Technology

Dr. Sreemanta Mitra

Assistant Professor & MURTI Faculty Fellow

Physics of Electronic Quantum Matters Group

Department of Physics, GITAM School of Science

Bengaluru, India



ABSTRACT

Back in the early 2000s, the concept of two-dimensional materials was not on everyone's radar. But then, enter the brilliant minds at Manchester University, who managed to fabricate the first devices using a single atomic plane of carbon. This groundbreaking achievement opened up a whole new realm of possibilities. Fast-forward to today, and we're witnessing an exponential surge in research and development focused on these atomic layers. Scientists and engineers are essentially playing with the building blocks of matter, creating materials with tailored properties. It's like constructing a LEGO set, but instead of plastic bricks, we're dealing with individual atoms. Atomic layers allow us to customize materials to our heart's content.

Quantum technology relies on the quirky behavior of particles at the atomic and subatomic scale. Think quantum computers, quantum sensors, and quantum communication. These devices often require materials with finely tuned properties. Enter our trusty atomic layers—they provide the raw ingredients for these quantum feats.

The talk will be divided into two broad sections: In the first part, I will be mostly concerned with the broader picture, and in the second part, I will try to describe some of my research results and what my group is currently exploring, just to give a hint on how this field is still rapidly evolving.

BIOGRAPHY

Born and raised in Kolkata, India, Dr. Sreemanta Mitra did his Bachelors & Masters in Physics from BidhanNagar Govt. College & University College of Science and Technology, University of Calcutta, in 2006 and 2008 respectively. He then joined Prof. Dipankar Chakravorty and Dr. Sourish Banerjee for his Ph.D. in experimental Condensed Matter Physics in Indian Association for the Cultivation of Science, India. During his PhD, Sreemanta worked on the transport and magnetic properties of low dimensional systems, graphene and nanocomposites prepared



thereof. After graduating from the University of Calcutta in 2013, he joined his first post-doctoral research assignments with Prof. Dan Shahar in the Condensed Matter Physics department of The Weizmann Institute of Science, Israel, where his research was centering around the superconductor to insulator transition in nanowire devices made up of amorphous indium oxide. After finishing his study there in 2015, he joined Prof. Christos Panagopoulos at Nanyang Technological University, Singapore for his second post doctoral study, where he worked on the low-temperature magnetotransport properties in the devices of Archemidean quantum magnets. Post his tenure in Singapore, Sreemanta spent a couple of months in Bose Institute as a visiting scientist with Prof. Achintya Singha to work on the Raman spectroscopy of 2D quantum matters and composite, before moving to the Physics department of the Indian Institute of Science with Prof. Arindam Ghosh as a Research Associate. Sreemanta joined the Physics department of GITAM University, Bangalore as a faculty member (Assistant Professor). He currently heads the Physics of Electronic Quantum Matter Lab at the host department and also associated with the Multidisciplinary Units of Research on Translational Initiatives (MURTI), Gandhi Institute of Technology and Management (GITAM) Deemed to be University as a Faculty Fellow



Contact-Electrification—A New Technology for Energy Harvesting and Self-Powered Sensing Delafossite

Dr. Sk Masum Nawaz

Assistant Professor, Department of Electrical and Electronics Engineering,

BITS-Pilani, Hyderabad Campus, Karimnagar, Hyderabad-500078,

Telangana, INDIA,



ABSTRACT

Contact-Electrification (CE) or the triboelectric effect is a known phenomenon since last 2600 years. Although, CE has always been regarded as a negative effect for electronic circuits and systems, it has been one of the hot areas of research in recent years when the triboelectric nanogenerator (TENG)^{a-c}, was introduced. TENG, which converts waste mechanical energy to electricity, works on the principle of CE charge transfer (between the layers of two dissimilar triboelectric materials) followed by electrostatic induction of charges on the metal electrodes attached to the triboelectric layers. Hence, an electric field is created between the charged surfaces of the triboelectric layers.^d If the metal electrodes are connected with external wires, a current will flow through the wires due to time varying surface charge density under mechanical excitation.^e The power generated by TENG is enough to drive small electronic gadgets, internet-of-things (IoT) sensors, etc.

Recently, we demonstrated high-performance TENG fabricated by recycling waste-polystyrene (WPS) from waste thermocol packaging boxes.^f Output performance of this device was further improved by embedding tea-leaf microparticles in WPS.^g We also demonstrated another performance enhancement method by means of molecular self-assembly of small molecules.^h

Since TENG generates output voltage/current when one triboelectric layer touches other or when the triboelectric surface charge varies, TENG or the CE effect can be utilized as self-powered sensors to detect/monitor a wide range of dynamic systems. We also demonstrated self-powered sensors by employing the CE effect.

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This presentation will focus on all these aspects of synthesis and applications of this novel nanomaterial along with important output parameters.

BIOGRAPHY

Dr. Sk Masum Nawaz obtained his Ph.D. in Electronic Science in 2018 from University of Calcutta under the guidance of Prof. Abhijit Mallik. He continued with the same institute as a Postdoctoral Research Associate (2019-2022). Currently he is an Assistant Professor in the Department of Electrical and Electronics Engineering (EEE) of BITS-Pilani (Hyderabad Campus). His current research interests include devices for neuromorphic computing, energy harvesting and self-powered sensing.



Light-Induced Motion in Metal-Organic Crystals

Dr. Basudeb Dutta

Assistant Professor, Department of Chemistry, School of Applied Sciences,

Kalinga Institute of Industrial Technology (KIIT)

Deemed to be University,

Bhubaneswar-751024, Odisha, India



ABSTRACT

The development of materials capable of converting light energy into mechanical motion has attracted considerable attention due to their potential in photo-induced technologies. These materials are expected to transform applications in optical actuators, soft robotics, smart biomedical systems, artificial muscles, and flexible electronics. Among them, metal–organic single crystals i.e. crystalline coordination complexes and related crystalline compounds have emerged as promising hybrid materials, displaying dynamic behaviors such as bending, jumping, hopping, and splitting upon exposure to light.¹⁻³ In this case, I want to present about the photo salient behaviour of a series of metal-organic crystals which are mainly synthesized from photo-responsive ‘C=C’ appended olifinic ligands such as: 4-(1-naphthylvinyl)pyridine}, which undergo topochemical [2 + 2] cycloaddition reactions upon exposure to UV irradiation as well as sunlight. The compounds exhibit pronounced photosalient behaviour, characterized by crystal jumping, splitting, rolling, and swelling upon UV irradiation.⁴⁻⁵ These observations propose that the photomechanical properties can be modulated through the selection of the structural components of the compounds. In addition to this, the mechano-structure-property relationship is elucidated through complementary nanoindentation measurements.⁵

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BIOGRAPHY

Dr. Basudeb Dutta, joined (Dec,2024) as an Assistant Professor at Department of Chemistry, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University just after completing his JSPS Post-doctoral work under Nobel laureate Prof. Susumu Kitagawa at Kyoto University. Dr. Dutta's research topic includes the design and synthesis of coordination compounds, coordination polymers, metal-organic frameworks (MOFs) and their application photo-responsive activity.



Software analysis in for low dimensional materials: Probing beyond instruments

Dr. Nirmalya Sankar Das

Assistant Professor, Department of Basic Science and Humanities,

Techno International Batanagar, Maheshtala, Kolkata 700141, West Bengal,

India



ABSTRACT

Since the development of unique and multifunctional materials and relevant research, a number of advanced tools and sophisticated instruments were fabricated to characterize their optical, electrical, morphological and application related properties. Despite requirement of special supportive arrangements, most of such instruments like electron microscopes, diffractometers etc. are remarkably useful and accurate offering precise measurements. However, like all advanced systems, all such instruments have their own limitations. In advanced research fields, AI assisted softwares therefore have emerged as suitable alternatives for probing low dimensional systems beyond the resolution of actual traditional instrument. For example, software analysis of a micrograph of system of particles often predict the roughness, particle sizes, distribution of pores which could require separate instruments for each feature to be measured individually. Additionally, different characterization techniques often require special sample preparation and thus may adversely affect the financial aspect of rigorous investigation. Analysis by software like ImageJ has been emerged as a good alternative in such cases. Using such virtual technique different features like porosity, particle dimension, average roughness and possible 3D projection can be anticipated sparing researchers from repeated attempts in wrong directions. We have recently applied this technique as supportive tool for field emission analysis, photocatalytic analysis and hydrophobicity related studies. Further application of such simulative method may be explored to open up easier solution for challenges in materials science research.

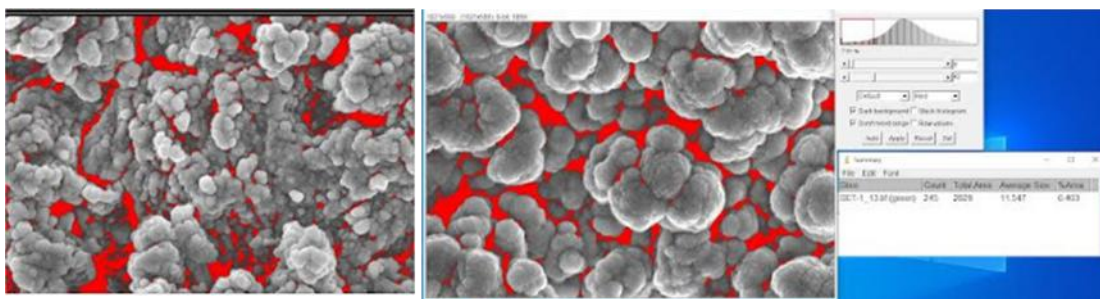


Figure: Analysis of porosity using ImageJ



BIOGRAPHY

Dr. Nirmalya Sankar Das has been working in the field of solid state physics and Nanotechnology since last 15 years. He started his academic career under scholastic environment of Ramakrishna Mission at Malda. After district level topper position in higher secondary he completed his graduation from Jadavpur University in 2005. Continuing his post graduation from Jadavpur University he started his research career in nanoscience and technology in thin film and nanoscience laboratory and received his doctorate degree from Jadavpur University in 2014. During his academic career, he has been awarded with prestigious fellowships like Research fellowship in science for meritorious students and post doctoral fellowship from University with Potential for Excellence scheme.

He has published more than 100 research articles so far and authored 2 book chapters. He has authored two books and contributed in a patent along with steel authority of India limited. He has supervised more than 17 students in their master degree thesis and has supervised one PhD scholar. He is currently the academic coordinator at Techno International Batanagar, a unit of Techno India Group and the Head of the department of Basic Science and Humanities. He is also leading his institute as the examination coordinator.

Along with regular academic activities, he is also an artist contributing in different scientific graphic works and artistic projects



Nano-Architectonics beyond Graphene Nanofabrications: Current Research Avenues Shaping Smart, Sustainable, and Adaptive Materials

Dr. Kaushik Pal

Associate Dean-Research, University Centre for Research and Development,

Department of Physics, Chandigarh University,

Gharuan, Mohali, Punjab, 140 413, India,



ABSTRACT

Dielectric relaxations are studied at three different frequencies of a hydrogen bonded liquid crystal chloro benzoic acid with nonyloxy benzoic acid. The process of synthesis is described and the synthesized mesogen is a monophasic variant with nematic phase. Carbon-based nanomaterials (CNMs), like CNTs, graphene, carbon dots (C-dots), and some other CNMs, have recently drawn a lot of interest in their future application as an elevated-performance sensor implementation. For the first time in the history of liquid crystal dielectric work, we observed that in the present sample at higher frequency the process mentioned above is reversed. All the dielectric data points obtained at various temperatures when plotted they are found to converge at the ∞ values and diverge at ϵ_0 values. This process is referred as frequency cross over. Nematic growth order derived from dielectric studies is also presented. We explored that qualitatively different behaviors could emerge via the specific nature of the inter-component interaction. Mastering this mechanism could lead to various applications based on phase tunable properties and novel switching.

Keywords: Nanomaterials; Graphene; Hybrid Nanocomposites; Spectroscopy; Switching

BIOGRAPHY

Professor (Dr.) Kaushik Pal belongs to an Indian citizen. He currently leads as a ‘Associate Dean Research’ at University Center for Research and Development (UCRD), Chandigarh University, Punjab (India). He was the former “Distinguished Chair Professor” at Laboratório de Biopolímeros e Sensores, Instituto de Macromoléculas, Universidade do Rio de Janeiro, Brazil and Advisory Chair Professor in Liquid Complex System and Solid State Research Laboratory, University of Maribor, Slovenia. Most recently, achieved Honoris Causa DOCTOR OF SCIENCE (D.Sc.) award from Ministry of Education, Govt. of Malaysia IKTBN Sepang, Selangor in this session June, 2020. He also acts as Distinguished Chair Professor in Wuhan University, Hubei, Republic of China. Before, he worked as a “Visiting Professor” at IIUCN, School of Energy Materials, Mahatma Gandhi University, Kottayam, Kerala. As a full-time “Research Professor” in the Department of Nanotechnology worked at Bharath University



(BIHER), Chennai. He completed a Doctorate in Philosophy (Ph.D.) in Physics (Expt. Materials Science and Nanotechnology) from University of Kalyani, Govt. of India. Most significant prestigious awards “Marie-Curie Experienced Researcher (Postdoctoral Fellow)” offered by the European Commission in Greece and “Brain Korea (BK-21) National Research Foundation Visiting Scientist Fellowship” in South Korea achieved in his research career. He was appointed “Senior Postdoctoral Fellow” at Wuhan University, China and within a year achieved a prestigious position “Chief-Scientist & Faculty Fellow” offered by Chinese Academy of Science. His current spans are focusing e.g. Nanofabrication, Chemical nanoengineering, solid-state condensation chemistry, Renewable green energy revolution, functional Materials hybridization, CNTs/Graphene, Liquid crystalline optical materials, Polymeric nanocomposite, Switchable device modulation, Spectroscopy and electron microscopy, Bio-inspired materials for Nanobiotechnology, Drug delivery, Tissue engineering, Nano-imaging and cell culturing and integration, Flexible and transparent electrodes, Supercapacitor, Optoelectronics, Green nanotechnology and novel biosensor applications. He supervises a significant number of Bachelors, Masters, Ph.D. and Postdoctoral scholar’s thesis in Foreign University collaborations. His outstanding research finding and novelty published around 250+ significant research/review articles in SCI & SCOPUS based peer-reviewed international top-tier journals likewise: IOP Nanotechnology, Royal Chemical Society, Elsevier, Springer, InTech, Taylor & Francis, Wiley-Scrivener, IEEE publications got the highest citation in every year and leading editors more than 15- SCI/SCOPUS journal. Throughout his academic experiences, skills and research backgrounddeserve him as an editorial member of Elsevier, Springer, IOPSciences, Wiley, Taylor & Francis, InTech Open, CRC Press etc. as well as edited several 32-Book’s along with Authored and Coauthors chapters and since several last decades reviewed approximate 450-articles and expert editor of Elsevier, Springer, Wiley, IOP journals. Prof. Pal is an expert group leader as well as the associate member in various scientific societies, reorganizations and professional bodies. In past decades, he organized mostly 52-National or International Conferences and workshops leaded as Chairperson/Convener/Co-convener, Workshops, Summer Internship program, and himself contributed around 40-Plenary, 38-Keynote and 45-Invited lectures worldwide. Outstanding achievements belongs to Prof. Kaushik Pal was selected worldwide as highly cited researcher leading Top 2% Scientist based Stanford University SCOPUS database since in the year 2022,2023,2024,2025.



Oral Presentation





Oral Presentation – OOP-01

Electric Field Aided Phase Transition and Thermal Properties in CNT- Liquid Crystal Composite

Subhayan Biswas,^{1,2} Arunava Jha¹

¹Department of Physics, Vivekananda College, Thakurpukur, Kolkata 700063, India

²Department of Physics, Aliah University, Kolkata 700160, India

E-mail (arunava.jha@gmail.com)

ABSTRACT

This study investigates the impact of electric field-driven isotropic (I) to nematic (N) phase transition in a CNT-liquid crystal (LC) composite. Our key findings reveal that the introduction of CNTs significantly enhances this first-order characteristic, with the transition becoming more pronounced as the CNT volume fraction increases. Additionally, the application of an external electric field fundamentally alters the phase transition dynamics and therefore the thermal properties of the composite.

INTRODUCTION

Liquid Crystals (LC) primarily shows isotropic to nematic (I-N) phase transition on cooling from liquid to solid transition and it is weekly first order in nature. LC shows very low sensitivity to the external field. [1]. Effect of electric and magnetic field in I-N transitions are reported previously but the influence of external field on LCs are hardly shown [2,3]. Without applied field the composite shows isotropic nature above the TNI (transition temperature) and nematic ordering below TNI. Sometimes an external field (electric/magnetic/surface ordering field) can induce a partial orientational ordering (paranematic phase) in the composite above the zero-field TNI [4]. In this paper we are going to show the effect of electric field on the CNT-LC composite. The theoretical explanation is based on Landau–de Gennes type free energy theory [5].

MATERIALS AND METHODS

It is essential to construct the free energy profile of CNT-LC composite under the influence of electric field (E) in order to investigate the effect of various parameters including electric field on the properties of the composite. The overall free energy can be written as,

$$F = F_0 + F_{CNT} + F_{LC} + F_{CNT-LC} + F_E$$

The dimensionless form of free energy is,

$$f = \frac{FV_1}{k_B T} = \phi \ln \phi + R(1 - \phi)[\ln(1 - \phi) + \chi \phi] + \phi \left[\frac{1}{2} \left(1 - \frac{U}{3} \right) S_1^2 - \frac{U}{9} S_1^3 + \frac{U}{6} S_1^4 \right] + (1 - \phi) \left[\frac{3}{2} a \left(1 - \frac{T^*}{T} \right) S_2^2 - \frac{3}{4} b S_2^3 + \frac{9}{4} c S_2^4 \right] - \phi(1 - \phi) \left(\delta_1 S_1 S_2^2 - \delta_2 \frac{S_1^2 S_2^2}{2} \right) - \frac{1}{3} [\phi h_1 S_1 + (1 - \phi) h_2 S_2]$$



RESULTS AND DISCUSSION

The free energy constructed above is renormalized mathematically, and LC order parameter (S_2) is plotted against temperature (T) for different applied electric field (h_1) and shown in fig.1

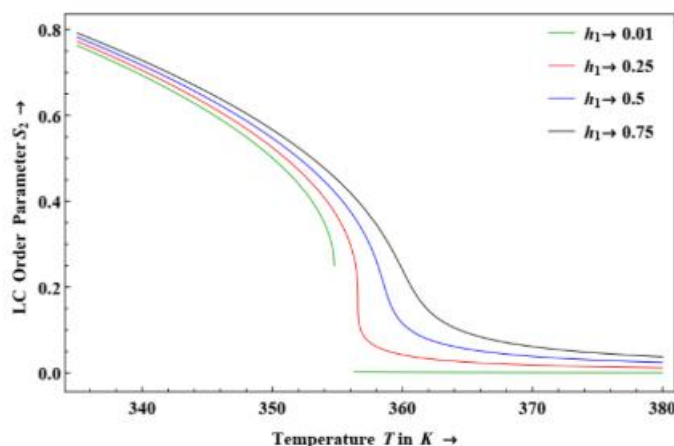


Figure 1. S_2 versus T plot for different field h_1

S_2 shows discontinuity in low h_1 proving that phase transition is first order by nature. With increasing h_1 curves become continuous with shifting of transition temperature towards higher value asserting a second order nematic to paranematic phase shift.

CONCLUSION

In this work effect of electric field (h_1) on I-N phase change of LC-CNT composite has been explained theoretically with the help of Landau–de Gennes free energy theory. Results shows regular 1st order transition for low h_1 , however anomalous behaviour of phase transition appears for higher h_1 characterizing 2nd order transition due to paramagnetic nature.

ACKNOWLEDGMENT

The authors would like to express heartfelt regards towards Vivekananda College, Thakurpukur for providing laboratory support for the work .

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ECG-BASED CONGESTIVE HEART FAILURE DETECTION USING OPTIMIZED FEATURE SELECTION

Lumbini Bhaumik^{1,2}, Abhishek Bandopadhyay², Kasturi Barik¹

¹JIS Institute of Advanced Studies and Research (JISIASR), JIS University, India

²Asansol Engineering College, Dept. of CSE, India)

E-mail: lumbini.cse@aecwb.edu.in

INTRODUCTION

Congestive Heart Failure (CHF) is a major cause of mortality worldwide, requiring early and reliable detection. Electrocardiography (ECG), being a non-invasive and cost-effective diagnostic tool, has been widely used for automated CHF detection using machine learning techniques [1], [2].

Most existing studies primarily focus on maximizing classification accuracy by utilizing large and high-dimensional feature sets. However, such approaches increase computational complexity, reduce interpretability, and may lead to overfitting. Although several feature selection methods have been explored [3-5], limited attention has been given to identifying minimal yet highly informative feature subsets. This work proposes a comparative and systematic evaluation of filter, wrapper, and embedded feature selection methods to obtain an optimized minimal feature subset. Unlike existing approaches, the proposed method demonstrates that competitive performance can be achieved using significantly fewer features, improving efficiency, robustness, and practical applicability.

RESULTS AND DISCUSSION

The proposed framework consists of preprocessing, feature extraction, feature selection, and classification, as shown in Figure 1.

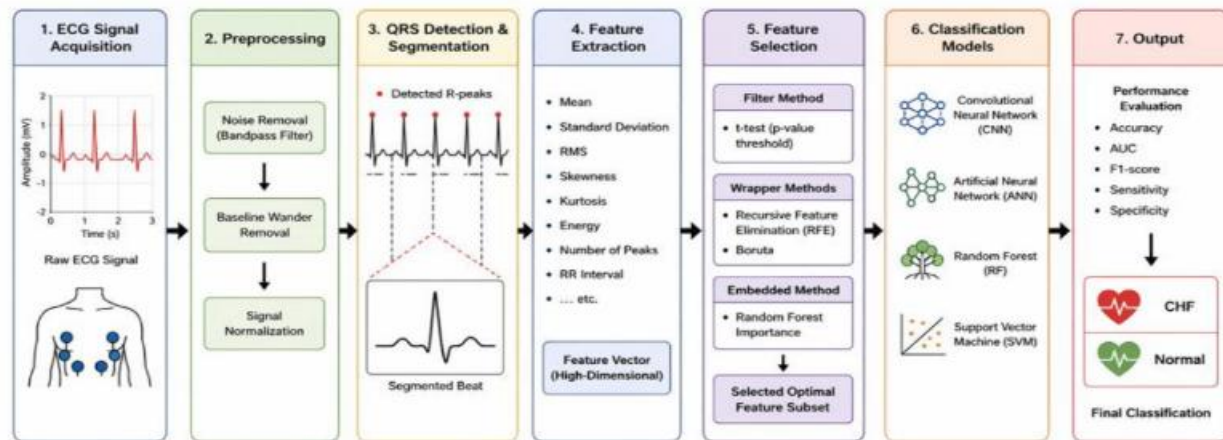


Figure 1. Proposed ECG-based CHF detection framework using feature selection and machine learning.

ECG signals are segmented using QRS detection, and 16 statistical and morphological features are extracted. Multiple feature selection methods were initially evaluated; for brevity, only the most effective are reported: t-test, RFE, Boruta, and Random Forest importance. These methods yield a compact subset of key features (mean, standard



deviation, energy, RMS, skewness, peaks, and zero-crossings), reducing dimensionality while preserving performance. The selected features are evaluated using CNN, ANN, Random Forest, and SVM, with performance measured by accuracy and AUC.

RESULTS AND DISCUSSION

Feature selection reduces the original 16 features to a compact subset (mean, standard deviation, energy, RMS, skewness, peaks, zero-crossings) while maintaining performance.

Table 1. Summary of Performance Across Feature Selection Methods

Method Type	Method	Accuracy (%)	AUC	Observation
Filter	t-test ($p < 0.15$)	75	0.75	Strong baseline with minimal features
Wrapper	RFE/ Boruta	72	0.71	Captures feature interaction; higher complexity
Embedded	RF Importance	75	0.76	Balanced performance and feature reduction
Classifier	Random Forest	75	0.78	Most consistent across feature subsets

The results indicate that effective CHF detection can be achieved using a reduced feature set. Although some studies report higher accuracy, they rely on larger feature spaces, whereas the proposed approach achieves comparable performance with fewer features, improving efficiency and generalization.

CONCLUSION

This study presents a feature selection-based framework for ECG-based CHF detection using a minimal feature subset. The results show that effective classification can be achieved by significantly reducing feature dimensionality without major loss in performance. Random Forest provides the most consistent results, while embedded feature selection offers a good balance between accuracy and efficiency. Unlike existing studies that rely on large feature sets [2-5], the proposed approach achieves comparable performance with fewer features, improving efficiency, interpretability, and generalization, making it suitable for practical deployment.

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Design and Analysis of Pipe Inspection Robot for Gas Pipeline

Omkar Rewale*, Pratiksha Bhosle, Harshad Talekar, and Ashwini Gotmare

Mechanical Engineering, DJ Sanghvi College of Engineering, Mumbai, India

Corresponding author: rewale.omkar.18@gmail.com

Keywords—Pipe inspection robot, gas pipeline, wall-press mechanism, IoT.

INTRODUCTION

Gas pipeline inspection is essential for identifying cracks, corrosion, blockages, and leaks that can lead to safety risks and service interruptions. Traditional manual inspection methods are often unsafe, slow, and expensive, especially inside confined pipelines. Existing pipe robots also face limitations in bend negotiation, pipe-diameter adaptation, and real-time visual monitoring. This work addresses those gaps by proposing a compact, low-cost wheeled wall-press pipe inspection robot for gas pipelines.

MATERIALS AND METHODS

The proposed robot combines a wheeled drive with spring-based wall pressing for traction, servo-actuated steering for lateral bend negotiation, and a hinge-type articulated body for vertical and inclined bends. An ESP32-CAM provides wireless video feedback, while an Arduino Nano coordinates steering and auxiliary control. The power system uses a 2S2P 18650 lithium-ion battery pack with buck converters for regulated 5 V supply. Structural and electrical sizing were carried out analytically to verify feasibility for small-diameter pipeline traversal.

RESULTS AND DISCUSSION

Design calculations indicate a total spring normal force of about 62.8 N and an estimated frictional force of about 37.7 N, sufficient for stable motion in horizontal, inclined, and vertical pipe conditions. The calculated drive torque requirement per motor is approximately 0.359 N·m, while the steering mechanism requires about 0.98 N·m of servotorque. The total electrical load is about 21 W, and the estimated runtime of the battery pack is about 1.32 h under the assumed load. These results support the feasibility of a compact inspection robot with stable traction and real-time monitoring.

CONCLUSION

The study presents a practical design direction for an affordable pipe inspection robot suited to gas pipelines. Compared with inchworm-style mechanisms, the proposed wheel-based wall-press system offers simpler fabrication and faster motion while retaining the ability to negotiate bends through integrated steering and articulation. The work remains at the design stage; future work will focus on prototype fabrication and experimental validation in actual pipes.

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A Predictive HR Analytics Framework for Optimizing Employee Promotion Cycles in MNCs using Machine Learning

Mr. Shashank Shekhar¹, Dr. Chandrima Chakrabarti², Ms. Jayita Pal³, Dr. Nabanita Das⁴, Mr. Rohit Kumar⁵, Mr. Ashish Raj⁶, Mr. Rishi Kumar Manjhi⁷

¹³⁵⁶⁷ Department of CSE, Narula Institute of Technology, Kolkata, India

Email: parmarshashank8210@gmail.com

²⁴ Department of CSE (Data Science), Narula Institute of Technology, Kolkata, India

Email: chandrima.narula@gmail.com

ABSTRACT

Human Resource (HR) Analytics has emerged as a transformative approach in modern organizations. With the advent of Machine Learning (ML) and data analytics, HR departments can now leverage large volumes of employee data to extract meaningful insights and improve organizational outcomes. This project focuses on applying predictive analytics to address one of the most critical HR challenges, i.e., identifying employees most likely to be promoted.

Promotion decisions are typically based on multiple factors such as performance ratings, training scores, experience, and behavioral attributes. However, manual evaluation of these parameters is time-consuming and prone to inconsistencies. Therefore, there is a strong need for an automated, scalable, and accurate system that can assist HR professionals in making objective promotion decisions.

In this paper, various machine learning techniques are applied to analyze employee-related data, including demographic details, performance indicators, and training outcomes. The objective is to build a classification model that predicts whether an employee will be promoted or not. The dataset used in this paper contains multiple features such as employee ID, department, education level, previous performance ratings, length of service, and key performance indicators (KPIs).

Data preprocessing techniques such as handling missing values, encoding categorical variables, and feature scaling are implemented to ensure data quality and improve model performance. Several machine learning models, including Decision Trees, Logistic Regression, Random Forest, XGBoost, LightGBM, and CatBoost, are evaluated and compared based on performance metrics such as F1-score, accuracy, and precision.

Among these, boosting algorithms, particularly CatBoost, demonstrate superior performance due to their ability to handle categorical variables effectively and reduce overfitting. Additionally, ensemble techniques such as voting classifiers are employed to further enhance prediction accuracy.

The proposed system provides a data-driven framework that enables organisations to identify high-potential employees earlier to reduce delays in the promotion cycle. It not only improves decision accuracy but also enhances transparency and fairness in HR processes. Furthermore, the system can be extended to other HR applications such as employee retention, performance evaluation, and workforce planning.



Overall, this project highlights the significance of integrating machine learning with HR analytics to achieve organizational efficiency, optimize talent management, and support strategic decision-making.

Keywords: HR Analytics, Machine Learning, Predictive Modeling, Employee Promotion, Workforce Optimization

**AI Face Recognition Attendance System**

Madhabendra Maity¹, Pritusna Banik², Aditya Raj Yadav³, Sayan Dutta⁴, Jit Das⁵, Sohinee Mondal⁶, Dr. Chandrima Chakrabarti⁷, Dr. Nabanita Das⁸

¹²³⁴ Department of Computer Science and Technology, Narula Institute of Technology, Kolkata, India

⁵ Assistant Professor (CST), Narula Institute of Technology, Kolkata, India

⁶ Assistant Professor (CSE), Narula Institute of Technology, Kolkata, India

⁷⁸ Department of CSE (Data Science), Narula Institute of Technology, Kolkata, India

E-mail: madhabendramaity04@gmail.com

ABSTRAC

Traditionally, attendance management in institutions has been based on manual roll-calls and time-sheet recording, which is inefficient and error-prone. In today's settings, such as in large-scale educational institutions, high-density manufacturing workplaces, and public event spaces, manual methods are proving inefficient and do not offer the efficiency, precision, and real-time reliability needed in today's administrative systems. Additionally, manual processes are vulnerable to "buddy-punching", or proxy attendance, which renders institutional data integrity questionable, and calls for automated biometric attendance verification. Although early attempts to automate attendance, such as Radio Frequency Identification (RFID) and fixed-position biometric scanners, have successfully replaced traditional approaches, they also bring in new limitations, particularly related to the high cost of hardware maintenance, contact-based verification, and scalability limitations. Although earlier automation approaches, namely Radio Frequency Identification (RFID) and static biometric recognition, have replaced manual data entry, they come with their own limitations, mainly related to high maintenance costs for biometric equipment, the need for physical contact, and a lack of scalability. In the context of evolving corporate needs to support hybrid and highly mobile workforces, there is a need for a contactless, scalable and efficient attendance system that can also function under variable network conditions. In this paper, we review and compare 24 recent automated attendance management studies, assess the shift from classical Computer Vision (CV) methods to modern Deep Learning (DL) approaches, and then introduce a secure and scalable attendance system based on edge computing that addresses the challenges observed in the literature reviewed. Our extensive review of 24 research papers demonstrates a stark divide in the current technological approaches: the use of traditional algorithms versus current neural networks. Classical methods, primarily using Haar Cascade and Local Binary Pattern Histograms (LBPH) classifiers, are widely favoured in computer-efficient studies. Our review suggests that these approaches, while computationally efficient, are commonly used in systems deployed on low-powered devices such as the Raspberry Pi, or other microcontrollers, but tend to have reduced accuracy when exposed to environmental challenges such as poor lighting, facial pose, or partial occlusion. In contrast, deep-learning models, especially Convolutional Neural Networks (CNNs) and Multi-task Cascaded Convolutional Networks (MTCNN), are a leap forward in the field and consistently perform well in recognition accuracy within the mid-90th percentile range under optimal conditions. Yet, our review also reveals the key research gaps with these high-accuracy models; these models are often not scalable in real-time scenarios with high density, and are often constrained by high-latency server processing. The research also points to emerging directions in masked-face recognition and multimodal biometric fusion (such as face-voice biometric recognition) to



improve recognition accuracy in post-pandemic environments where face masks are prevalent. However, a critical practical challenge remains: most proposed systems do not consider "offline resilience," a common cause of data loss for large-scale deployments due to network outage issues. Following these observations, this paper presents the design and implementation of a future generation contactless attendance system that fills the gap between deep-learning-based accuracy and real-time (edge-device) deployment. Our design approach moves the processing from the core of the network to the "edge" by leveraging edge devices (such as NVIDIA Jetson or ARM-based accelerators) to detect and identify multiple people in real-time at the entry point. This design addresses some of the common points of failure in cloud-based systems, facilitating seamless business operations even in the absence of internet connectivity. Local processing of video streams enables sub-second responsetimes and significantly reduces the cost of video streaming to the cloud. A key contribution of the proposed system is its "Offline First" storage engine, where the system continuously detects, matches and records attendance information in a secure local database, even in the absence of an external network. This enables uninterrupted attendance logging in factories, remote schools or -scale venues where the network infrastructure may be intermittent or unreliable. Through a background synchronisation layer, the system automatically activates once the network is stable again to securely batch and upload the offline attendance data to a cloud-based server. This approach guarantees data retention and allows administrators to access real-time attendance metrics seamlessly, following the network's recovery, without further manual effort. To overcome the challenges mentioned in the literature on occlusion and lighting conditions, the proposed system adopts a hybrid identification model. This uses the MTCNN model to accurately align and detect faces, and a powerful, pre-trained CNN model to extract features, which was fine-tuned to recognise partially occluded faces, a common issue in health and safety applications. This hybrid approach not only ensures high-precision facial recognition but also enables the use of lightweight models capable of running on edge devices. Moreover, the proposed structure compiles with basic security considerations to protect the privacy of sensitive data, such as converting facial images to encrypted embeddings before storing them, meaning that biometric data is never stored in its raw form. This not only improves the effectiveness of attendance recording but also mitigates the problem of proxy fraud where a colleague could be "impersonated" by another person due to the biometric matching being based on the person's unique facial biometric data. This study concludes that the next generation of institutional attendance monitoring systems must be smart and edge-based, with a focus on environmental adaptability, data continuity and real-time identification. Moreover, introducing such technology creates an open and auditable environment, essential in ensuring compliance with regulatory requirements in critical industrial and education settings. Our approach makes a substantial contribution to the state-of-the-art by providing a scalable system that does not require network connectivity at all, thus overcoming the main source of failure in current systems that are tied to the cloud. This combination of the high-precision results from contemporary deep learning research and the practicality of edge computing solves a "win-win" problem: it reduces the amount of administrative work while improving the integrity of attendance records. We contend that this contactless, smart system is not only technically viable to implement in large-scale environments (such as factories, schools and large public events) but is also a necessary advancement in institutional management, providing reliable, secure and accurate performance, regardless of network and environmental conditions. Future research will be dedicated to the implementation of this architecture in test-bed environments to determine precisely the time savings in manual attendance recording as well as the error rate in comparison to traditional log-book recording, further establishing the efficiency and need for this proposed contactless system



HYBRID AMORPHOUS CARBON NANOTUBES: SYNTHESIS, STRUCTURE, AND DOPING STRATEGIES FOR ENERGY APPLICATIONS

Rabindranath Sinha, Sagar Chakroborty, Saikat Khan, Suryasoumya Jana, Tamim Izaz Sardar, Debaprasad Adikari

Department of Computer Science Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer Math, Kolkata-700074
(rabindranathsinha35@gmail.com)

INTRODUCTION

Hybrid amorphous carbon nanotubes (HACNTs) represent a novel class of nanostructured materials that combine the structural advantages of conventional carbon nanotubes with the tunability of amorphous carbon. Unlike highly crystalline nanotubes, HACNTs exhibit partially disordered atomic arrangements, enabling enhanced surface reactivity, defect density, and functionalization potential. These characteristics make them highly promising for energy-related applications such as super capacitors, lithium-ion batteries, fuel cells, and hydrogen storage systems. This study focuses on the synthesis routes, structural properties, and doping strategies that influence the performance of HACNTs in energy applications.

MATERIALS AND METHODS

HACNTs are typically synthesised using methods such as chemical vapour deposition (CVD), plasma-enhanced CVD, and arc discharge techniques under controlled conditions. Hydrocarbon precursors like methane, acetylene, or ethanol are decomposed in the presence of transition metal catalysts (e.g., Fe, Ni, Co). The degree of amorphization is controlled by adjusting parameters such as temperature, gas flow rate, and catalyst composition. Doping strategies involve introducing heteroatoms such as nitrogen (N), boron (B), sulphur (S), or phosphorus (P) during or after synthesis. In-situ doping is achieved by adding dopant-containing precursors, while post-synthesis treatments include plasma modification or chemical functionalization. Characterisation techniques such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopy, and X-ray diffraction (XRD) are used to analyze morphology, crystallinity, and bonding structures.

RESULTS AND DISCUSSION

The synthesised HACNTs exhibit a hybrid structure consisting of crystalline graphitic domains embedded within an amorphous carbon matrix. This structure leads to increased defect sites and higher surface area compared to pristine carbon nanotubes. Raman spectra show a prominent D-band, indicating structural disorder, alongside a G-band corresponding to graphitic structures. Doping significantly enhances the electrochemical performance of HACNTs. Nitrogen doping improves electrical conductivity and introduces active sites for charge transfer, making it suitable for supercapacitors and battery electrodes. Boron doping enhances p-type conductivity, while sulphur and phosphorus doping improve catalytic activity in fuel cell reactions.

Electrochemical studies demonstrate improved capacitance, cyclic stability, and charge-discharge efficiency in doped HACNTs. The synergistic effect of amorphous structure and heteroatom doping results in better ion diffusion and electron transport, making these materials highly efficient for energy storage and conversion systems.



CONCLUSION

Hybrid amorphous carbon nanotubes offer a versatile platform for advanced energy applications due to their unique structural and electronic properties. Controlled synthesis techniques allow tuning of amorphous and crystalline phases, while doping strategies significantly enhance performance characteristics. The study highlights that HACNTs, particularly when doped with heteroatoms, exhibit superior electrochemical behaviour compared to conventional carbon nanomaterials. Future research should focus on scalable synthesis methods and optimization of doping concentrations to further improve efficiency and commercial viability.

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**Oral Presentation – OOP-07****QUANTAM DOT ENHANCE TERAHEARTZ ANTENNA INTERATED WITH VLSI ARCHITECTURE FOR ECO SAFE AND BIRD SAFE 6G COMMUNATIONS**

Dr. Mithu Dey¹, Akash Sutradhar², Swastik Mukherjee³, Suchetana Chakraborty⁴, Jyotirmoy Chatterjee⁵, Swastika Banerjee⁶

¹Department of Basic Science & Humanities , Asansol Engineering College, Asansol-713305, West Bengal, India.

²³3rd year student, Computer Science and Business Systems, Asansol Engineering College, Asansol-713305, West Bengal, India.

⁴3rd year student, Electrical and Electronics, Asansol Engineering College, Asansol-713305, West Bengal, India.

⁵3rd year student, Information Technology, Asansol Engineering College, Asansol-713305, West Bengal, India.

⁶2nd year student, Computer Science and Business Systems, Asansol Engineering College, Asansol-713305, West Bengal, India.

INTRODUCTION

The rise of sixth-generation (6G) wireless networks is driven by the demand for ultra-fast data speeds, real-time communication, and immersive applications. Central to this vision is the terahertz (THz) spectrum, offering vast bandwidth but facing challenges such as high path loss, short propagation, and energy efficiency concerns. At the same time, ecological impacts of traditional antennas—like bird collisions and heating effects—have raised sustainability issues. Quantum dots, with their tunable properties, combined with low-power VLSI circuitry, present a promising solution. This paper explores an integrated antenna system designed for high-performance communication and environmentally responsible 6G infrastructure.

METHODOLOGY

The proposed THz antenna integrates quantum dots into a compact patch structure, enhancing radiation efficiency, tunable resonance, and impedance matching while reducing thermal stress. Coupled with VLSI control, it supports real-time reconfigurability, beam steering, and adaptive frequency operation, ensuring efficient, reliable, and ecologically safe performance for 6G communication.

RESULTS AND DISCUSSION

The quantum-dot-assisted THz antenna with its VLSI control unit was evaluated using electromagnetic and circuit-level simulations. Results showed that embedding quantum dots enhanced permittivity and field confinement, yielding an 18–25% gain improvement over conventional THz patch antennas. The design also enabled wide tunability from 0.3 to 1.2 THz through bias control. Radiation analysis confirmed a stable directional beam across the tuning range, with reduced side lobes and narrower beamwidth, minimising stray radiation and supporting ecological safety. Thermal testing indicated device temperatures remained below 40°C even at peak transmission, while environmental stress tests verified material reliability under varying conditions. The VLSI subsystem demonstrated strong energy efficiency, consuming ~30–40 mW during full transmission and less than 2 mW in standby, aided by dynamic voltage scaling and power gating. Ecological modeling further showed negligible absorption and heating in avian tissues, confirming bird-safe operation. Overall, the integrated system achieved higher gain, broad frequency



agility, efficient power use, thermal stability, and minimal ecological impact—making it a promising solution for sustainable 6G infrastructure.

Table 1. Simulation Results Summary

Metric	Outcome
Antenna Gain Enhancement	Approximately 18–25% improvement compared to standard designs
Frequency Tunability	Operational range spanning 0.3 to 1.2 THz
Side Lobe Characteristics	Noticeably reduced side lobe levels
VLSI Power Performance	High efficiency: ~30–40 mW during operation, <2 mW in standby
Thermal Performance	Maintained device temperature below 40°C
Bird-Safe Functionality	Verified minimal radiation absorption and negligible heating

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CRYOSENSE: COLD CHAIN DAMAGE MEMORY SYSTEM FOR FLORAL AND FOOD STORAGE

Keerthivasan, S., Udhayaraj, T., and Vidhya, G.

Department of Electronics and Communication Engineering, Jerusalem College of Engineering.

Velachery Main Road, Narayanapuram, Pallikaranai, Chennai, Tamil Nadu, 600100, India

Corresponding author e-mail: Kvasan2019@gmail.com

INTRODUCTION

INTRODUCTION

The cold chain is a critical logistics system that maintains low-temperature conditions for perishable goods such as flowers, fruits, vegetables, and dairy products throughout storage and transport. Failures in cold chain integrity — such as temperature excursions, vibration-induced damage, or elevated ethylene gas levels — result in significant economic losses and food waste worldwide. Conventional monitoring systems record data passively without integrating multi-sensor inputs into a unified spoilage risk metric. This work presents CryoSense, an Arduino UNO-based embedded system that continuously acquires temperature, humidity, atmospheric gas concentration, and vibration data, and computes a cumulative Damage Index (DI) that quantifies spoilage risk in real time. The system provides tiered alert outputs — visual LED indicators, an audible buzzer, and an automatically activated cooling fan — enabling immediate corrective action by storage personnel. The proposed system is low-cost, self-contained, and suitable for deployment in cold storage rooms, refrigerated transport vehicles, and floral preservation chambers.

MATERIALS AND METHODS

The CryoSense hardware platform is built around an Arduino UNO microcontroller interfacing with five sensor modules. A BME280 sensor (I2C, address 0x76) measures ambient temperature, relative humidity, and barometric pressure at 12-bit resolution. A DS18B20 digital temperature sensor (OneWire protocol, Pin D2) provides an independent secondary temperature probe, enabling cross-validation and average temperature computation. An MQ135 electrochemical gas sensor samples the analog output on pin A0 to detect volatile organic compounds (VOCs) and ethylene — gases associated with biological spoilage. A digital vibration sensor on Pin D3 counts shock events. A 16×2 LCD with I2C backpack (address 0x27) displays live data on three rotating pages. Outputs include three status LEDs (green/yellow/red on Pins D5–D7), an active buzzer (Pin D9), and a 5V relay module (Pin D8) that switches a DC fan from a 9V supply. The Damage Index (DI) is calculated every two seconds according to Equation [1], accumulating weighted penalty scores based on deviations from safe operating conditions. The DI is bounded in the range [0, 100].

$$DI(t) = DI(t-1) + P\_temp + P\_gas + P\_vib \quad [1]$$

where the penalty terms are defined as:

Condition	Penalty Applied



Average temperature > 12°C (critical high)	$P_{temp} = 2.0 \times (T_{avg} - 12)$
Average temperature 8–12°C (mild high)	$P_{temp} = 1.0 \times (T_{avg} - 8)$
Average temperature < 2°C (freeze risk)	$P_{temp} = 0.5 \times (2 - T_{avg})$
MQ135 analog count > 600	$P_{gas} = 3.0$
MQ135 analog count 400–600	$P_{gas} = 1.0$
Vibration events > 10 (counter reset)	$P_{vib} = 2.0$

Table 1. Damage Index penalty parameters for CryoSense.

RESULTS AND DISCUSSION

The system was bench-tested over a 60-minute monitoring session under three controlled conditions simulating safe storage, mild temperature excursion, and advanced spoilage. During the SAFE phase ($DI < 30$), the BME280 and DS18B20 readings were consistent within $\pm 0.3^\circ\text{C}$ of each other, and the green LED remained active with DI accumulating at < 0.5 units per cycle due to negligible penalty scores. In the WARNING phase ($30 \leq DI < 70$), an induced temperature rise to 10°C caused the yellow LED to activate, with DI growing at approximately 2 units per 2-second cycle. Gas sensor values rose from a baseline of ~ 180 counts to ~ 450 counts upon introduction of ethylene-generating ripening fruit, confirming sensor sensitivity. In the SPOILAGE phase ($DI \geq 70$), the red LED activated, the buzzer produced an intermittent 500 ms alert tone, and the relay closed to engage the cooling fan — all within one sampling cycle of threshold crossing. The LCD rotated across three information pages at 3-second intervals: (1) average temperature and humidity, (2) gas analog reading and vibration event count, and (3) current DI value and system status string. Serial monitor output at 9600 baud allowed real-time logging of all sensor values for post-session analysis. Table 2 summarises the system state transitions observed during testing.

Test Phase	Avg Temp ($^\circ\text{C}$)	MQ135 Count	DI Range	State
Cold storage baseline	5.2	182	0 – 8	SAFE
Mild temp excursion	10.1	210	8 – 38	WARNING
Ethylene exposure	10.5	463	38 – 65	WARNING
Simulated spoilage	13.2	618	65 – 100	SPOILAGE

Table 2. System state transition results during bench testing.

The dual-temperature sensor approach proved beneficial: a single faulty reading from either sensor did not trigger a false alarm, since the average was used in penalty computation. Vibration events were accurately counted when the storage unit was subjected to simulated transport jolts, contributing a discrete penalty increment after every 10 registered events. The system's total bill of materials cost approximately ₹1,200 ($\approx$ USD 14), making it significantly



more affordable than commercial cold chain loggers while offering comparable multi-parameter sensing capability.

CONCLUSION

CryoSense demonstrates that a low-cost, microcontroller-based multi-sensor platform can effectively monitor cold chain integrity for floral and food storage applications. The cumulative Damage Index approach provides a more informative spoilage risk metric than simple threshold-based alarms, as it accounts for the duration and magnitude of adverse conditions across temperature, gas concentration, and physical shock dimensions. The system correctly identified all three operational states — SAFE, WARNING, and SPOILAGE — during bench validation, with appropriate activation of LED, buzzer, and fan outputs. Future work will integrate GSM/IoT connectivity for remote monitoring, incorporate a real-time clock module for timestamped event logging to EEPROM, and evaluate performance under extended field deployment in commercial cold storage facilities.

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Hand Exoskeleton Suit for People with Parkinson's Disease

Tanishque Mondal¹, Srideep Ghosh², Prashun Kumar Shaw³, Adrita Das⁴, Sanskriti Gupta⁵, Dr. Susmita Das⁶

¹²³⁴⁵⁶Narula Institute of Technology, 81, Nilgunj Road, Agarpara, Kolkata - 700109, West Bengal, India

E-mail : susmitad2011@gmail.com (corresponding author)

INTRODUCTION

The symptoms of Parkinson's arise when large groups of neurons abnormally fire in unison. Parkinson's disease is a brain disorder that causes uncontrollable movements such as shaking, stiffness, and difficulty with balance and coordination. It has been found that aged people face problems gripping any object. These are the symptoms of Parkinson's disease Tremors in hands, arms, legs, jaw, and head. For example, people may have difficulty getting out of the chair.

MATERIALS AND METHODS

In the device, we are using a hand glove. A total of five Servo motors (SG90) are connected to the Arduino Uno servo driver (PCA9685). IR sensor is also connected to the Arduino Uno board. A total of five mini-vibrating motors are used in the glove. To solve this kind of problem we introduce a device that will help to reduce muscle tremors. In this device, we are making hand gloves that will control hand movement using servo motors.

RESULTS AND DISCUSSION

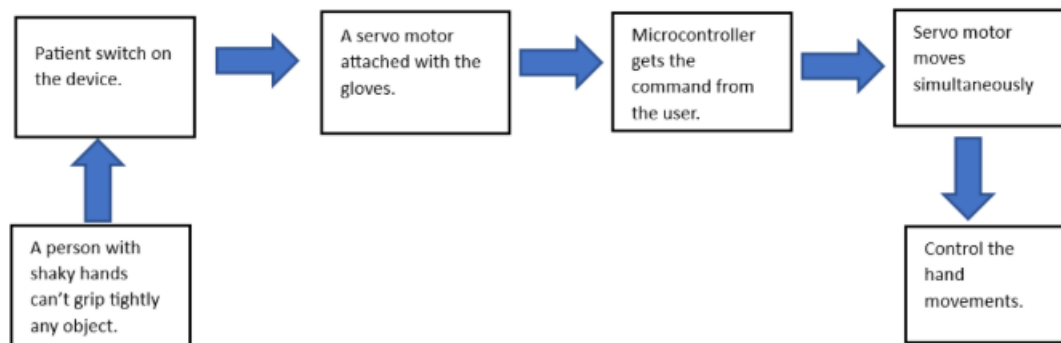


Figure 1. Block Diagram of Hand Exoskeleton System Design

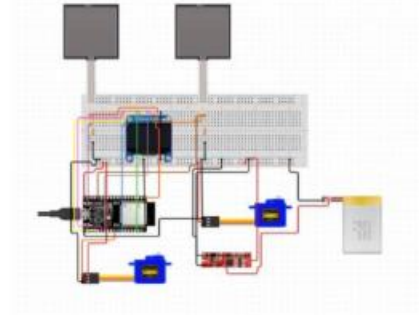


Figure 2. Connection Diagram of Hand Exoskeleton Design

The focus is on upper-limb exoskeletons, specifically the wrist exoskeleton. This type of exoskeleton typically incorporates a joint design for each hand. By adjusting various parameters like torque output, joint location, and movement patterns, we aim to optimize the exoskeleton's performance for the user. The level of assistance provided by the exoskeleton can range from partial to full weight support and gripping.

CONCLUSION

The solution solves the tremoring or shaking of hands. The system can be developed using EMG sensor with biofeedback. The exoskeleton solution is justified for the workshop to learn new methodology for the specially abled persons.

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Ultra-fast Charge Dynamics at F16CuPc/Au Heterostructure

Sumona Sinha¹, Michael Vorokhta², Manabendra Mukherjee³, A. K. M. Maidul Islam⁴

¹Department of Basic Science and Humanities, Institute of Engineering and Management, Kolkata,
University of Engineering and Management, Newtown, Kolkata–7000160, India

²Faculty of Mathematics and Physics, Department of Surface and Plasma Science, Charles
University, V Holešovičkách 2, 18000 Prague, Czech Republic

³Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata – 700064, India

⁴Department of Physics, Aliah University, IIA/27, New Town, Kolkata–7000160, India

E-mail (sumona.net.09@gmail.com)

INTRODUCTION

Ultra-thin organic molecular films are important for next-generation biocompatible electronics and optoelectronics. Organic semiconductor/metal interfaces govern device performance through complex mechanisms such as charge transfer, dipoles, and hybridisation, which remain incompletely understood. Molecular orientation significantly affects energy alignment. Metal phthalocyanines, especially fluorinated F16CuPc, show tunable properties and promising n-type behaviour, though intrinsic charge transfer at such interfaces requires further investigation [1, 2]. We investigate charge transfer, molecular alignment, and interactions of F16CuPc on Au(111) using various synchrotron-based photoemission spectroscopy techniques. Core-hole clock analysis reveals ultrafast charge dynamics across the interface in detail.

MATERIALS AND METHODS

The sample preparation and all experiments were carried out in situ in a UHV system (pressure P : 2×10^{-10} mbar) at the Elettra synchrotron radiation facility (Material Science Beamline endstation), Italy. Before deposition, the Au(111) surface was cleaned by repeated cycles of Ar⁺ sputtering and subsequent annealing at high temperature. XPS characterisation was carried out to ensure no contamination on the sample. For depositing ultrathin films on Au(111), F16CuPc molecules were thermally evaporated with an evaporation rate of about 0.1 Å/s. The nominal thicknesses of the F16CuPc films were calibrated by monitoring the evaporation rate with a quartz crystal microbalance (Inficon GmbH, Germany). Photoelectron spectra were recorded at the valence band and various core levels. The peak fitting of XPS spectra was performed using the Peakfit data evaluation software. Near-edge X-ray absorption fine structure spectroscopy (NEXAFS) measurements were carried out at C, N and F K-shell ionisation thresholds using three different angular configurations in Auger yield mode. The valence region (0–25 eV) resonance photoemission spectroscopy (RPES) spectra were recorded by varying the photon energy across the C, N and F K-shell absorption edges [2, 3].

RESULTS AND DISCUSSION

Angle-dependent carbon and nitrogen K-edge NEXAFS data indicate that F16CuPc molecules adopt a lying-down geometry on Au (111). This molecular configuration remains unaltered with thickness. Moreover, the C1s and N1s XPS spectra reveal the creation of an interfacial layer between the molecules and the Au(111) substrate. The results



further illustrate that the molecules were in a flat shape and not deformed in close contact with Au (111) substrate. After that, we studied charge transfer time across the interface. The two-dimensional RPES maps, showing photon energy versus electron-binding energy plots, consist of a collection of valence band photoemission spectra acquired at various photon energies, spanning the N K-edge threshold and displayed on the scale of coloured intensity. In the present study, RPES images for both F16CuPc films on Au (111) are exhibited in Fig. 1 (a) and (c), respectively. On the other hand, corresponding N K-edge NEXAFS spectra for 5 Å and 50 Å films on Au(111) are displayed in figure 1(b) and (d), respectively [2, 3].

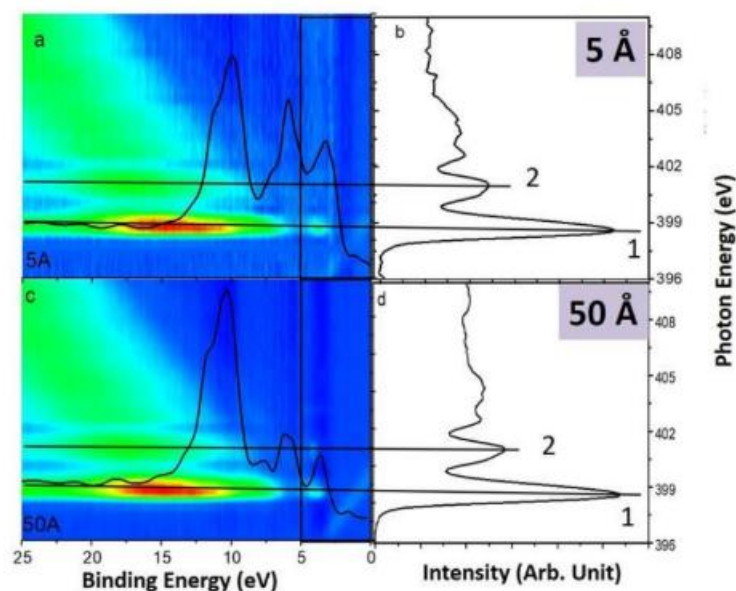


Figure 1: N K-edge RPES intensity contour maps of F₁₆CuPc on Au(111) for (a) submonolayer (5 Å) and (c) multilayer (50 Å) films. The displayed spectra represent valence band data acquired at a photon energy of 110 eV. Corresponding N K-edge NEXAFS spectra are shown in the right panels for (b) 5 Å and (d) 50 Å films on Au(111).

Then charge transfer time was calculated using the following expression, equation (1) [3, 4],

$$\tau_{CT} = \tau_{CH} \frac{I_{RPES}^{COUP} / I_{NEXAFS}^{COUP}}{I_{RPES}^{ISO} / I_{NEXAFS}^{ISO} - I_{RPES}^{COUP} / I_{NEXAFS}^{COUP}} \quad [1]$$

Where τ_{CH} symbolizes the charge-transfer time with a value of about 6 fs for the N 1s of phthalocyanine lifetime



[4, 5]. and represent the integrated intensities of LUMOs for the RPES spectra as collected for the coupled sub-monolayer and multilayer of F16CuPc systems, respectively. Similarly, and are the LUMO intensities in the NEXAFS spectra for sub-monolayer and multilayer scenarios. The charge transfer time from F16CuPc molecules to the Au substrate is computed around 12 fs due to the interfacial interaction at the F16CuPc/Au interface. Overall, these findings clarify the fundamental charge-transfer behaviour of a photoexcited n-type molecule on a metal surface and guide for optimizing the use of F16CuPc in electronic devices.

CONCLUSION

Angle-dependent NEXAFS measurements indicate that F16CuPc predominantly adopts a planar adsorption geometry on Au(111). Core-level photoemission analyses further reveal the formation of an interfacial layer arising from molecule–substrate coupling. Moreover, using the core-hole clock method, we determined an ultrafast interfacial charge-transfer timescale of about 12 fs at the F16CuPc/Au(111) interface.

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A comparative study on Methyl Orange Degradation by gamma Iron oxide and nano zero valent Iron (nZVI)

Avik De^{*1}, Biplab Saha², Gourab Mondal², Pawan Kuma^{r3}, Dibyendu Banerjee³

¹*Assit. Professor, Department of BS&HU (Chemistry), Asansol Engineering College, Asansol-713305,
E-mail: avik.chem@aecwb.edu.in

²Assit. Professor, Department of Civil Engineering, Asansol Engineering College, Asansol-713305,
E-mail: biplab.ce@aecwb.edu.in, gourab.mondal13@gmail.com

³Department of Civil Engineering, Asansol Engineering College, Asansol-713305,
pk9148442@gmail.com, dibyendubanerjeeab@gmail.com

Corresponding author mail id: avik.chem@aecwb.edu.in

INTRODUCTION

The critical need for an environmentally friendly and clean chemical process has been brought to light by global environmental pollution. Strict laws governing waste production and effluent quality standards are posing problems for wastewater treatment procedures (WWTP) (De et al., 2016).

Methyl orange is an anionic dye due to the presence of sulfonic acid group. Dyes are extremely stable due to their complex aromatic molecular structure and are thus difficult to biodegrade. [Konicki et.al., 2018] Methyl orange (C₁₄H₁₄N₃NaO₃S), known for its biorecalcitrant property with molecular weight 327.33 g/mol and characteristic wavelength λ_{max} of 465nm, was degraded. In present work, it was degraded at optimum condition as mentioned earlier both by gamma and nZVI.

MATERIALS AND METHODS

(i) FeCl₃, 6H₂O Ferric chloride hexa hydrate (ii) Ethyl alcohol (iii) Ferrous chloride tetrahydrate (iv) Distilled water from Merck, India (v) Sodium Hydroxide (vi) Hydrochloric acid (vii) NaBH₄ Sodium borohydrate (viii) n- butanol. ix) Methyl Orange were purchased from: Merck (India) and all chemicals procured are of analytical grade.

i) XRD measurement: XRD analysis was carried out by: PANalytical Machine Model No.PW.3040/60. All powdered nanoparticle samples are undergone XRD analysis.

ii) FESEM and EDX: FESEM images are taken by JEOL-ZSN-7600S-FESEM.

RESULTS & DISCUSSION:

All the above nanoparticles are undergone XRD analysis & Particle size calculations are (As per Debye Scherrer Equation and JCPDS file no. 19-0629, 44-1415, 34-0529) shown in following table:



Table 4.1: Comparison of Nanoparticles in terms of Particle Size

Name of the particle	Average Nano Particle Diameter
Gamma nanoparticle	52 nm
nZVI particles	32 nm

The samples are also characterized by FESEM analysis

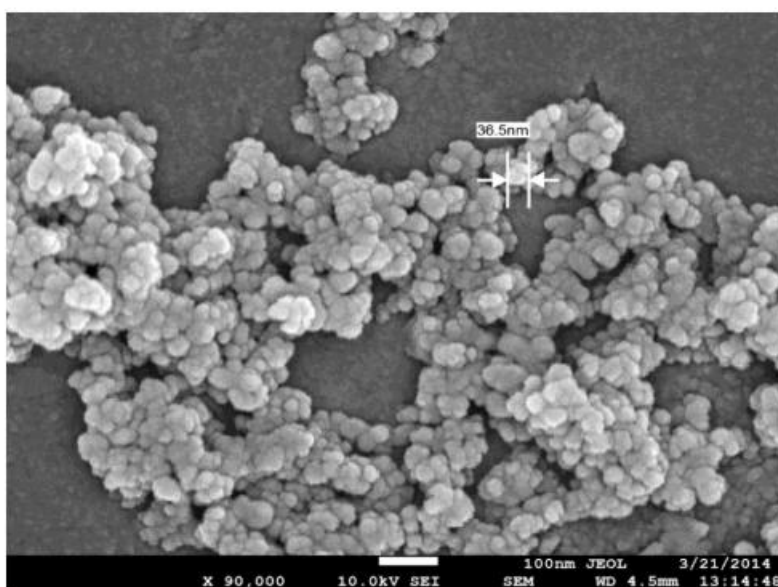


Figure 3.1: FESEM image of nano gamma particles

Methyl orange ($C_{14}H_{14}N_3NaO_3S$) with molecular weight 327.33 g/mol and characteristic wavelength λ_{max} of 465nm was degraded. It was degraded at optimum condition as mentioned earlier both by gamma and nZVI. Out of this nZVI showed better reactivity towards MO degradation within 150 minutes of reaction. The first-order degradation kinetics pattern is shown in figure 5.2 where C/C_0 represents fraction of methyl orange degraded over time.



Figure 3.2 Gradual decrease in color with the progress of the reaction

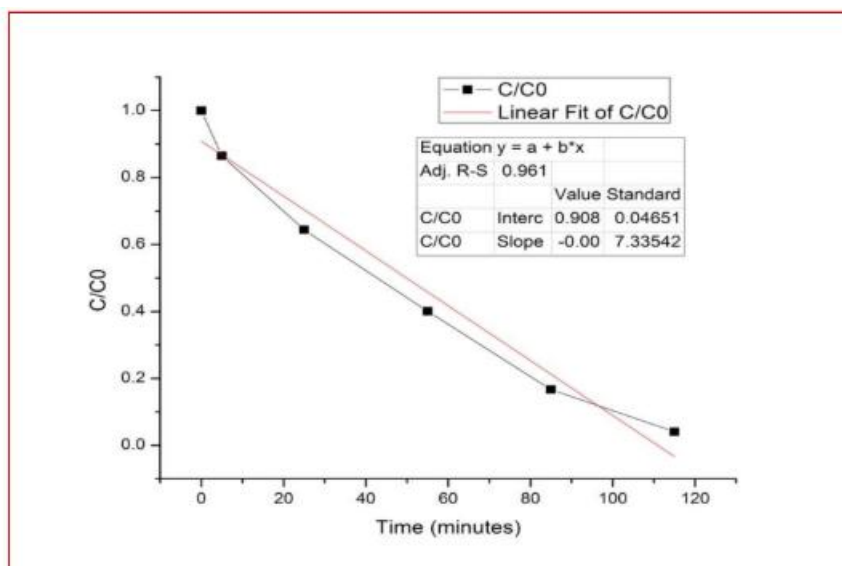


Figure 3.3 Degradation kinetics of methyl orange dye

After completing almost 38 no of experiments as per RSM depicted values of process variables, an optimum condition is achieved or reached.

CONCLUSION

In the present work it has been found that nZVI acts as a better catalyst towards methyl orange dye degradation compared to gamma. This may be attributed due to the lower particle size of nZVI over gamma. The optimum reaction condition for dye degradation reaction is: Initial Dye 200 mg/l, nanoparticle concentration: 0.6 g/l. Reaction time: 15 minutes. pH = 7.8, temperature = 35o C. Reaction volume = 100 ml. H2O2 = not used. In order to maximize the conversion of Phenol, the standard Response surface Methodology (RSM) was used to determine the optimum condition. For the present study, the well-known central composite design (CCD) scheme was chosen for its flexibility.



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Hybrid Deep Learning Approach for Skin Lesion Classification Using Image and Metadata Fusion

Mr. Sandipan Biswas¹, Ms. Jayita Pal², Dr. Chandrima Chakrabarti³, Debsurya Das⁴, Sharanya Sinha⁵, Amarjit Dey⁶, Arunabha Bhattacharyya⁷

^{1,4,5,6,7} Department of CST

Narula Institute of Technology, Kolkata, India

E-mail: sandipanbiswas714@gmail.com

³Department of CS (Data Science)

Narula Institute of Technology, Kolkata, India

E-mail: chandrima.narula@gmail.com

²Department of CSE

Narula Institute of Technology, Kolkata, India

E-mail: jayitapal.it@gmail.com

INTRODUCTION

Skin lesion classification using deep learning has gained significant attention due to its potential in assisting the early detection of skin cancer, particularly melanoma, which is one of the most aggressive and life-threatening forms of the disease. Early and accurate diagnosis is critical for improving patient survival rates; however, manual diagnosis based on dermoscopic analysis is often time consuming and highly dependent on clinical expertise. Although deep learning based approaches have demonstrated promising performance in automated skin lesion classification, many existing models rely exclusively on image-based features. This unimodal approach limits their ability to incorporate clinically relevant contextual information, such as patient demographics and lesion location, which are known to influence diagnostic decisions in real world clinical settings.

To address this limitation, the present study proposes a hybrid deep learning framework that integrates dermoscopic image data with structured patient metadata to enhance classification performance. The central objective is to leverage both visual and contextual information through a multimodal learning strategy, thereby improving the robustness and generalization capability of the model, particularly in cases involving visually similar lesion classes.

The dataset used in this study is the HAM10000 dataset, a widely recognized benchmark in skin lesion analysis, which contains 10,015 dermoscopic images categorized into seven diagnostic classes: actinic keratoses (akiec), basal cell carcinoma (bcc), benign keratosis-like lesions (bkl), dermatofibroma (df), melanoma (mel), melanocytic nevi (nv), and vascular lesions (vasc). In addition to image data, associated metadata including patient age, sex, and lesion localization were incorporated into the learning process. These metadata attributes provide valuable clinical context that complements visual features and contributes to improved classification accuracy.

Data preprocessing was performed to ensure consistency and quality of both image and metadata inputs. Missing



values in the age attribute were handled using mean imputation, while categorical metadata such as sex and localization were transformed using one-hot encoding to enable numerical representation. The age feature was normalized using MinMax scaling to ensure compatibility with neural network training. Dermoscopic images were resized to a fixed resolution of 224×224 pixels and processed using EfficientNet-specific normalisation to align with the pretrained model requirements. Furthermore, a custom multi-input data generator was developed to efficiently load and preprocess image and metadata inputs in parallel during training, enabling seamless integration of multimodal data within the training pipeline.

The proposed model architecture follows a dual-branch design. The image branch utilizes a pretrained EfficientNetB0 model as a feature extractor, leveraging transfer learning from ImageNet weights to capture rich hierarchical visual features. The metadata branch consists of fully connected dense layers that process structured tabular inputs and learn meaningful representations from patient specific attributes. The outputs of both branches are combined through feature-level fusion using concatenation, resulting in a unified representation that captures both visual and contextual information. This fused representation is further processed through additional dense layers with dropout regularization to mitigate overfitting and improve generalization. The final classification is performed using a softmax activation function over seven output classes.

The model was trained using the Adam optimization algorithm with categorical cross entropy as the loss function. An 80–20 stratified train-validation split was employed to preserve class distribution across subsets, ensuring fair evaluation. Performance was assessed using standard classification metrics, including accuracy, precision, recall, and F1 score, providing a comprehensive evaluation of model effectiveness across all classes.

Experimental results demonstrate that the proposed hybrid model achieves an overall accuracy of 86% on the validation dataset, along with a weighted F1 score of 0.85, indicating strong overall performance. The model exhibits high classification accuracy for majority classes such as melanocytic nevi (nv), which dominate the dataset. However, comparatively lower performance is observed in minority classes such as dermatofibroma (df) and melanoma (mel), primarily due to class imbalance and limited sample representation. This imbalance poses a significant challenge, as minority classes often correspond to clinically critical conditions.

A detailed analysis of the confusion matrix reveals that misclassification predominantly occurs between visually similar classes, particularly between melanoma and melanocytic nevi. This observation highlights the inherent difficulty in distinguishing between certain lesion types based solely on visual characteristics. Importantly, the integration of metadata contributes to improved contextual understanding, enabling the model to make more informed predictions in ambiguous cases and reducing misclassification in some instances.

Despite the promising results, several challenges remain. The presence of class imbalance significantly impacts the model's ability to generalize across all categories, particularly rare and clinically significant classes. Additionally, the reliance on a limited dataset restricts the diversity of training samples, which may affect model robustness in real-world scenarios. Future work will focus on addressing these limitations through the incorporation of advanced techniques such as focal loss for handling class imbalance, enhanced data augmentation strategies to improve generalization, and fine-tuning of pretrained network layers to extract more domain-specific features. Furthermore, the integration of explainability methods such as Grad-CAM may enhance interpretability and facilitate clinical adoption.



In conclusion, this study demonstrates that a multimodal deep learning approach combining dermoscopic images with patient metadata can significantly enhance skin lesion classification performance compared to conventional image-only models. The proposed framework provides a scalable and effective solution for computer-aided diagnosis systems and holds strong potential for supporting dermatologists in clinical decision-making processes.

Keywords: Hybrid Deep Learning, EfficientNetB0, Multi-Input Neural Network, Image- Metadata Fusion, HAM10000 Dataset, Transfer Learning, One-Hot Encoding, MinMax Scaling, Custom Data Generator, Stratified Sampling, Categorical Crossentropy, Adam Optimizer, Confusion Matrix, Classification Report.



Transition Metal Oxide Based Resistive Switching Memory Devices for Non- Volatile Memory Applications

Sarbojit Ghosh, Shubham Dutta, Soumik Haldar, Shubhadip Saha, Satyam Chakrabarty

Department of Computer Science Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer Math, Kolkata – 7000741

E-mail :sarbojitghosh16@gmail.com

INTRODUCTION

Transition metal oxide based resistive switching memory is an innovative non-volatile storage technology that encodes data by toggling a thin oxide layer between high and low electrical resistance states. By utilizing a simple metal-insulator-metal architecture, these devices achieve high-speed, energy-efficient, and highly scalable performance. Because they are compatible with standard CMOS fabrication, they represent a key solution for future high-density memory and advanced computing applications.

MATERIALS AND METHODS

Transition metal oxide (TMO) based resistive switching memory utilizes specific materials and mechanisms to store data through controlled electrical resistance changes.

1. Materials: The core of the device is a thin-film switching layer typically composed of transition metal oxides such as Hafnium Oxide (HfO_x), Tantalum Oxide (TaO_x), or Titanium Oxide (TiO₂). These materials are selected for their excellent CMOS compatibility and ability to maintain stable resistance states under external electrical stress.

2. Switching Mechanisms: Operation primarily occurs via two processes: Valence Change Memory (VCM), which relies on the movement of oxygen vacancies, and Electrochemical Metallization (ECM), which is driven by the migration of metallic ions. These mechanisms facilitate the formation and rupture of nanoscale conductive filaments, allowing the device to toggle between high and low resistance levels.

3. Fabrication: Production typically involves depositing the oxide switching layer between metal electrodes using thin-film deposition techniques such as atomic layer deposition or physical vapor deposition. Success in creating reliable memory devices depends heavily on optimizing the interface between the metal electrodes and the oxide layer to ensure uniform switching performance.

RESULTS AND DISCUSSION

Transition metal oxide (TMO)-based resistive switching memory devices are gaining attention as a promising option for non-volatile memory. Researchers have been exploring these materials because they can outperform many traditional memory technologies in key areas.

Performance Achievements: Studies show that TMO-based RRAM devices can switch extremely quickly—often in less than 10 nanoseconds—while maintaining long lifetimes of over 10 billion cycles and data retention that can last more than a decade. Materials like hafnium oxide (HfO_x) and tantalum oxide (TaO_x), especially when deposited using atomic layer deposition, tend to operate at relatively low voltages and provide strong differences between their



on and off states. These characteristics make them well-suited for use in dense memory architectures such as crossbar arrays.

Key Challenges and Solutions: One ongoing challenge is variability in device behavior, which is largely caused by the random nature of conductive filament formation inside the filament . To address this, researchers have experimented with bilayer oxide structures—for example, combining TaO_x with Ta_2O_5 —which has helped reduce fluctuations between switching cycles. Scaling these devices down to around 10 nm is possible, but it introduces issues like unwanted current paths. To manage this, configurations such as one-transistor–one-resistor (1T1R) and one-selector–one-resistor (1S1R) are commonly used

Table 1. Key TMO-Based RRAM Materials for NVM Applications

oxide	Switching Type	On/off ratio	endurance	Key Feature
HfO_2	Filamentary	10^3 - 10^5	10^{10}	CMOS Compatible
TaO_x	Filamentary	10^3 - 10^6	$>10^{12}$	Highest Endurance
TiO_2	Interface	10^2 - 10^4	10^6	First PRAM material

Emerging Applications: Beyond traditional data storage, TMO-based RRAM is also being explored for neuromorphic computing, where it can mimic the behaviour of biological synapses by gradually adjusting conductance. This makes it particularly useful for AI hardware, where it has the potential to achieve much higher energy efficiency compared to conventional CMOS systems. With ongoing development and support from semiconductor manufacturers, these devices are expected to play a role in future embedded memory solutions, especially in IoT and edge computing applications.

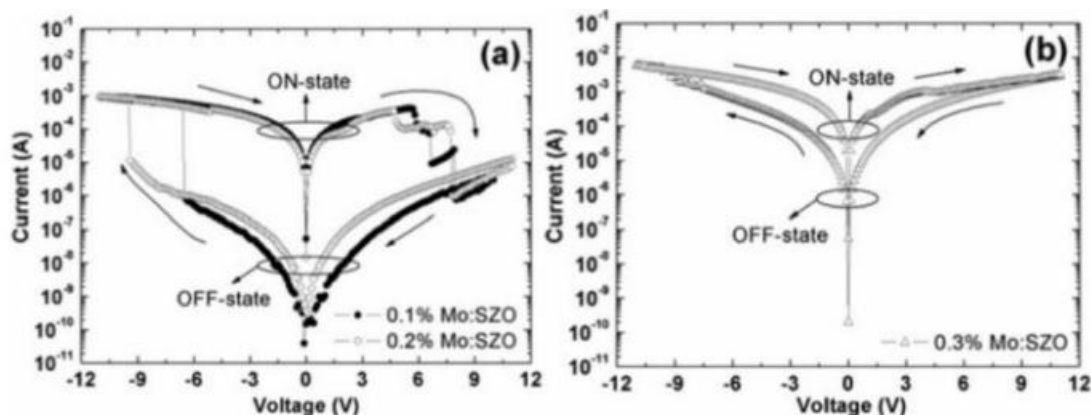


Figure 1. I –V curves of various 0.1, 0.2, 0.3% Mo doping SZO-based memory devices



CONCLUSION

Transition metal oxide (TMO)-based RRAM devices, such as HfO₂, TaO_x, and TiO₂, are promising candidates for next-generation non-volatile memory because of their strong endurance, reliable retention, and compatibility with CMOS technology. Although issues like device variability and scaling still pose challenges, ongoing improvements suggest they will play an important role in future data storage and neuromorphic computing systems.. 5.

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RIDGE VS. LASSO REGRESSION: AN ML-BASED STUDY FOR PREDICTING THE SEEBECK COEFFICIENT OF THERMOELECTRIC MATERIALS

Arun KP¹, Jehan Taraporewalla², Amarnath Samanta³, Biswajit Das⁴, and Dipankar Saha³

¹Department of Electronics and Telecommunication Engineering, Indian Institute of Engineering Science and Technology Shibpur, Howrah-711103, India

²Department of Electrical Engineering, Indian Institute of Technology Delhi, New Delhi-110016, India

³Department of Electronics and Communication Engineering, Narula Institute of Technology, Agarpara, Kolkata, 700109, India

⁴Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, Kolkata - 700074, India

INTRODUCTION

In today's world, the demand for energy is rapidly rising. The growing energy consumption requirements are often met by burning fossil fuels, which have a catastrophic effect on the environment [1][2]. In order to address these issues, a sustainable and effective solution is needed. One such method is the harvesting of electrical energy from waste heat [2][3]. Thermoelectric conversion is achieved by solid-state devices that have no moving parts, making them a silent and reliable source of electricity [3, 4]. The selection of a good thermoelectric material is based on ZT or thermoelectric figure of merit [4, 5]. The dimensionless thermoelectric figure of merit, $ZT = (\sigma_e \times S_B^2 \times T) / (\kappa_{ph} + \kappa_e)$ where σ_e , S_B , $\kappa_{ph} + \kappa_e$, and T are the electrical conductivity, Seebeck coefficient, total thermal conductivity, and temperature value respectively [4-8]. For a thermoelectric material to be considered for industrial applications it must have $ZT \geq 1$, stable at high temperatures and cost effective [9, 10].

The primary challenge in maximizing the thermoelectric figure of merit lies in optimizing the mutually conflicting thermoelectric properties, i.e., to have a high ZT value for a material, it must have a high Seebeck coefficient, high electrical conductivity and low thermal conductivity [11, 12]. The expression for Seebeck coefficient for a metal or degenerate semiconductor considering parabolic band approximation is given by the Mott equation [7, 13].

$$S_B = \frac{\pi^2}{3} \left(\frac{K_B^2 \times T}{q} \right) \left[\frac{d[\ln(\sigma(E))]}{dE} \right]_{E=E_F} = \left(\frac{8\pi^2 K_B^2 T}{3qh^2} \right) m_d^* \left(\frac{\pi}{3n} \right)^{2/3} \quad (1.1)$$

Here K_B is Boltzmann constant, n is carrier concentration, m_d^* is effective mass calculated from the density of states function, and h is Planck's constant. Moreover, electrical conductivity is defined by the equation below [4, 11, 12].

$$\sigma_e = nq\mu = \frac{nq^2\tau}{m} \quad (1.2)$$



METHODOLOGY

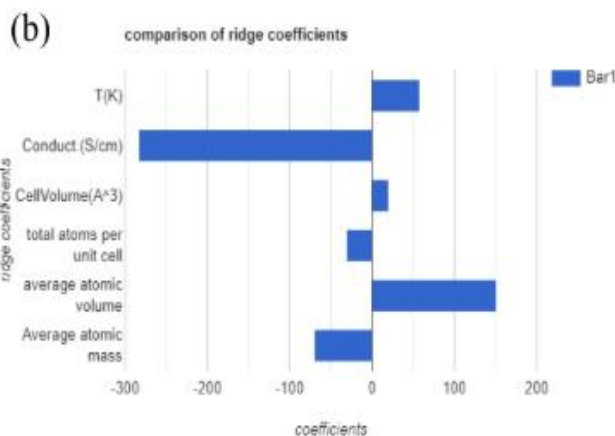
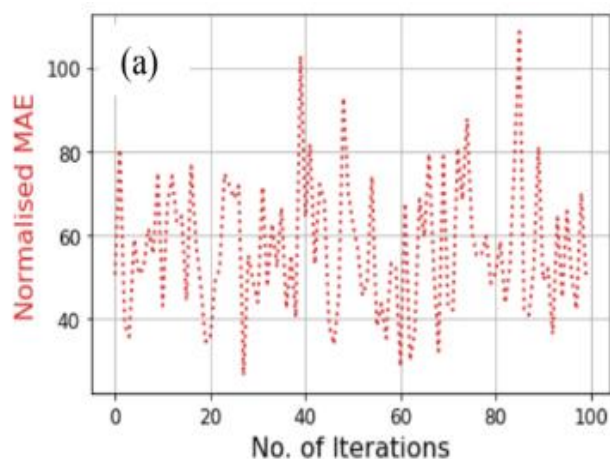
In this study, the dataset is sourced from the UC Santa Barbara database [18, 19], from which 202 non-oxide thermoelectric material entries were collected [19]. The entries are divided randomly into two sets for training purpose and predicting purpose. The data set for training purpose is assigned around 85 percent of the entries and for prediction rest 15 percent of the entries are assigned. To implement the ML methods, Python is used along with the external library Scikit-learn [20–22]. Two ML algorithms are considered for this prediction, namely (i) Ridge Regression and (ii) Lasso Regression. The following properties for various thermoelectric materials are considered for the prediction of Seebeck coefficient.

(i) Temperature, (ii) Conductivity, (iii) Cell volume, (iv) Total atoms per unit cell, (v) Average atomic volume, and (vi) Average atomic mass

PREDICTION OF SEEBECK COEFFICIENT USING MACHINE LEARNING

In the case of linear regression, a limited number of samples may result in overfitting, leading to an unreliable model. This can be mitigated using Ridge Regression and Lasso Regression techniques. Ridge Regression modifies the mean squared error by adding a penalty on the model parameters. Thus, it aims to reduce both the prediction error and the size of the coefficients. However, the sign of model parameters may decrease the loss function instead of increasing it [23, 24]. Hence, in Lasso Regression, the absolute values of the model parameters are considered, unlike Ridge Regression, where the model parameter values are squared [23, 24].

Next, two types of graphs are plotted to analyze the results, viz. (i) Mean Absolute Error (MAE) vs. number of iterations, and (ii) bar plots of Ridge/Lasso coefficient values.



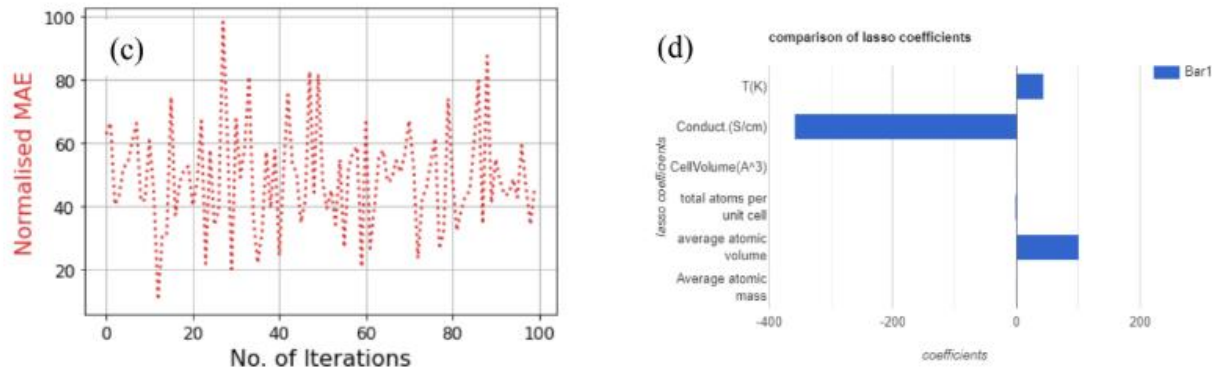


Figure 1: (a) Ridge mean average error versus number of iterations, (b) Ridge coefficient values of the parameters passed to the model, (c) Lasso mean average error versus number of iterations, and (d) Lasso coefficient values of the parameters passed to the model.

Analysis of the Ridge Regression bar graph reveals that conductivity and average atomic volume have a strong influence on the Seebeck coefficient, whereas temperature and average atomic mass exhibit a moderate influence. Considering the Lasso Regression bar graph, it is observed that only temperature, conductivity, and average atomic volume are significant coefficients. The mean absolute error plots indicate that Lasso Regression is more suitable for predicting the Seebeck coefficient and better highlights the key influencing parameters.

CONCLUSION & FUTURE WORK

In this work, a comparison between Ridge Regression and Lasso Regression for predicting the Seebeck coefficient of thermoelectric materials is presented. Analysis of the mean absolute error plots suggests that Lasso Regression is a more effective method for predicting the Seebeck coefficient. Moreover, it offers better interpretability by identifying the most relevant parameters. However, the oscillatory nature of the error plot, instead of convergence to a local minimum, indicates that the model requires further refinement for improved accuracy.

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Tuning of photo-inert to Photo-salient effects of a series of Zn(II)/Cd(II) metal-organic single crystals

Arindam Patra¹, Basudeb Dutta*¹,

Department of Chemistry, School of Applied Sciences,
Kalinga Institute Of Industrial Technology Deemed To Be University,
Bhubaneswar, Odisha

ABSTRACT

Metal–organic crystalline coordination compounds have recently emerged as a promising class of smart hybrid materials, capable of exhibiting remarkable dynamic behaviours such as jumping, hopping, and splitting under light stimulation.¹⁻³ In this work, we focus on the photo salient behaviour of a series of metal–organic crystals synthesized from photo-responsive olefinic ligands. These ligands undergo topochemical [2 + 2] cycloaddition reactions—green, solvent-free transformations—when exposed to UV light or natural sunlight. The resulting compounds display pronounced photo salient effects, including crystal jumping, splitting, rolling, and swelling upon irradiation.⁴⁻⁵ These observations indicate that the photomechanical response can be finely tuned through deliberate selection of structural components. Additionally, the relationship between crystal structure and mechanical behaviour is elucidated through complementary nanoindentation studies, which show good agreement with single-crystal elastic properties predicted by DFT calculations.⁵

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Institute: ¹Department of Chemistry, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar-751024, Odisha, India.

Email ID: dutta.basu11@gmail.com /basudeb.duttafch@kiit.ac.in



Facile Synthesis of Carbon-Coated Graphitic Carbon Nitride for Energy Storage

M. Parashar), D. Banerjee*), A K Upadhyay

Thin Film and Nanotechnology Laboratory

Department of Physics , Faculty of Engineering

Teerthanker Mahaveer University, Moradabad; UP 244001; India

Corresponding author nilju82@gmail.com#)

ABSTRACT

In the present study carbon-coated graphitic carbon nitride was synthesized via thermal polymerization of urea coupled with in situ carbonization of glucose, yielding a structurally integrated carbon–nitride hybrid also called as carbon coated GCN (TCN-200). The phase and morphology of the obtained sample were characterized by XRD and FESEM whereas, EDX analysis verifies elemental composition of the sample. Cyclic voltammetry demonstrates promising capacitive behaviour of the material with the specific capacitance value reaches 435.6 F/g at scan rate of 5mVs whereas, the energy and power density came ought to be $\sim 180 \text{ W h kg}^{-1}$ and $\sim 32,000 \text{ W kg}^{-1}$, respectively indicating its capability to deliver balanced energy storage with high power output. This study demonstrates that such system can be taken as a promising candidate for advanced supercapacitor applications.

Keywords: Graphitic carbon nitride, Specific capacitance, Cyclic voltammetry, charge storage

INTRODUCTION

The increasing global demand for sustainable and efficient energy systems has intensified research on advanced energy storage technologies. Among various storage devices, electrochemical supercapacitors have attracted considerable attention due to their high-power density, rapid charge–discharge capability, and long cycle life [1]. However, their relatively low energy density compared to batteries remains a major limitation, which necessitates the development of advanced electrode materials. Carbon-based materials have been widely explored as electrode candidates owing to their high surface area, excellent electrical conductivity, chemical stability, and cost-effectiveness [2]. In particular, graphitic carbon nitride (g-C₃N₄) has emerged as a promising material due to its layered structure, high nitrogen content, and potential for pseudocapacitive charge storage [3]. Despite these advantages, the practical application of g-C₃N₄ is restricted by its poor electrical conductivity and limited charge transport properties.

To overcome these limitations, hybridization with conductive carbon materials has been recognized as an effective strategy to enhance the electrochemical performance by improving electron transport and increasing active surface area. In this context, carbon-coated graphitic carbon nitride structures offer a synergistic advantage by combining the conductivity of carbon with the redox-active nature of nitrogen functionalities. Therefore, in the present work, carbon-coated graphitic carbon nitride (TCN-200) has been synthesized via thermal polymerization of urea with in situ carbonization of glucose, aiming to achieve enhanced capacitive performance for supercapacitor applications [4,5].



MATERIALS AND METHODS

Carbon-coated graphitic carbon nitride was synthesized via thermal polymerization of urea in the presence of glucose. Briefly, 6 g of urea and 200 mg of glucose were dissolved in 10 mL of deionized water under continuous stirring to obtain a homogeneous solution. The solution was dried at 80 °C, followed by calcination at 550 °C for 2 h in a muffle furnace. The obtained product was collected after cooling and designated as TCN- 200. The as synthesized material was studied by XRD, FESEM (equipped with EDX) and cyclic voltametric analysis

a. Structural and Morphological Characterization

Figure 1 (a and b shows the XRD and FESEM spectra of the as synthesized sample).

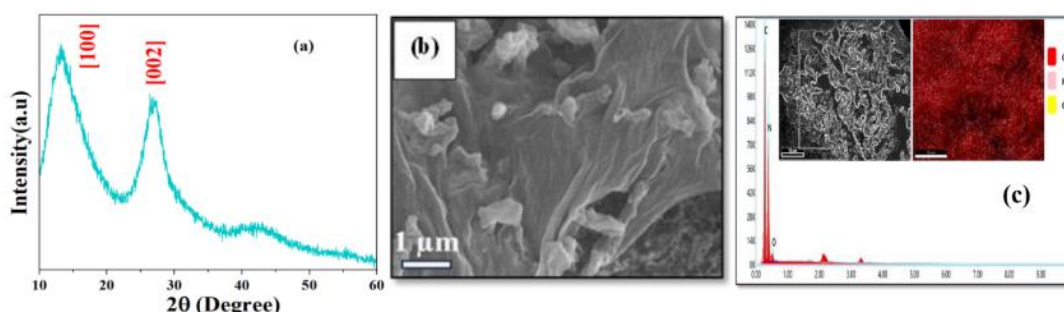


Figure 1: XRD (a) FESEM (b) and EDX (c) pattern of as-synthesized sample

RESULTS AND DISCUSSION

The XRD pattern from **Fig.1(a)** shows two characteristic peaks at $2\theta \sim 13.1^\circ$ and $\sim 27.4^\circ$, corresponding to the (100) in-plane structural packing of tri-s-triazine units and the (002) interlayer stacking in conjugated aromatic systems respectively.

The FESEM image in **Fig.1 (b)** reveals that the sample exhibits a wrinkled nanosheet morphology. Here the precursor interactions between urea and glucose favor planar layer formation, resulting in large, flexible 2D layers with prominent surface ridges and "folds." Enhancing the effective surface area favourable for charge storage capacity

EDX spectra of the sample along with the elemental mapping is shown in **Fig.1 (c)**. The presence of carbon, nitrogen and oxygen confirms the absence of unwanted impurities in the sample.



b. Electrochemical Analysis

The electrochemical properties of the sample electrode were evaluated using cyclic voltammetry (CV) within a potential window of 0.0 to 0.65 V. Fig.2 illustrates the CV curves at varying scan rates. The curves exhibit a quasi-rectangular shape integrated with distinct, broad anodic and cathodic peaks, signifying a hybrid charge storage mechanism comprising electric double-layer capacitance (EDLC) and Faradaic pseudo-capacitance. The specific capacitance was calculated from the equation gives as:

$$C_{sp} = \frac{\text{Area}}{\text{Scan rate} \times \text{Mass of the sample} \times \text{voltage window}} \quad (1)$$

The prominent redox peaks are attributed to the reversible intercalation/de-intercalation of electrolyte ions into the nitrogen-rich framework of the GCN. Specifically, the lone pair of electrons on the pyridinic nitrogen atoms in the carbon nitride lattice facilitates redox reactions. The broadening of these peaks suggests that the redox process is not confined to a single crystalline phase but occurs across a distribution of energetically different active sites on the wrinkled nanosheet surface. the maximum specific capacitance of 435.6 F g⁻¹ was achieved at a low scan rate of 5 mV s⁻¹.

The energy and power density (U) and (P) were also calculated from the formula:

$$U (\text{WhKg}^{-1}) = \frac{1}{2} C_{sp} V^2 \quad (2)$$

$$P (\text{WKg}^{-1}) = \text{Energy density} \times 3600/t \quad (3)$$

where C_{sp} = specific capacitance in F/g, V = voltage window in volts, t = discharge time in seconds.

The energy and power densities of TCN-200 were evaluated at a current density of 0.5 A g⁻¹, are found to be approximately ~180 W h kg⁻¹ and ~32,000 W kg⁻¹, respectively, indicating its capability to deliver balanced energy storage with high power output.

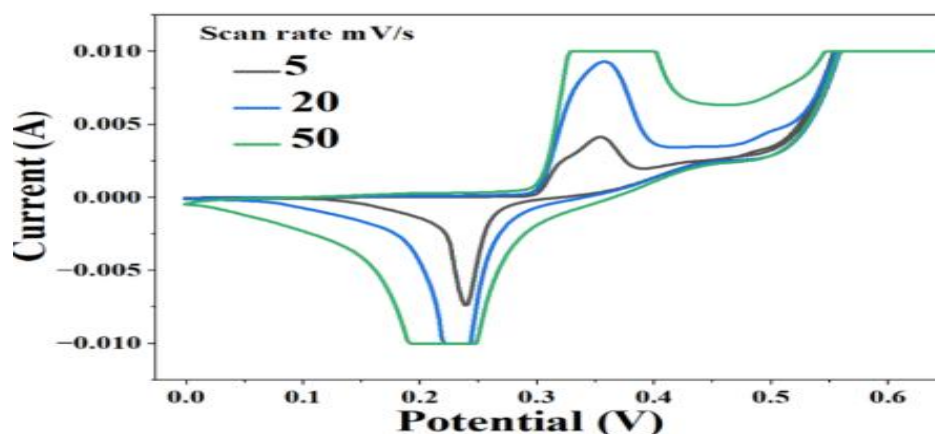


Fig.2: CV characteristics of the sample at different scan rates



Conclusion

In this study, a structurally integrated carbon-coated graphitic carbon nitride hybrid was successfully synthesized via a facile one-pot thermal polymerization of urea combined with in situ carbonization of glucose. XRD confirmed the formation of the conjugated aromatic system. FESEM analysis revealed a wrinkled nanosheet structure, attributed to the lack of a templating mechanism

CV characteristics of the sample exhibits hybrid charge storage mechanism of both EDLC and Faradaic pseudo-capacitance. The material achieved a significant specific capacitance of 435.6 F/g at a scan rate of 5 mV/s. Furthermore, the system delivered a balanced energy density of $\sim 180 \text{ Wh kg}^{-1}$ alongside a high-power density of $\sim 32,000 \text{ W kg}^{-1}$. All these speculating the use of the as synthesized sample as promising charge storage system.

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Hetero-Bridged Zn(II) 2D Coordination Polymer for Schottky Diodes: Structure and Theory

Arnab Samanta¹

¹Department of Chemistry, Brainware University, Barasat, Kolkata 700125

E-mail: anuparnab@gmail.com

ABSTRACT

Using two distinct bridging ligands, 4,4'-Dipyridylsulphide (4,4'-DPS) and 5-Nitroisophthalic acid (5-H₂NIA), we have prepared a hetero-bridging Zn (II)-coordination polymer {[Zn(4,4'-DPS)₂(5-HNIA)₂(H₂O)]_n} (Zn-CP) and characterized the crystalline compound with Single Crystal X-ray diffraction (SCXRD) technique. Through a variety of non-covalent interactions, a 2D network self-assembles to produce a 3D supramolecular structure. Hirshfeld surface analysis is carried out to understand the possibilities of non-covalent interactions present in Zn-CP. Density functional theory (DFT) based numerical calculation using crystallographic parameters has estimated the band gap 3.51 eV which the value is closer to the experimental value (3.71 eV) indicating the semiconducting nature of Zn-CP. The Zn-CP shows good electrical conductivity ($8.54 \times 10^{-7} \text{ S m}^{-1}$) at room temperature.

INTRODUCTION

In recent years, metal organic frameworks (MOFs) and co-ordination polymers (CPs) are utilized to fabricate active electronic devices. [1-2] In order to produce the difference in polarity on the surface of such systems, mixed ligand-based CPs are purposefully made so that one of the components is electron rich and the other is electron deficient. In that way, the redox inefficiency of metal nodes may be ignored. Despite being redox inactive, Zn-based coordination systems are typically quite stable and capable of forming long-range crystalline systems. The Zn (II) metal center is capable of designing a wide range of regulated dimensional coordination polymeric systems in the varied coordination atmosphere. Keeping in mind all these facts, we carefully chose electron-rich 4,4' dipyridyl sulphide (4,4'-DPS) and electron-deficient 5-nitroisophthalic acid (5-H₂NIA) ligand systems to co-ordinate with Zn(II) centre and successfully built 2D CP having outstanding crystallinity [3]. SCXRD is used to structurally analyze well-diffracted single crystals, while PXRD is used to confirm the phase purity of the bulk materials. TGA and UV-Vis spectroscopic study are used to support thermal consistency and electronic nature of CP, respectively. It is interesting to note that this material exhibits electrical conductivity at room temperature and in dark conditions when used to manufacture Schottky interface electronic devices. The Schottky character of the metal-semiconductor contact is confirmed by the non-linear rectifying nature of current-voltage. The Zn-CP displays optical band gap 3.71 eV within semiconducting region and exhibits high electrical conductivity ($8.54 \times 10^{-7} \text{ S m}^{-1}$) at ambient temperature.

MATERIALS AND METHODS

A solution of 4,4'-DPS (0.036 g, 0.2 mmol) in Methanol (2 mL) was slowly and carefully layered onto a solution of Zn(NO₃)₂ · 6H₂O (0.060 g, 0.2 mmol) in H₂O (2 mL) using DMF and MeOH (2 mL, 1:1 (v/v)) mixture as buffer followed by layering of 5-H₂NIA (0.042 g, 0.2 mmol) neutralized with Et₃N (0.042 g, 0.4 mmol) in ethanol (2 mL). Then the whole solution was kept undisturbed for a week. The yellowish white, block-shaped crystals of {[Zn(4,4'-



DPS)2(5-HNIA)2(H₂O)]_n} (Zn-CP) were obtained after a week.

RESULTS AND DISCUSSION

The crystal belongs to monoclinic crystal system with space group P 21/c and Z = 4 ; D_x = 1.482 g.cm⁻³, according to X-ray crystallographic data analysis. The distorted pentagonal bipyramidal geometry of the architecture is represented by the ZnO₃N₂ unit (Fig. 1(a)), where 5- nitroisophthalateion (5-HNIA-) acts as monoanionic carboxylate-O bridging agent; one water molecule coordinates and Pyridyl-N of two 4,4'-Dipyridylsulphide (4,4'-DPS) bridges Zn (II). The two ligands function as a two-dimensional network to construct a 2D rectangle framework.

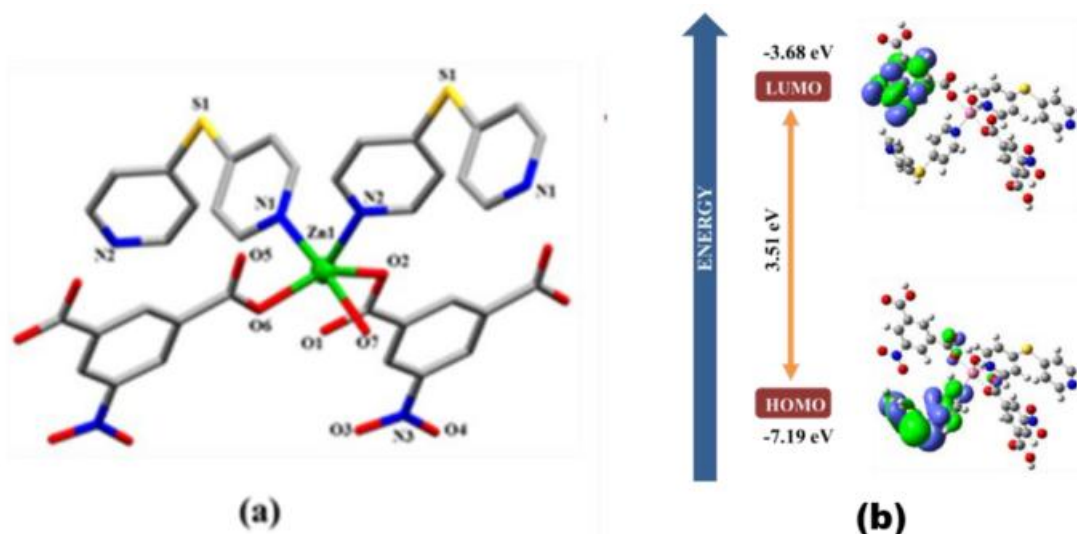


Fig. 1. (a) Coordination environment around Zn(II)-metal of Zn-CP; (b) Schematic representation of HOMO-LUMO gap of Zn-CP obtained from DFT computation.

The geometry of Zn-CP is optimized by DFT computation method by using Single crystal X-ray diffraction coordinates. In DFT computation, a discrete molecular synthon is considered. The energy of frontier molecular orbitals (FMOs) is calculated and the energy gap, (E_{LUMO} (-3.68 eV) – E_{HOMO} (-7.19 eV)) is 3.51 eV and the value is closer to the experimental value (3.71 eV). The Zn-CP displays optical band gap 3.71 eV within semiconducting region and insists for studying the Schottky diode behaviour (Fig. 1(b)). The Zn-CP demonstrates good electrical conductivity at room temperature with the value of $8.54 \times 10^{-7} \text{ S m}^{-1}$. The DC activation energy of the device is found to be $9.05 \times 10^{-19} \text{ eV}$ with the conductivity limit $4.71 (\Omega\text{-m})^{-1}$ having Richardson constant value of $7.07 \times 10^{-10} \text{ Am}^{-2} \text{ K}^{-2}$ which suggest this Zn-CP can be categorized as an n-type material. The temperature-dependent barrier height indicates that the MS-junction has a non-uniform barrier height distribution at 0.87 eV. The device also exhibits good ideality factor of 2.64 and reasonably low series resistance with values of 991 k Ω .



CONCLUSION

In summary, a Zn (II)-coordinated 2D CP using 4,4'-Dipyridylsulphide and 5-Nitroisophthalic acid is structurally characterized. The purity of crystal is confirmed by the PXRD of the as-prepared Zn- CP, which likewise matches the simulated spectrum quite well. At room temperature, the Zn-CP displays good electrical conductivity with the value of $8.54 \times 10^{-7} \text{ S m}^{-1}$. In light of technological considerations in this period of rising energy consumption, the new study may offer a simple route for laboratory-to-land use of such energy materials.

ACKNOWLEDGMENT

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INTERFACIAL ELECTRON RELAY ENGINEERING IN 2D BIOCL NANOPLATES/MWCNT NANOCOMPOSITES FOR ENHANCED PHOTOCATALYTIC DEGRADATION OF ORGANIC DYES

Shreyasi Pal^{1*}, Shibsankar Dutta², Sukanta De³ and Kalyan Kumar Chattopadhyay⁴

¹ Department of Physics, Raidighi College, South 24 Parganas, Diamond Harbour Subdivision, Raidighi, West Bengal, 743383, India

² Ruby Park Public School, P 17, Transport Depot Road Behind Alipore Mint, Kolkata 700088, West Bengal, India

³ Department of Physics, Presidency University, 86/1 College Street, Kolkata, 700073, India

⁴ Thin Films and Nanoscience Laboratory, Department of Physics, Jadavpur University, Kolkata 700032, India.

*E-mail : shreyasi.tua@gmail.com

INTRODUCTION

The rapid discharge of organic dye pollutants from textile and pharmaceutical industries poses a significant threat to environmental sustainability and human health. Dyes such as Rhodamine B (RhB) and Methylene Blue (MB) are chemically stable and resistant to conventional treatment techniques, including biological degradation and adsorption. Semiconductor-based photocatalysis has emerged as an effective and environmentally benign approach for the mineralization of such pollutants.

Bismuth oxychloride (BiOCl), a layered semiconductor with a unique internal electric field arising from alternating $[\text{Bi}_2\text{O}_2]^{2+}$ slabs and halide layers, has shown promise in photocatalytic applications. Its two-dimensional (2D) nanoplate morphology provides a high surface area and abundant active sites. However, its wide bandgap ($\sim 3.2\text{--}3.5$ eV) and rapid electron–hole recombination limit its efficiency.

To address these challenges, coupling BiOCl with conductive carbon materials such as multi-walled carbon nanotubes (MWCNTs) has been proposed. MWCNTs offer high electrical conductivity and act as electron acceptors, facilitating charge separation and transport. Additionally, strong $\pi\text{--}\pi$ interactions enhance dye adsorption, improving photocatalytic performance.

In this work, BiOCl/MWCNT nanocomposites are investigated as efficient photocatalysts for dye degradation, with emphasis on interfacial electron transfer and reactive oxygen species (ROS) generation.

MATERIALS AND METHODS

BiOCl nanoplates were synthesized via a hydrothermal method using bismuth nitrate and chloride precursors. MWCNTs were incorporated in varying weight percentages to form BiOCl/MWCNT nanocomposites through in situ mixing followed by thermal treatment.

Structural characterization was performed using X-ray diffraction (XRD) and electron microscopy techniques



(SEM/TEM). Optical properties were analyzed using UV–Vis diffuse reflectance spectroscopy (DRS) and photoluminescence (PL) spectroscopy. Electrochemical measurements, including photocurrent response and electrochemical impedance spectroscopy (EIS), were conducted to evaluate charge transport properties.

Photocatalytic activity was assessed by degrading RhB and MB under light irradiation. The concentration change was monitored using UV–Vis spectroscopy, and degradation kinetics were analyzed using a pseudo-first-order model:

$$\ln(C_0/C) = kt \quad [1]$$

Radical scavenging experiments and electron paramagnetic resonance (EPR) spectroscopy were used to identify dominant reactive species.

RESULTS AND DISCUSSION

XRD analysis confirmed the formation of highly crystalline tetragonal BiOCl, while electron microscopy revealed well-defined 2D nanoplates integrated with MWCNT networks, indicating strong interfacial contact. The incorporation of MWCNTs did not significantly alter the crystal structure but improved electrical connectivity.

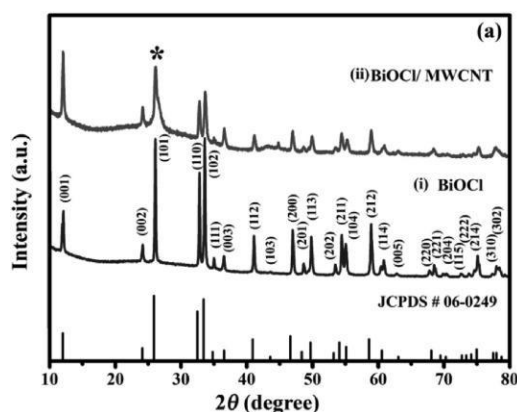


Figure 1. XRD patterns of BiOCl and BiOCl/MWCNT nanocomposites

Field emission scanning electron microscopy (FESEM) analysis (Fig. X) reveals that the pristine BiOCl exhibits well-defined two-dimensional (2D) nanoplate morphology with lateral dimensions in the range of ~0.5–2 μm. These nanoplates appear thin, with smooth surfaces and partial stacking, indicative of anisotropic growth along the crystallographic planes. Upon incorporation of MWCNTs, an interconnected network of entangled nanotubes is observed, uniformly distributed across the BiOCl nanoplates. The nanotubes act as conductive bridges between adjacent plates, preventing excessive agglomeration and promoting intimate interfacial contact.

The photocatalytic performance of BiOCl/MWCNT nanocomposites was evaluated by the degradation of Rhodamine B (RhB) and Methylene Blue (MB) under visible light irradiation ($\lambda \geq 420$ nm). Prior to illumination, the suspension was stirred in the dark to establish adsorption–desorption equilibrium. The degradation process was monitored using UV–Vis spectroscopy, and the kinetics followed a pseudo-first-order model:

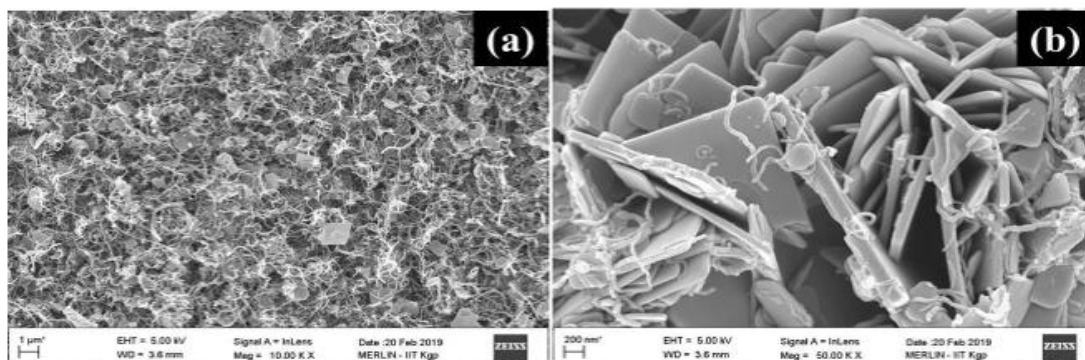


Figure 2. FESEM images of BiOCl/MWCNT nanocomposites.

$$\ln(C_0/C) = kt \quad [1]$$

The BiOCl/MWCNT composites exhibited significantly enhanced activity, showing an approximately 3–4-fold increase in the apparent reaction rate constant compared to pristine BiOCl.

The enhanced performance is attributed to a synergistic mechanism involving dye sensitization and efficient interfacial electron transfer. Under visible light, dye molecules are photoexcited and inject electrons into the conduction band of BiOCl. These electrons are subsequently transferred to MWCNTs, which act as electron acceptors and conductive pathways, thereby suppressing charge recombination. The transferred electrons reduce dissolved oxygen to generate superoxide radicals ($\cdot\text{O}_2^-$), while holes in BiOCl produce hydroxyl radicals ($\cdot\text{OH}$). These reactive oxygen species drive the degradation and mineralization of dye molecules. The formation of a 2D/1D heterostructure enables efficient electron relay and improved photocatalytic efficiency.

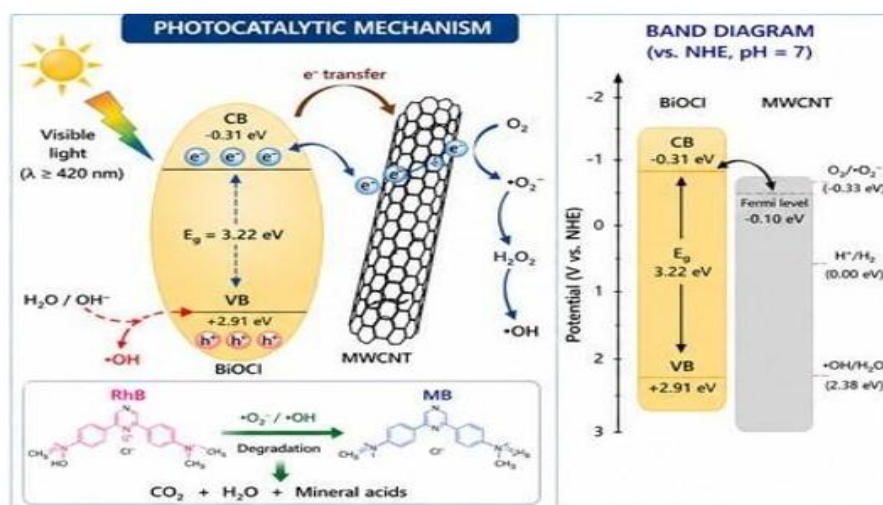


Figure 3. Photocatalytic mechanism and possible band diagram of BiOCl/MWCNT nanocomposites.

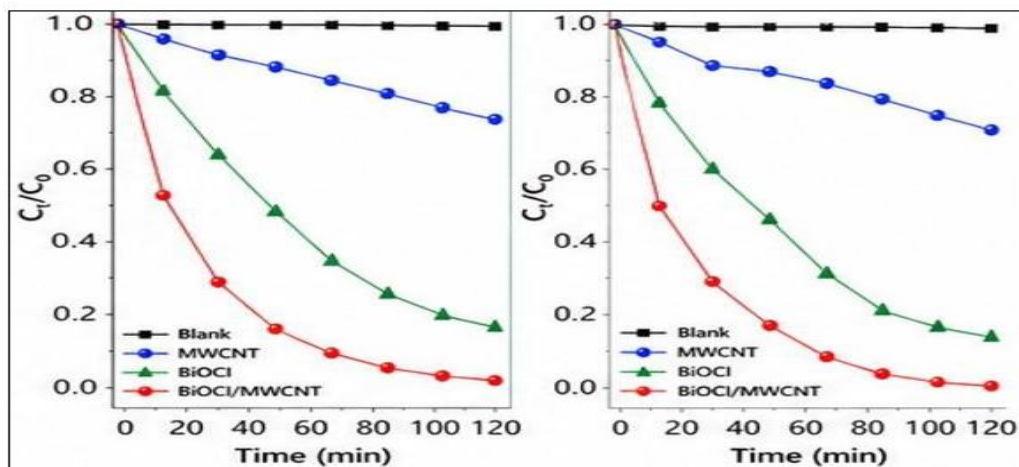


Figure 3. Photocatalytic mechanism and possible band diagram of BiOCl/MWCNT nanocomposites

Photocatalytic studies demonstrated that BiOCl/MWCNT nanocomposites exhibit significantly enhanced degradation efficiency toward RhB and MB compared to pristine BiOCl, with an approximately 3–4-fold increase in the apparent reaction rate constant. The enhanced performance is attributed to efficient charge separation and rapid electron transfer through the MWCNT network.

CONCLUSION

BiOCl/MWCNT nanocomposites demonstrate significantly enhanced photocatalytic performance for the degradation of organic dyes due to improved charge separation and interfacial electron transfer. The MWCNTs act as efficient electron relay channels, facilitating reactive oxygen species generation and accelerating degradation kinetics. This study highlights the importance of interface engineering in designing high-performance photocatalysts for wastewater treatment applications.

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A Short Review Last Five Years Development in Removing Textile Dyes by Copper oxide Nanostructures

Vaishali Chauhan[#], Diptonil Banerjee^{*}

Thin Film and Nanotechnology Laboratory
Department of Applied Sciences (Physics) Faculty
of Engineering
Teerthanker Mahaveer University, Moradabad, UP
244001, India

Abstract:

In the present era, among the different forms of pollutions water pollution may be considered as one of the most acute problems in both the rural and urban area. Water may be polluted by different sources that includes different inorganic heavy metals, large organic molecules, dyes, as well as biological micro-organism threats etc. Of which, one of most dangerous threat, specially in the vicinity of paper or textile industry is different dyes that completely destroy the life cycle of aquatic flora and fauna causing several diseases that may be as deadly as cancer. The dyes from water thus needs to be removed through different processes that includes like coagulation, catalysis, sedimentation, filtration, adsorption, reverse osmosis, ion exchange and many others of which photon induced catalysis has specific importance in terms of its process simplicity and cost effectiveness. Of which photocatalysis is one of the most effective processes to remove the dyes and different oxide systems like TiO₂, CuO, ZnO, V₂O₅ have shown their potentials in removing dyes through photocatalysis. Among this CuO has the further advantages over other regarding its easy and cost-effective synthesis processes.

Keeping this in mind this short article reviews the last few years development in use of CuO as photo-catalyst to remove the textile dyes.

Keyword: Copper oxide, Textile dye, photon, catalysis, nanostructure, Optical band gap

#) E-mail: vc4585611@gmail.com (VC), Research Scholar (Presentation Author),
drdiptonil.engineering@tmu.ac.in (DB) Corresponding author;

Introduction:

Any technical advancement in the present era of civilisation may be said to broadly address two issues: energy and the environment. It would not be incorrect to state that success in one area always comes at the expense of the other. For example, the careless use of fossil fuels causes issues with CO₂ emissions, the greenhouse effect, and global warming, yet when alternative green energy sources are prioritised, the system begins to struggle with efficiency. Pollution has always been a serious issue in growing nations like India, particularly when it comes to water pollution. Among the different form of water pollution and its subsequent remedial the most prominent name that comes in mind, respectively are textile dyes and photocatalysis as well as adsorption. It is now well established that different oxide systems like TiO₂, CuO, ZnO, V₂O₅ have shown their potentials in removing dyes through photocatalysis.



Among this CuO has the further advantages over other regarding its easy and cost-effective synthesis processes [1, 2]. Copper oxide may be formed in two different ways i.e. cupric oxide (CuO) and cuprous oxide (Cu₂O)

Copper (I) oxide melts at a little lower but still high temperature than copper (II) oxide, which has a high melting point of around 1,300 °C. Due to their practical insolubility non water, both substances are stable in a variety of watery conditions. In terms of chemistry, copper oxides stand out for being amphoteric, which means they may react with both strong bases and acids. They can react with concentrated alkaline solutions to generate complex ions, but they will easily dissolve in strong acids to form copper salts. Moreover, both types of copper oxide serve as semiconductor materials. Specifically, cuprous oxide exhibits a narrow band gap that controls its electrical behaviour. This work develops a mini review mainly focussing on the performance of copper oxide based nanostructures in removing textile dyes through the process of photocatalysis. Mainly work in the duration of last few years have been considered [3]

Basic Mechanism of Photocatalysis

The process of photocatalysis consists of several steps where the suitable semiconductor (here copper oxide) absorbs light to catalyse the removal process. Photon incident generates electron-hole pairs that remains at the edges of the conduction and valence bands respectively. These generated electron-hole pairs interact with surrounding media to produce reactive radicals which initiate the dye degradation process converting them into harmless water and carbon di oxide. Here, the activation of the catalysis depends upon the optical band gap of the material which determines whether the catalyst will be activated in the visible light or under UV radiation. Fig.1 shows the schematics of the process along with different steps

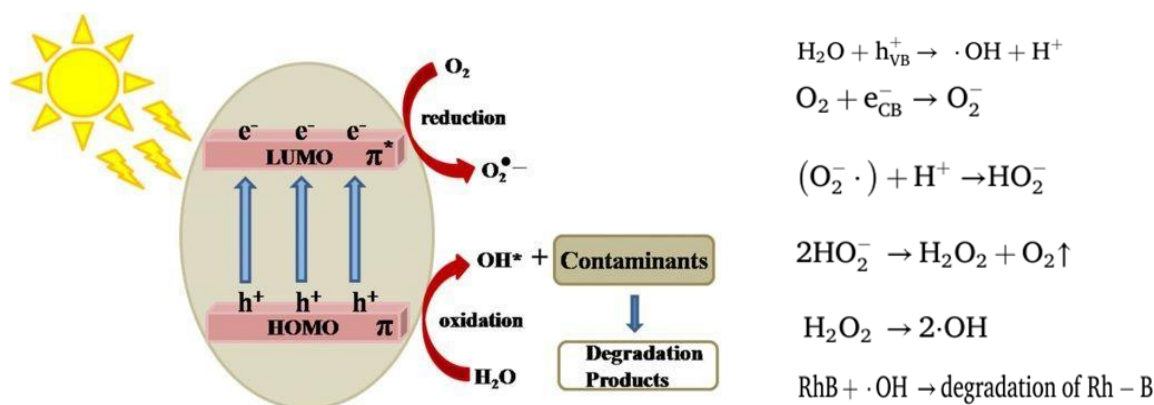


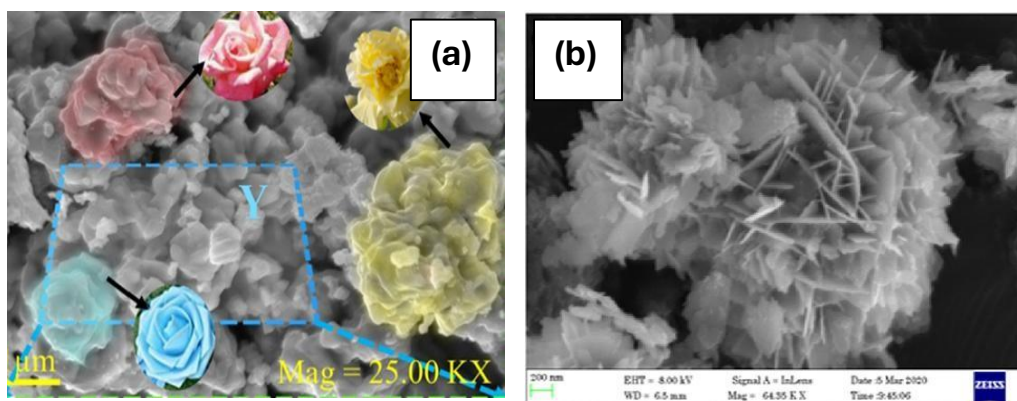
Fig.1.: Schematic diagram of photocatalysis dye degradation mechanism



Copper oxide as photocatalyst

In the year of 2021, Fekri et al. reported visible-light induced photocatalytic removal of methylene blue by copper oxide decorated zinc oxide nanorods [4]. They found that under suitable condition the material can remove around 100 % dye within a time interval of 45 minutes. In the next year 2022 Hilkart et al. reported the removal of congo dye by CuO-ZnO hybrid with efficiency more than 95 % within 50 minutes [5]. The same dye was removed by pure CuO nanoparticles with efficiency over 85 % in the time period of 75 minutes as shown by Sidra et al. in the same year 2022 [6]. A nice flower-like morphology of CuO was developed by Kaur et al. (shown in **Fig.2 a**) which found application in removing dyes like RY-86 and RO-4 with efficiency more than 95 % [7].

Fig.2: (a) Flower-like CuO nanostructure and (b) CuO decorated over ZnO rod-like nanostructures



Ternary system consisting of CuO/ZnO and graphene as efficient photocatalyst was developed by Rajapaksha et al. that was capable of removing numbers of dyes but the removal was mainly by adsorption rather than photocatalysis [8]. Another binary oxide-based (CuO-NiO) catalyst was developed by Ahsan et al. [9]. They have shown that at optimum concentration RR-2, RB-5, and OII dyes, NiO-NPs degraded 90, 82 and 83%, CuO-NPs degraded 49, 34, and 44%, whereas the nanocomposite NiO/CuO-NC degraded 92, 93, and 96% of the said dyes respectively. Shanmugam et al. in the next year of 2023 reported the development CuO decorated ZnO rod-like nanostructures (**Fig.2 b**) to remove methylene blue with efficiency more than 98 % [10]. Very recently Yousefzadeh and group reported the photocatalytic degradation of water-soluble organic pollutants in aqueous solution by thulium copper oxide nanostructures [11]. In their case the targeted dye was erythrosine and removal efficiency was 100 % just within 35 minutes. However, all these reports are lab scale only and there exists challenges in converting its utility in real industry scale.

Conclusions

This mini review discusses the performance of copper oxide-based nanostructures in removing textile dyes that include both cationic as well as anionic. It has been shown that as per the various reports in the recent times came from the different workers in the last few years CuO has shown promising efficiency in removing textile dyes. The efficiency sometimes reaches even above 95 % within a time interval of just 30 minutes. In maximum instances the reaction kinetics mainly followed the 1st order mechanism. The review work also concludes that though CuO shows good performance in laboratory scale but its industry scale test is yet to be taken



which is the biggest challenge in implementing the material in large scale.

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Oral Presentation – OP-01

Arsenic Mobilization in Aquifers and its Implications on Groundwater Safety

Sathi Das

Molecular Biology and Biotechnology (MBBT), Sripat Singh College

*-Corresponding author email: sathid56432@gmail.com

Abstract

Arsenic contamination in groundwater of the Bengal Delta Plain (BDP) poses a severe environmental and public health concern due to its widespread occurrence and adverse effects. The study investigates the hydrogeochemical behaviour of arsenic in shallow aquifers of the Chakdah block, Nadia District, India, with specific emphasis on its reason for mobilization, controlling factors, and very close correlation with coliform contamination and its causal biological agent: FeRB and DARPS. Groundwater samples collected from multiple sites were analysed for their physicochemical parameters, dissolved ions concentration (specifically- concentration of Total arsenic (AsT)), and coliform bacteria. The findings from the study revealed elevated levels of arsenic concentrations ranging from (0.069–0.178 mgL⁻¹) (Mean: 0.119 mgL⁻¹), significantly exceeding recommended drinking water limits. A clear depth- dependent trend was observed, with higher arsenic levels in shallow aquifers, indicating strong control of anoxic conditions of groundwater. The groundwater which is predominantly characterized by its reductive environment, where arsenic mobilization is more dominant due to reduction of iron oxyhydroxides which releases arsenic in its Arsenate form As(V) in the water increasing concentration of free arsenic and that again on reduction by the groundwater turns into more mobile As; Arsenite As(III). High bicarbonate levels further support active geochemical processes facilitating arsenic release. Microbial contamination, including total and fecal coliforms was detected across all sites- particularly in wells located near surface water bodies and sanitation sources. While the correlation between arsenic concentration and microbial indicators is moderate, the coexistence of these contaminants suggests that microbial activity may indirectly influence arsenic mobilization through organic matter degradation and reduction of iron oxyhydroxides. Sanitary risk assessment classified most drinking water sources (aquifers) as high to very high risk (83.3% of all sourced samples from tubewells across Chakdah block), emphasizing role of anthropogenic factors as the main reason for groundwater vulnerability.

Keywords: Groundwater, Arsenic, Coliform, Sanitary Risk, Anthropogenic Factors.



Oral Presentation – OP-02

Paper-Based Flexible Pressure Sensor Using Aligned Carbon Nanotubes (aCNT)

Bipul Maity¹, Ayan Saha², Sudip Shau³, Souvik Dey⁴

Department of Electronics and Communication Engineering, Dr. Sudhir Chandra Sur Institute of
Technology and Sports Complex,

540, Dum Dum, Surer Math, Kolkata - 700074

E-mail: bipulmaity12345@gmail.com

INTRODUCTION

Flexible pressure sensors are becoming very important for applications like wearable devices, electronic skin, and health monitoring. Traditional rigid sensors cannot adapt to curved or moving surfaces, which makes them less suitable for such uses. To solve this problem, paper-based substrates are being explored because they are low-cost, flexible, and environmentally friendly. They also support easy and large-scale fabrication. Carbon nanotubes (CNTs) are commonly used in flexible sensors due to their excellent electrical conductivity and sensitivity to pressure. However, when CNTs are randomly distributed, the performance is not optimal because the electron flow becomes inefficient. To improve this, aligned carbon nanotubes (aCNTs) are used. In this structure, the nanotubes are arranged in a single direction, which allows better electron transport and higher sensitivity. In this work, a paper-based flexible pressure sensor using aligned CNTs is developed, aiming to achieve a low-cost, highly sensitive, and real-time sensing solution for wearable health monitoring applications.

MATERIALS AND METHODS

Multi-walled carbon nanotubes (MWCNTs, purity > 95%) were procured commercially and functionalized via acid treatment ($\text{H}_2\text{SO}_4:\text{HNO}_3 = 3:1$) to introduce carboxyl groups for improved dispersion. An aCNT ink was formulated by dispersing functionalized MWCNTs (2 mg/mL) in an aqueous surfactant solution (0.5 wt% sodium dodecyl sulfate) using probe sonication (500 W, 30 min, ice bath). Alignment was achieved through a shear-coating process on A4 cellulose paper (80 g/m²) using a customized doctor-blade at a controlled velocity of 5 mm/s, which imparted hydrodynamic shear forces sufficient to orient CNTs parallel to the coating direction. The coated papers were dried at 60°C for 2 h. Finally, conductive silver electrodes were applied on both sides to complete the sensor structure, with an active sensing area of 1 cm × 1 cm. The alignment of carbon nanotubes was analyzed using standard characterisation techniques. The electrical performance of the sensor was evaluated by measuring its resistance. Pressure was applied using a motorized universal testing machine (UTM) in the range of 0.1 Pa to 50 kPa. The sensitivity of the sensor was determined based on the change in resistance with respect to the applied pressure. Cycling durability was tested at 10 kPa over 5000 loading–unloading cycles.

RESULTS AND DISCUSSION

From the usual SEM imaging confirmed a high degree of CNT alignment along the shear-coating direction, with an angular distribution of $\pm 12^\circ$ relative to the coating axis. Further analysis also confirmed that the nanotubes were properly aligned. The baseline resistance of the aCNT layer was 1.8 k Ω , compared to 8.5 k Ω for a randomly oriented CNT film of equivalent loading, reflecting the enhanced percolation efficiency of aligned structures. The aCNT pressure sensor demonstrated a sensitivity of 12.6 kPa⁻¹ in the low-pressure regime (0.1–1 kPa) and 1.4 kPa⁻¹ in the mid-pressure regime (1–50 kPa), with a limit of detection

(LOD) of 0.5 Pa. The high sensitivity at sub-kPa pressures is attributed to the progressive



reconnection of aligned CNT junctions under compression, amplifying the change in percolation pathways. Response and recovery times were 85 ms and 110 ms respectively, suitable for dynamic physiological signals.

Table 1. Performance comparison of the aCNT paper sensor with literature values.

Sensor Type	Substrate	Sensitivity (kPa ⁻¹)	LOD (Pa)
aCNT (This work)	Paper	12.6	0.5
rCNT/PDMS	PDMS	3.8	5
Graphene/PET	PET film	5.2	10
MXene/paper	Paper	7.4	1.2

rCNT: randomly oriented CNT; LOD: limit of detection

The durability test revealed less than 4.2% variation in sensitivity after 5000 loading–unloading cycles at 10 kPa, indicating robust aCNT adhesion within the paper fiber network. A humidity sensitivity test (30–90% RH) showed a resistance drift of 6.3%, which was mitigated by applying a thin polydimethylsiloxane (PDMS) encapsulation layer, reducing drift to below 2%. As a proof-of-concept wearable application, the sensor was laminated on the wrist and successfully captured radial pulse waveforms at 72 bpm, resolving distinct features including the percussion wave, tidal wave, and dicrotic notch.

CONCLUSION

A paper-based flexible pressure sensor incorporating shear-aligned carbon nanotube (aCNT) active layers was successfully demonstrated[1]. The alignment strategy resulted in a 3.3-fold reduction in baseline resistance and a sensitivity of 12.6 kPa⁻¹ with an LOD of 0.5 Pa, outperforming randomly oriented CNT counterparts[2]. The sensor exhibited fast response (85 ms), excellent durability over 5000 cycles, and reliable pulse waveform acquisition on human skin[3]. The combination of an eco-friendly paper substrate, scalable shear-coating fabrication, and high-performance aCNT sensing establishes this approach as a promising platform for next-generation low-cost wearable health monitoring devices[4]. The proposed sensor shows strong potential for future integration in smart wearable and IoT-based healthcare systems.

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The authors would like to express their sincere appreciation to the Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, for their support in carrying out this work.

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Oral Presentation – OP-03

Defect Engineering in Oxide Thin Films for Enhanced Resistive Switching PerformanceSrija Hazra¹, Aneek Banik², Sudip Saha³, Akash Mondal⁴, Aryan Roy⁵, Soumajit Maity⁶ - (DS)

Department of CSE Data Science, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,

540, Dum Dum, Surer Math, Kolkata – 700074

E-mail: akashmonda8574@gmail.com**INTRODUCTION**

The rapid growth of AI and IoT technologies requires non-volatile memory solutions that surpass the limits of conventional Flash. Resistive random-access memory (RRAM) has emerged as a promising, scalable, and energy-efficient platform. Its core mechanism involves the voltage-driven formation and dissolution of conductive filaments within an oxide layer. However, RRAM faces significant hurdles such as high device variability and poor data retention at high temperatures. To combat these issues, defect engineering has become the most impactful strategy between 2023 and 2025. This approach includes techniques like nitrogen ion implantation and interfacial tungsten doping. By manipulating oxygen vacancy density, researchers can better control the percolation pathways of filaments. This report specifically investigates tantalum oxide (TaO_x) thin films engineered via heterogeneous stacking. The goal is to provide a robust solution that stabilizes switching performance across multiple cycles. Ultimately, these advancements aim to benchmark engineered RRAM against current state-of-the-art memory results.

MATERIALS AND METHODS

Tantalum oxide (TaO₂) thin films (~15nm) were deposited on TiN/SiO₂/Si substrates using reactive RF magnetron sputtering. The process utilized a high-purity Ta target in an Ar/O₂ atmosphere with a 4:1 flow ratio at 5×10^{-7} Torr. Precise oxygen stoichiometry was controlled to achieve sub-stoichiometric compositions, as verified by Rutherford Backscattering Spectrometry (RBS). Nitrogen implantation (N⁺, 5 keV) was then performed at doses between 1×10^{14} and 5×10^{15} cm⁻² to introduce controlled trap states. To enhance performance, a 1nm tungsten (W) seed layer was inserted, and heterogeneous TaO₂/HfO₂ stacks were fabricated via ALD. Top electrodes of TiN (50nm) were patterned into circular cells of varying diameters (2μm to 10 μm) using lift-off lithography. Electrical characterization included DC quasi-static I-V sweeps, pulsed endurance cycling, and high-temperature retention baking at 150° C. Finally, multi-level cell (MLC) programming was executed using ISPV algorithms on a Keysight B1500A analyzer.

RESULTS AND DISCUSSION

XPS deconvolution of the Ta 4f spectra reveals that nitrogen implantation at a dose of (1×10^{15} cm⁻²) reduces the oxygen vacancy concentration by ~35% compared to pristine TaO_x, while simultaneously introducing N–Ta–O bonding configurations that act as shallow trap sites. The W:TaO_x bilayer devices show an ultrathin (~1.2 nm) interfacial WO_x layer formed spontaneously during thermal budget, which serves as a controlled nucleation site for the conductive filament, drastically suppressing random CF nucleation variability



Oral Presentation – OP-04

Low Power Resistive Switching Devices for Artificial Intelligence HardwareSudhansu Tudu¹, Md Mobinul Islam², Sanu Mondal³, Susmita Halder⁴, Anushree Mondal⁵, Soumili Das⁶

Department of Computer Science & Engineering (Cybersecurity & Data Science),

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,

540, Dum Dum, Surer Math, Kolkata – 700074

E-mail: sudhansutudu45000@gmail.com

INTRODUCTION

In the current big data era, the exponential growth of data-intensive tasks has exposed the limitations of traditional Von Neumann computing. The physical separation of memory and processing unit results in the “memory wall,” where significant energy is consumed by data movement. To address this, Resistive Switching (RS) devices have gained significant attention for neuromorphic computing. These devices facilitate In-Memory Computing (IMC), allowing for high-speed, parallel processing with significantly reduced power consumption.

MATERIALS AND METHODS

The resistive switching behavior is investigated in Metal-Insulator-Metal (MIM) configurations. Transition metal oxides (e.g., HfO₂, TiO₂, Ta₂O₅) and perovskite oxides (e.g., PCMO) are selected for their reliable switching and CMOS compatibility. Synthesis methods range from Physical Vapor Deposition (PVD) to low-cost solution-based processing. Electrical characterization is performed using DC voltage sweeps to evaluate the device’s ability to transition between High Resistance States (HRS) and Low Resistance States (LRS).

RESULTS AND DISCUSSION

The switching mechanism is primarily attributed to the formation and rupture of conductive filaments. Under an applied electric field, ion migration creates a path for electron transport. For AI applications, achieving “analog” switching is vital to represent synaptic weights.

Figure 1. Illustrates the typical hysteric I-V behavior required for these operations.

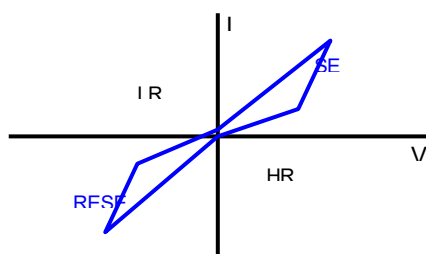


Figure 1. Typical bipolar resistive switching characteristics illustrating LRS and HRS.

Low power consumption is achieved by optimizing the SET/RESET voltages and limiting the compliance current to the nano-ampere range. This enables switching energies in the picojoule range, crucial for portable edge-AI devices. Table 1 summarizes the performance matrices of common RS materials.

Material Layer	Switching Type	Power Level	Target AI Task
HfO _x	Bipolar	Low	Image Recognition
Perovskite Oxide	Analog	Ultra-Low	Neuromorphic Computing
TaO _x	Bipolar	Low	Data Storage / Logic

Table 1. Performance matrices of common RS materials.



CONCLUSION

Resistive switching devices provide a promising path toward high-efficiency AI hardware. By integrating memory and processing, these devices bypass the energy-intensive data transfer of conventional architectures. Materials like HfOX and perovskites offer the stability and low-power operation required for scalable synaptic arrays. Future research should focus on minimizing device-to-device variability.

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The authors would like to express their sincere appreciation to the Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, for their support in carrying out this work.

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Oral Presentation – OP-05

Comparative Reliability Analysis of Bifacial Photovoltaic Modules: Glass-Glass vs Glass-Transparent Backsheet PerformanceShraboni Kundu¹, Partha Sarathi Ghosh¹, Debjit Misra¹, and Sugato Ghosh^{1*}¹JIS Institute of Advanced Studies and Research, JIS University, Kolkata

E-mail: shraboni.kundu1986@gmail.com

INTRODUCTION

In today's world, cost savings with the highest enhanced performance are prioritized in every sector, so in PV technologies, awareness and interest are focused on making PV modules in such a way to harvest sunlight from both front and rear sides as a bifacial module to keep the concern of effective efficiency to cost ratio [1]. The architecture of a bifacial module is similar to that of a monofacial module. However, the rear side is designed with either glass or a transparent backsheet, allowing reflected light to pass through while ensuring transparency and durability. Initial performance results of these bifacial modules are promising. However, uncertainties remain regarding their long-term reliability, particularly under varying environmental conditions such as UV exposure, humidity, and temperature fluctuations [2]. Therefore, the concern the main is to build the reliability strengths and weakness of this new technology. Between these two constructions, glass/glass modules have an impact on long term performance because of low moisture ingress, symmetrical sandwich of solar cell string whether glass/transparent backsheet modules give better electrical performance, heat dissipation property, light weight, low cost and easy maintenance [3]. So this current study is motivated by the industry's predominant adoption of glass-glass bifacial modules, largely due to concerns about long-term transparency retention, which remains a key challenge for glass/transparent backsheet bifacial modules. Accordingly, this paper presents a comparative reliability assessment of glass-glass and glass/transparent backsheet bifacial modules.

**Figure 1. Installation of Bifacial modules****MATERIALS AND METHODS**

Electrical performance for potential induced degradation is carried out for both G/G and G/TB bifacial modules. To perform PID test some pre-test measurements such as visual inspection, electroluminescence was done for visual defect, microcrack and inactive region. After PID cycle similar post test was also done in order to assess any degradation or performance changes in the module. As per the prescribed method, the test conditions are maintained at a module temperature of 85 ± 2 °C and a relative humidity of $85 \pm 5\%$, with a test duration of 96 hours. During this period, an applied potential of -1500 V DC is imposed to induce potential-induced degradation (PID).

RESULTS AND DISCUSSION

Glass/transparent bifacial modules are promising due to their lighter weight. As shown in Fig. 2, these modules operate at a lower average temperature than glass/glass bifacial modules, which leads to improved efficiency. The lower temperature results in a higher open-circuit voltage (VOC), thereby increasing the overall power output [2]. Besides that, it is checked to validate sustainability under harsh environmental conditions by performing a potential-induced degradation (PID) test result in table 1 shows that both module can pass the module level testing according to IEC standard and provide 25-30 years of service. But the chances of moisture ingress are still under observation in glass/transparent bifacial modules, whereas glass/glass bifacial modules have very little chance of moisture ingress.



Table 1. Comparison of PID data for glass/glass and glass/transparent backsheet bifacial module

Module	P _{max} [W]	FF	V _{oc} [V]	I _{sc} [A]	V _{mp} [V]	I _{mp} [A]	Degradation %
G/TB	438.409	0.84	48.36	10.77	42.2	10.39	0.2
G/G	578.138	0.81	52.754	13.504	45.507	12.704	0.07

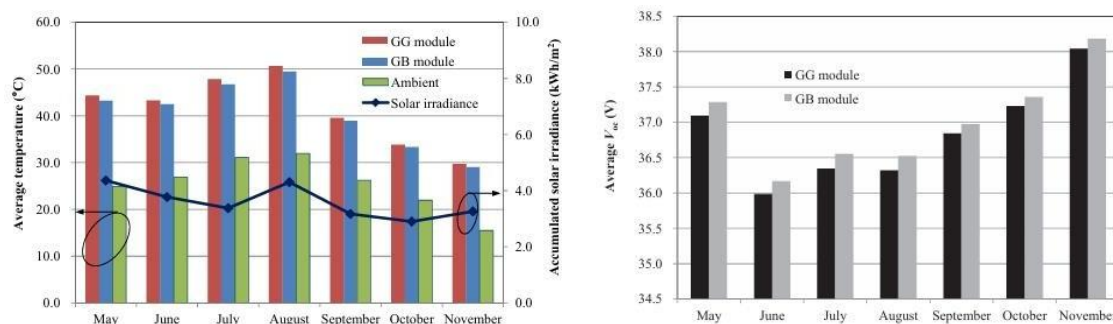


Figure 2. Average temperature and average Voc of g/g and g/tb modules

CONCLUSION

The long-term durability of the glass/transparent backsheet bifacial module was compared with that of the glass/glass bifacial module by conducting an extended cycle test according to the IEC standard. Further testing for more than 96 hours can mitigate the moisture ingress behavior of the glass/transparent backsheet, which can help the industry gain acceptance. Less degradation percentage for glass/glass bifacial module is observed, however in case of glass/transparent backsheet gain in VOC is profound because of low module temperature.

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Oral Presentation – OP-06

Nanostructured Materials for Artificial Synapse Devices in Neuromorphic Computing

Rupak Ghosh, Akash Tarafdar, Sagnik Sarma, Somnath Karmakar, Jyoti Paul

Dr. Sudhir Chandra Sur Institute of Technology & Sports Complex

E mail: rupakghosh2006@gmail.com

INTRODUCTION

Nanostructured materials are essential for artificial synapse devices in neuromorphic computing, which aims to mimic the human brain's efficient and low-power information processing. These materials enable synaptic behaviours like memory and learning by changing their electrical properties in response to stimuli. As a result, they help develop faster, energy-efficient systems for artificial intelligence and advanced computing.

MATERIALS AND METHODS

Different categories of nanostructured materials are widely used in artificial synapse devices. Such as,

- Oxide-Based Nanomaterials [Examples: Titanium dioxide, tantalum oxide.]
- Two-Dimensional (2D) Materials [Examples: Graphene, hexagonal boron nitride.]
- Phase-Change Nanomaterials [Example: GST ($\text{Ge}_2\text{Sb}_2\text{Te}_5$).]
- Organic/Polymeric Nanostructures [Examples: PEDOT: PSS, conjugated polymers.]
- Perovskite Nanostructures [Example: MAPbI_3 .]
- Synaptic Behaviours Achieved

These materials allow artificial synapses to achieve important biological-like behaviours, including short-term and long-term plasticity, spike-timing-dependent plasticity (STDP), facilitation, and depression. Such functions are necessary for adaptive learning and intelligent computation.

RESULTS AND DISCUSSION

Nanostructured artificial synapse devices show strong potential for neuromorphic computing due to their scalability, low power use, and adaptive learning ability. Memristors and ECRAM provide efficient analog control, while ferroelectric and optogenetic devices expand functionality in advanced applications. These systems are effective in AI, robotics, biomedical engineering, and energy-efficient computing. Despite challenges such as variability and endurance limits, innovations like 3D stacking and hybrid materials continue to improve performance. Future trends, including spiking neural networks and crossbar arrays, indicate significant progress toward practical large-scale deployment.

Device Type	Key Advantage	Main Application
Memristors	Scalability	Neural networks
ECRAM	Analog precision	Learning systems
Ferroelectric Devices	Reliable switching	Memory functions
Optogenetic Synapses	Light integration	Hybrid computing

CONCLUSION

Nanostructured materials enable artificial synapse devices to emulate brain-like learning through tunable electrical properties and multi-level states.

Like a bird's brain that adapts quickly during flight, these systems support dynamic, real-time learning, while traditional computers (like drones) rely on fixed instructions.

They offer high switching speed, low power consumption, and scalability for dense neuromorphic architectures.

However, challenges such as device variability, endurance limits, and CMOS integration still require further research.



Overall, they are a promising foundation for next-generation, energy-efficient, and adaptive computing systems.

ACKNOWLEDGMENT

The authors would like to express their sincere appreciation to the Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, for their support in carrying out this work.

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Oral Presentation – OP-07

Lamellar-Templated Ultrathin CuInSe₂ Nanoplatelets as Heavy-Metal-Free 2D Emitters for Bioimaging

Bikram Das,^{1,¶} Farhin Islam,^{1,¶} Amarnath Pal,¹ Uttam Pal,² Sourik Dutta,¹ Shubhasis Haldar,^{1,2} Rajib Kumar Mitra,^{1,2,*} Tanusri Saha-Dasgupta,^{2,3,*} Ali Hossain Khan^{1,2,*}

¹Department of Chemical and Biological Sciences, S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700106, India;

²Technical Research Centre, S. N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700106, India;

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

E-mail : alikhan@bose.res.in

INTRODUCTION

Colloidal semiconductor nanocrystals (NCs) are promising for next-generation optoelectronic and photonic technologies due to their tunable properties governed by quantum confinement. However, widely studied Cd- and Pb-based systems raise toxicity concerns, motivating the development of heavy-metal-free alternatives. Ternary I–III–VI semiconductors, particularly CuInSe₂ (CISE), offer attractive features including a direct band gap, strong absorption, and a large excitonic Bohr radius, enabling efficient and tunable optical responses.

In addition to size and composition, shape control provides a powerful route to tailor NC properties. Two-dimensional nanoplatelets (NPLs), with confinement along the thickness direction, exhibit narrow emission linewidths and enhanced excitonic behavior. Despite these advantages, CISE NPLs remain largely unexplored due to synthetic challenges associated with multicomponent systems and defect formation.

Here, we demonstrate a ligand-directed synthesis of ultrathin CISE NPLs and establish their structure–property relationships, highlighting their potential as efficient, heavy-metal-free emitters for optoelectronic and bioimaging applications.

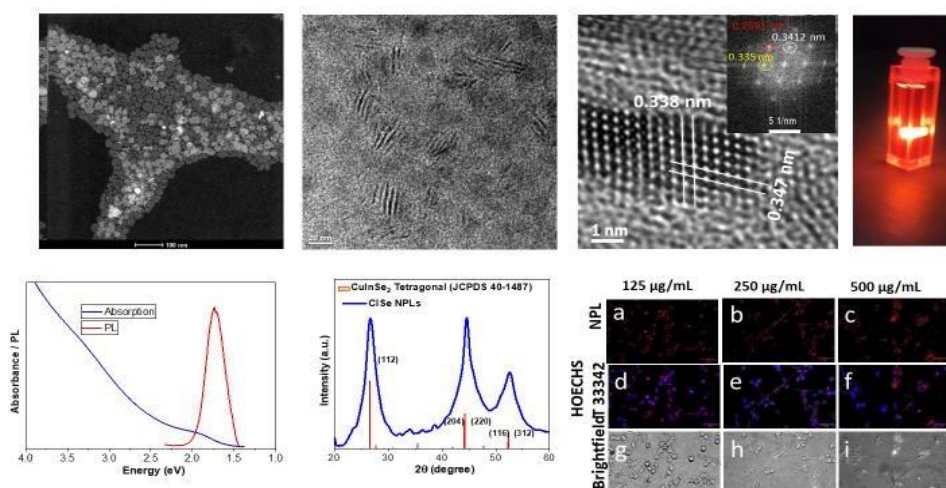
MATERIALS AND METHODS

CuInSe₂ (CISE) nanoplatelets were synthesized using a colloidal solution-phase approach. Copper, indium, and selenium precursors were combined in a reaction flask, followed by the addition of coordinating ligands such as oleylamine and a thiol-based ligand. The mixture was degassed to remove oxygen and moisture, resulting in a homogeneous solution. Subsequently, the reaction was carried out under an inert atmosphere with continuous stirring to promote nucleation and anisotropic growth of the nanoplatelets. After completion of the reaction, the mixture was allowed to cool to ambient conditions. The resulting nanocrystals were isolated by centrifugation and purified through repeated washing using a nonpolar solvent and a polar antisolvent to remove unreacted species and excess ligands. Finally, the purified nanoplatelets were redispersed in a suitable nonpolar solvent for further characterization and storage.

RESULTS AND DISCUSSION

Ultrathin CuInSe₂ (CISE) nanoplatelets (NPLs) were successfully synthesized via a ligand-directed, lamellar-templated growth mechanism, yielding uniform quasi-2D nanodiscs with ~2 nm thickness and ~24 nm lateral dimensions. Structural analyses (XRD, TEM, SAED) confirm a single-crystalline tetragonal chalcopyrite phase with preferential {112} facet exposure and high compositional purity. The formation of NPLs is governed by a transient oleylamine/dodecanethiol lamellar mesophase, which acts as a soft template for anisotropic growth.

Optical studies reveal sharp band-edge emission (FWHM ~0.26 eV) and significantly faster radiative recombination compared to CISE quantum dots, attributed to strong quasi-2D quantum confinement and enhanced excitonic coherence. Density functional theory calculations further show that confinement modifies conduction band dispersion and carrier localization, explaining the observed optical behavior.



ZnS shell passivation enhances photoluminescence efficiency (~51%) and stability, while ligand exchange enables water dispersibility without degrading optical properties. The resulting NPLs exhibit efficient cellular uptake and low cytotoxicity, highlighting their potential as biocompatible, heavy-metal-free emitters.

CONCLUSION

In summary, we report a ligand-templated colloidal strategy for the synthesis of ultrathin CuInSe₂ nanoplalelets via a lamellar intermediate. The resulting quasi-2D nanostructures exhibit high crystallinity, preferential {112} facet exposure, and distinct optical properties arising from strong quantum confinement. Compared to quantum dots, the NPLs show narrower emission and faster radiative recombination. ZnS shell passivation significantly enhances photoluminescence efficiency and stability, while ligand exchange enables aqueous dispersibility and biocompatibility. The CISE/ZnS NPLs demonstrate efficient cellular uptake with low cytotoxicity, highlighting their potential as heavy-metal-free emitters for optoelectronic and bioimaging applications. This work also establishes lamellar templating as a general strategy for designing anisotropic multinary nanocrystals.

ACKNOWLEDGMENT

The authors acknowledge also establishes lamellar templating as a general strategy for designing anisotropic multinary nanocrystals.

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Oral Presentation – OP-08

Perovskite Oxide Electrocatalysts for Electrochemical Water Splitting and Green Hydrogen Production

Uday Chowdhury , Sayan Roy, Rajdeep Bhowmik , Pritam Gain, Raja Kumar Sharma , Agnibha Mukharjee

Department of Computer Science and Engineering,
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,
540, Dum Dum, Surer math, Kolkata - 700074
E-mail: chowdhury1uday@gmail.com

INTRODUCTION

The increasing global energy demand and environmental concerns have driven the search for sustainable and clean energy sources. Green hydrogen production through electrochemical water splitting is considered a promising solution. However, the efficiency of water splitting largely depends on the performance of electrocatalysts. Perovskite oxide materials, with the general formula ABO_3 , have gained significant attention due to their excellent catalytic activity, structural flexibility, and cost-effectiveness compared to noble metal catalysts. This study focuses on the role of perovskite oxide electrocatalysts in enhancing the efficiency of hydrogen production through water splitting, highlighting their advantages, challenges, and future potential.

MATERIALS AND METHODS

Perovskite oxide catalysts were synthesized using methods such as sol-gel, hydrothermal, and solid-state reactions. The structural and morphological properties were analyzed using techniques like X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Electrochemical measurements, including cyclic voltammetry (CV) and linear sweep voltammetry (LSV), were carried out to evaluate catalytic performance. The oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) activities were studied in alkaline and acidic media.

RESULTS AND DISCUSSION

The results indicate that perovskite oxides exhibit high catalytic activity due to their tunable electronic structure and oxygen vacancy formation. Substitution at A-site and B-site significantly improves conductivity and catalytic efficiency. The OER performance was enhanced by optimizing transition metal ions such as Co, Fe, and Ni. Similarly, HER activity showed improvement with defect engineering and surface modification.

Table 1. Performance comparison of different perovskite catalysts

Catalyst	OER Activity	HER Activity	Stability
LaCoO ₃	High	Moderate	Good
SrFeO ₃	Moderate	High	Excellent
BaNiO ₃	High	High	Very Good

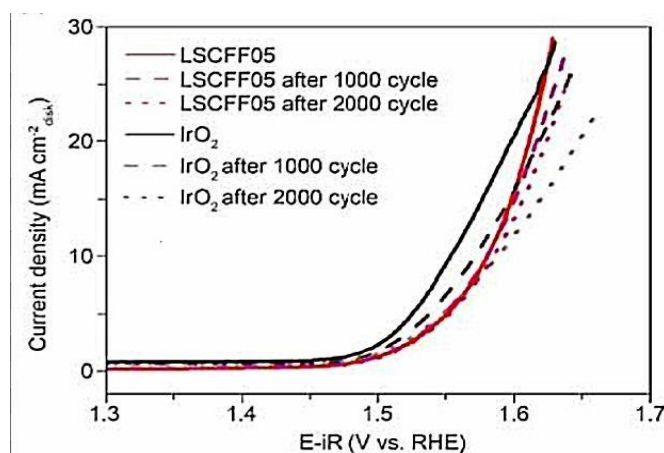


Figure 1. Electrochemical performance of perovskite catalysts in water splitting



CONCLUSION

Perovskite oxide electrocatalysts demonstrate great potential for efficient and cost-effective green hydrogen production. Their tunable structure allows optimization for both OER and HER processes. However, challenges such as long-term stability and scalability remain. Future research should focus on improving durability and developing hybrid materials for enhanced performance.

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Oral Presentation – OP-09

Enhancing Catalytic Activity of Titanium Dioxide Nanoparticles by Various Synthesis Methods

Ratna Sarkar¹, Aaishiki Saha², Sourav Sarkar², Kalyan Kumar Chattopadhyay¹

¹Department of Physics, Jadavpur University, Kolkata, 700032, India

²School of Materials Science and Nanotechnology, Jadavpur University, Kolkata, 700032, India

Email: ratnasarkar60@gmail.com

INTRODUCTION

Titanium dioxide (TiO₂) [1-3] nanoparticle sample was exhibiting with highly crystalline structure and exposed facets (101) have been synthesised by various technique. Several sophisticated techniques were used to characterise as-synthesised TiO₂ samples for detailed analysis of phase formation, chemical bonds, composition, morphology, and other characteristics. The phases, morphology, and photocatalytic activity of the sample were compared by varying the synthesis temperature and duration. Light absorption by a solid material can trigger a photocatalytic reaction [4]. Upon irradiation under UV light, organic toxic Rhodamine B dye was effectively degraded within few minutes. A plausible mechanism for understanding the chain of reactions has been proposed based on several variations of the parameters influencing reduction activity. Due to the ability of synthesised materials to degrade a wide range of hazardous pollutants and their mixtures, they can be used in practical applications as water remediation [5].

MATERIALS AND METHODS

97% purity, Titanium Isopropoxide [Ti{OCH(CH₃)₂]₄], Titanium (IV) Oxide, anatase [TiO₂] were purchased from Sigma Aldrich. 99% purity, 2-propanol or Isopropanol [C₃H₈O] was obtained from Merck Emplura. Deionized Water (18.3 MΩ) was used for all synthesis purposes.

The precursor, the reagents molar concentration, and the synthesis period are varied significantly in the current work. All of the reagents were of analytical quality and employed without further purification. Titanium Isopropoxide was used as the starting material to prepare TiO₂ Nanoparticles by Solvothermal, Hydrothermal and Annealing technique for different time and temperature.

RESULTS AND DISCUSSION

1.1 eV with change in the morphology obtained from diffuse reflectance spectra (DRS) analysis. The as-synthesized TiO₂ samples showed efficient degradation capability of Rhodamine B (RhB) organic textile dye within a very small time under visible light irradiation. Also the 1st order kinetics, the rate constants and the degradation 99.5% were evaluated.

CONCLUSION

The as-synthesized samples were characterized in details by several techniques to have a proper insight into the phase formations, chemical bonding, morphology and electronic band gaps. The X-Ray diffraction (XRD) analysis revealed the preferential growth in the (101) direction whereas the Fourier Transform Infrared (FTIR) analysis confirmed the presence of all the respective chemical bonds. The morphology of the samples was revealed from the Field Emission Scanning Electron Microscope (FESEM) and Transmission Electron Microscope (TEM) images. The band gaps of the as-synthesized samples varied from 2.8 to In conclusion, the as-synthesized morphology tuned TiO₂ samples prepared by variation in different synthesis methods with time and temperature was effectively exploited for degradation of organic toxic Rhodamine B (RhB) dye under UV-light irradiation.

ACKNOWLEDGMENT

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Oral Presentation – OP-10

MoS₂ Nanostructures for High Performance Supercapacitors

Anupam Laha¹, Soumyajit Baruri¹, Ronit Kumar², Shibam Roy², Indronil Rana²,
Soham Sarkar²,

¹Department of Computer Science Engineering (DS), Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex

²Department of Computer Science Engineering (CS), Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex

INTRODUCTION:

The growing demand for efficient energy storage systems has increased interest in advanced electrochemical devices such as supercapacitors. These devices offer high power density, rapid charge–discharge rates, and long cycle life, but suffer from low energy density. To address this limitation, the development of advanced electrode materials is essential. Molybdenum

disulfide (MoS₂), a transition metal dichalcogenide, has gained attention due to its layered two-dimensional structure and high surface area. Its rich redox activity enables both electric double-layer capacitance and pseudocapacitance. Moreover, MoS₂ nanostructures provide enhanced ion diffusion and more active sites for charge storage. Therefore, MoS₂-based

materials are promising for high-performance supercapacitor applications

MATERIALS AND METHODS:

The synthesis and characterization of the nanostructures were conducted through the following rigorous processes:

1. Hydrothermal Synthesis: A controlled hydrothermal method was employed to facilitate the growth of MoS₂ nanostructures, allowing for precise control over the phase and crystallinity of the resulting nanosheets.
2. Electrochemical Testing: The performance of the synthesized material was evaluated using a three-electrode configuration.
3. Analytical Techniques: Testing included Cyclic Voltammetry (CV) to assess redox behavior and Galvanostatic Charge-Discharge (GCD) to determine practical energy storage capabilities.

RESULTS AND DISCUSSION

The synthesized MoS₂ nanostructures exhibit a layered morphology with high surface area, which enhances ion accessibility and charge storage. The nanosheet structure provides efficient pathways for electron transport, improving overall electrochemical performance. Cyclic voltammetry (CV) analysis shows quasi-rectangular curves with distinct redox peaks, indicating the presence of both electric double-layer capacitance and pseudocapacitance. This dual charge storage mechanism significantly increases the specific capacitance of the material. The electrode demonstrates good rate capability, maintaining performance even at higher scan rates, which reflects fast ion diffusion. Charge–discharge behavior is symmetric, indicating high reversibility and low energy loss. Additionally, the material shows excellent cycling stability over repeated cycles. These results confirm that MoS₂ nanostructures are highly effective for high-performance supercapacitor applications.

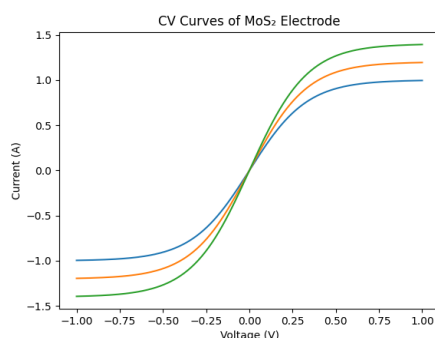


Figure 1. Cyclic Voltammetry curves of MoS₂ electrode showing strong capacitive behaviour.

CONCLUSION:

Organized by: Department of Basic Science & Humanities,
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), (Autonomous), Kolkata



MoS₂ nanostructures are promising electrode materials for high-performance supercapacitors. Their layered structure and high surface area enhance charge storage and electrochemical activity. The presence of redox sites improves pseudocapacitive behavior and overall performance. They also show good cycling stability and rate capability. Thus, MoS₂-based materials are suitable for advanced energy storage applications.

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Oral Presentation – OP-11

Synthesis, Characterization and Applications of doped Carbon Dots

Dipsikha Bhattacharya¹, Poushali De²

¹Department of Chemistry, School of Basic and Applied Sciences, Adamas University, Kolkata, India

²La Martiniere for Girls, Kolkata, Dr. U. N. Bhramachari Street, Kolkata

Email: dipsikha.chem@gmail.com

INTRODUCTION

From the last two decades, Carbon dots (CDs) have recently gained substantial attention as a fluorescent material due to their strong attributes including excellent photoluminescence properties, versatile surface functionalization efficiency, superior aqueous solubility, and low intrinsic toxicity. Compared to the traditional organic dye and inorganic semiconductor quantum dots, CDs have shown many advantages because of their good solubility in water, simple preparation techniques, high fluorescence intensity, good stability and good biological compatibility and hence it can be widely used in medicine, biology, energy, the sensors, photoelectric conversion and photoelectric catalysis.¹⁻² Among many synthesis techniques, doping with nonmetal heteroatoms into the carbon core is one of the most promising method to prepare CDs with enhanced fluorescence properties because these hetero atoms can change the electronic structure of the carbon core as well as incorporate multiple surface states, which in turn alter the properties from the undoped ones.³ Especially, the use of hetero atom doped CDs in the fluorescence detection of metal ions has become one of the most important applications where the highly photostable CDs can guarantee the stability of fluorescence signal to ensure the accurate detection of the analytes. Among many heavy metals, for our work, we have selected iron (Fe³⁺) as one of the most common metal pollutants detected in environmental water bodies as a trace amount of iron (Fe³⁺) plays an important role in the human body.⁴⁻⁵ Additionally, the accumulation of Fe³⁺ ions in the environment will cause a great threat to living organisms. In our work, cyan color emitting doped CDs were prepared using sulfanilic acid with excitation dependent emission properties and based on its luminescence properties, it has been used to detect the presence of Fe³⁺ ions by detecting changes in their fluorescence intensity.

MATERIALS AND METHODS

Sulfanilic acid, Ethanol, n-Hexane were purchased from SRL, India. 0.4 gm of Sulfanilic acid was dissolved in 1:1 ethanol and water mixture and it was completely dissolved in the reaction mixture after stirring the reaction mixture at 1000 rpm for 30 minutes and then the liquid was transferred to a Teflon-lined stainless-steel autoclave and kept in the oven at 180°C for 16 hours. The obtained as prepared brown colored liquid was transferred into a beaker and checked under UV lamp where a fluorescence glow was observed. These as prepared CDs was purified using the column chromatography technique using hexane and ethanol. After the purification, the solution containing carbon dots was dried in a rotatory evaporator.

RESULTS AND DISCUSSION

CDs was synthesized by the high temperature and high-pressure carbonization of Sulfanilic acid. The broad nature of the peaks in the XRD pattern indicates that the S, N doped CDs exhibit amorphous carbon nature. From the TEM images of S, N doped CDs, these CDs exhibited almost spherical shape with good dispersibility. The particle size of CDs was statistically analyzed, and its size is mainly distributed at about 5-7 nm. We used FTIR to characterize the structure and surface -lgroups of nitrogen and sulfur co-doped CQDs. The peaks at 1020, 1109, 1220, 1420 and 1630 cm strongly indicates the presence of C-S, SO₃⁻, C-O, C-N and C=C stretching vibrations of aromatic compounds. The presence of O-H and N-H stretching vibration peaks between 3000–3600 cm⁻¹ indicated the presence of amino and hydroxyl groups on the surface of the CDs. From the UV- Visible and fluorescence spectra of the purified CDs, a broad peak at 302 nm along with a sharp peak at 355 nm with a narrow



full width at 434 nm confirmed the characteristic of C=N bonds in aromatic rings and the presence of intrinsic surface states. The fluorescence emission peak at 502 nm exhibited the excitation independent nature. The fluorescence intensity of doped CDs was monitored through fluorescence spectra and it was decreased monotonically as the Fe(III) concentration increased⁵ which might be due to the strong coordination of Fe(III) to the oxygen-rich or amine groups on the surface of doped C-dots.

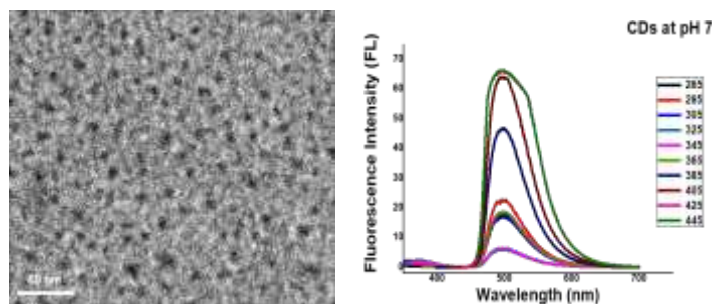


Figure 1. TEM and Fluorescence spectra of purified S, N doped CDs.

CONCLUSION

The study successfully demonstrates a simple and efficient method for synthesizing nitrogen and sulfur co-doped carbon dots using sulfanilic acid. These CDs exhibit strong fluorescence, excellent stability, and high selectivity toward Fe³⁺ ions. The sensing mechanism is based on photoinduced electron transfer, leading to fluorescence quenching upon interaction with Fe³⁺. The CDs show a low detection limit and a wide detection range, making them suitable for real-world applications, especially in environmental monitoring.

ACKNOWLEDGMENT

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Oral Presentation – OP-12

Donor-Bound Excitons and Intersubband-Driven Resistive Switching in Indium-Doped CdSe Nanoplatelets

Sourik Dutta¹, Uttam Pal², Bikram Das¹, Anusri Medda³, Suswapna Mukherjee⁴, Avanti Chakraborty¹, Ajoy Mandal⁵, Sudipto Chakrabarti⁴, Rajib Kumar Mitra^{1,2}, Tanusri Saha-Dasgupta^{2,6}, Ali Hossain Khan^{1,2,1}

Department of Chemical and Biological Sciences,² Technical Research Centre, S. N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata, India; ³ School of Materials Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India. ⁴ Surface Physics and Material Science Division, Saha Institute of Nuclear Physics, Kolkata, India; ⁵ Department of Physics, Govt. General Degree College Tehatta, Nadia, West Bengal; ⁶

Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata, India. Email: alikhan@bose.res.in

INTRODUCTION

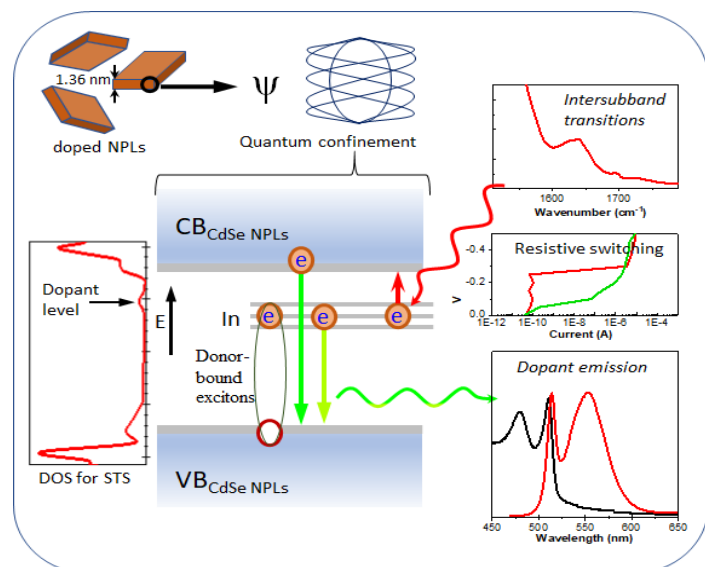
In Doping is a powerful strategy to tailor the optical and electronic properties of semiconductor nanocrystals without altering their size-dependent quantum confinement. While acceptor-bound excitons in p-type doped CdSe systems have been extensively studied, donor-bound excitons arising from n-type dopants remain largely unexplored. This is mainly because n-type dopants typically enhance electron transport without significantly affecting recombination dynamics. In this work, indium-doped CdSe nanoplatelets (NPLs) are employed as an ideal platform to probe donor states due to their narrow emission linewidth and well-defined thickness. The study demonstrates the formation of emissive donor-bound excitons associated with indium dopants, located close to the conduction band. This unique system enables the observation of intersubband transitions and novel electronic behaviors, including resistive switching. The findings provide new insights into charge carrier dynamics and establish a pathway for designing advanced optoelectronic and memory devices.

MATERIALS AND METHODS

CdSe nanoplatelets were synthesized using a hot-injection method involving cadmium myristate, selenium, and octadecene under inert conditions. Indium doping was achieved by introducing indium acetate during the growth stage. The resulting nanoplatelets were purified via centrifugation. Structural and compositional characterization was carried out using TEM, XRD, EDX, and XPS. Optical properties were studied using UV–Vis absorption, photoluminescence (PL), and time-resolved PL spectroscopy. Ultrafast carrier dynamics were investigated using femtosecond transient absorption spectroscopy. Additional analyses, including FTIR, scanning tunneling spectroscopy (STS), and density functional theory (DFT) calculations, were performed to probe electronic structure and dopant states.

RESULTS AND DISCUSSION

The synthesized CdSe nanoplatelets exhibited uniform morphology and high crystallinity, which remained largely unaffected after indium incorporation. Structural analyses confirmed successful substitutional doping without formation of secondary phases. Optical measurements revealed that absorption spectra of doped and undoped samples were nearly identical, indicating preservation of the host band structure. However, photoluminescence spectra showed a distinct new emission peak at ~554 nm in indium-doped samples, attributed to donor-bound excitons. This emission was narrower and exhibited significantly faster recombination compared to typical acceptor-bound excitons. Time-resolved PL studies revealed a reduction in band-edge lifetime upon doping, indicating enhanced carrier trapping, while the dopant-related emission showed a moderate lifetime (~14 ns), suggesting strong radiative recombination.



Ultrafast transient absorption spectroscopy provided deeper insight into carrier dynamics, showing additional excited-state absorption features linked to indium-induced localized states. These results confirm the presence of donor levels just below the conduction band. Further evidence of localized donor states was obtained through FTIR spectroscopy, which showed mid-infrared absorption corresponding to intersubband transitions (~ 0.2 eV). Scanning tunneling spectroscopy measurements directly identified a mid-gap state near the conduction band, consistent with optical findings. Theoretical DFT calculations supported the formation of a stable donor level that remains energetically fixed regardless of dopant concentration. Interestingly, unlike p-type systems, the dopant emission peak in In:CdSe

NPLs remained unchanged with increasing dopant concentration, indicating negligible band dispersion. This behavior was attributed to stabilization of conduction band sublevels by excess electrons introduced by indium.

Electrical measurements demonstrated resistive switching behavior in fabricated devices, where a sharp transition from high-resistance to low-resistance state occurred at low bias ($\sim \pm 0.2$ V). This switching originates from electron excitation from the donor state to the conduction band, effectively forming a three-level electronic system. The devices exhibited good endurance and retention, highlighting the functional relevance of the dopant states.

Overall, the results establish that indium doping introduces a robust donor state that governs both optical and electronic properties, enabling new functionalities such as intersubband absorption and low-voltage resistive switching.

CONCLUSION

This study demonstrates the successful realization of emissive donor-bound excitons in indium-doped CdSe nanoplatelets. The donor state, located near the conduction band, enables intersubband transitions and resistive switching behavior. Unlike p-type systems, the dopant emission remains stable with varying concentration, indicating a robust electronic structure. These findings provide new insights into n-type doping in nanocrystals and open avenues for developing advanced optoelectronic and memory devices based on engineered donor states.

ACKNOWLEDGMENT

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Oral Presentation – OP-13

Doping Engineering in Hybrid Amorphous Carbon Nanotubes: A Comprehensive Review for Energy Storage System

Niket Raj, Raj Narayan Ray, Atrim Das, Ishu Sharma, Atul Das, Sumit Shaw

Department of computer science engineering, Dr. Sudhir Chandra Sur Institute of Technology
and Sports Complex, 540, Dum Dum, Surer Math, Kolkata-700074
(info.niketraj@gmail.com)

Abstract

Amorphous carbon nanotubes (ACNTs) are a special form of carbon nanomaterials that possess a disordered atomic structure along with tubular nanoscale morphology. Unlike crystalline carbon nanotubes, ACNTs contain irregular arrangements of carbon atoms, which provide unique electrical, chemical, and surface properties. Due to their porous nature, large surface area, and low production cost, ACNTs are widely studied for doping applications and energy storage systems. Doping with heteroatoms or metals can significantly improve their conductivity and electrochemical activity. In batteries and supercapacitors, ACNTs enhance charge storage capacity, electron transfer, and stability. Therefore, ACNTs are promising materials for advanced nanotechnology and sustainable energy applications.

Introduction

Amorphous carbon nanotubes are nanoscale tubular structures made of carbon with a non-crystalline or partially disordered arrangement of atoms. They combine the shape advantages of nanotubes with the chemical flexibility of amorphous carbon. ACNTs can be synthesized through chemical vapor deposition, pyrolysis, arc discharge, and template methods. These materials have attracted attention because of their high surface area, lightweight nature, chemical stability, and tunable properties. Their disordered structure creates more active sites, which are useful in catalytic reactions, adsorption, doping, and charge storage. ACNTs are increasingly used in sensors, environmental treatment, batteries, and supercapacitors.

Materials Required

The following materials are commonly required for preparation and study of ACNT-based doping and energy storage systems: Amorphous carbon nanotubes (ACNTs) Carbon precursor materials (hydrocarbons, polymers, biomass sources) Dopants such as Nitrogen, Boron, Sulfur, Phosphorus Metal salts or nanoparticles for composite formation Solvents and chemical reagents Conductive substrates (graphite sheet, copper foil, aluminum foil) Electrolytes for batteries and capacitors

Role of ACNT in Doping

Doping is the process of introducing foreign atoms into a material to improve its electrical and chemical properties. ACNTs are highly suitable for doping because their disordered structure provides many defect sites where dopant atoms can be easily incorporated. Nitrogen-doped ACNTs improve conductivity and catalytic activity. Boron-doped ACNTs enhance hole transport and semiconductor behavior. Sulfur and phosphorus doping improve redox activity. Doped ACNTs are used in sensors, catalysts, solar cells, and fuel cells.

Role of ACNT in Energy Storage System

ACNTs play an important role in modern energy storage devices such as lithium-ion batteries, sodium-ion batteries, and supercapacitors. Their porous structure provides more space for ion storage, while the tubular network allows rapid electron movement. In batteries, ACNTs improve conductivity, charge capacity, and cycle stability. In supercapacitors, they offer high power density and fast charging-discharging performance. ACNT-based composites are also studied for hydrogen storage and fuel cell electrodes.



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Conclusion

Amorphous carbon nanotubes are advanced carbon nanomaterials with excellent potential in doping and energy storage applications. Their high surface area, porous structure, and defect-rich nature make them highly effective for introducing dopants and improving electrochemical performance. ACNTs enhance the efficiency of batteries, supercapacitors, sensors, and catalytic systems. With further research and industrial development, ACNTs are expected to contribute significantly to future clean energy and nanotechnology solutions.

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Oral Presentation – OP-14

Visible-Light-Active Heterostructured TiO₂-BNNS Nanocomposites for Photocatalytic Cr(VI) Reduction

Shaona Chatterjee^{1,3}, Soumita Samajdar^{2,3}, Maitrayee Biswas^{2,3}, Srabanti Ghosh^{2,3*}, Shirshendu Chakraborty^{1,3*}

¹Advanced Ceramics and Composites Division, CSIR-Central Glass and Ceramic Research Institute, Kolkata, West Bengal 700032, India

²Energy Materials & Devices Division, CSIR - Central Glass and Ceramic Research Institute, Kolkata, West Bengal 700032, India

³Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, Uttar Pradesh 201002, India E-mail: srabanti.cgcri@csir.res.in, shirshendu.cgcri@csir.res.in (Corresponding authors)

INTRODUCTION

Two-dimensional (2D) materials such as graphene and boron nitride nanosheets (BNNS) exhibit distinctive photocatalytic and mechanical properties compared to their bulk counterparts, making them highly attractive for applications in advanced catalysts as well as reinforcing composites. Owing to its exceptional features-including low density, high thermal stability, excellent mechanical strength, and strong corrosion resistance-boron nitride has garnered significant global interest^{1,2}. BNNS has emerged as a promising photocatalyst; however, its practical application is hindered by poor solar-light harvesting due to its wide band gap and rapid charge recombination. In this study, BNNS were synthesized via liquid-phase exfoliation and subsequently coupled with TiO₂ to form heterostructure for enhancing photocatalytic performance.

MATERIALS AND METHODS

Boron nitride nano sheet (BNNS) has been synthesized from bulk boron nitride (BN) through liquid phase exfoliation. 1 gm of BN and 3 gm cysteine have been taken in a 250 ml water and sonicated at 500W for 2 hours at pH=7. Upon completion of filtration, the residue was separated and dried at 60°C for 24 hours. The dried BNNS powder was sensitized with TiO₂. From the above-mentioned residue. The powder is then mixed with 230 ml water and 70 ml IPA to prepare 300 ml stock solution. In each 50 ml solution 5%, 10%, 20% TiO₂ added and placed the solution Under uninterrupted magnetic stirring conditions 48 hours.

RESULTS AND DISCUSSION

The photocatalytic performance and physicochemical properties of the synthesized TiO₂-BNNS nanocomposites were systematically investigated to elucidate the role of heterostructure formation in enhancing. To understand the structural and interfacial characteristics of the prepared samples, detailed analyses were carried out using XRD, FT-IR, and microscopic techniques. The enhanced photocatalytic reduction of Cr(VI) can be attributed to improved charge separation and interfacial interaction in the TiO₂-BNNS heterojunction system. XRD and FT-IR images has shown the characteristic peaks of pristine BNNS and TiO₂ present in the nanocomposites. The multilayer BNNS exhibits a band gap of 5.0 eV, whereas TiO₂ has a band gap of 3.2 eV. Following heterostructure formation, a significant enhancement in absorption within the visible region is observed, indicating that the synthesized heterostructures are well-suited for visible-light-driven photocatalytic applications. From the microstructural analysis BNNS nano sheets are visible and After sensitization the TiO₂ nano particles are dispersed on the BNNS is clearly observed. From HR-TEM crystalline planes are exactly matches with the corresponding planes observed from the XRD. Photo electro chemical measuement has been done to investigate the photo response of the composite material and chemical stability under vissible light. We have succesfully



reduce the Cr(VI) in to Cr(III) with our TiO₂-BNNS nanocomposites. We have achieved 95.6% Cr(VI) reduction within 180 min with a rate constant of 0.02 min⁻¹. And from the absorbance spectra band gap of the pristine TiO₂ and BNNS has been calculated and it comes out to be a direct z scheme mechanism.

Table: Percentage of Cr(VI) reduction value and rate constant of pristine and different composites

Material	Cr (VI) reduction/% in 180 mins	Rate constant/min
Dark	8.01	0.003
BNNS	51.3	0.005
10% TiO ₂ -BNNS	95.64	0.02
20% TiO ₂ -BNNS	77.3	0.006

CONCLUSION

The optimized TiO₂-BNNS heterostructure exhibits significantly enhanced visible-light photocatalytic performance, achieving ≥95% Cr(VI) reduction with a rate constant of 0.02 min⁻¹. This improvement is supported by a threefold increase in photocurrent density and a substantial decrease by a factor of around 10 in charge transfer resistance compared to pristine BNNS. Additionally, the composite shows a higher charge carrier concentration and a more negative flat-band potential. These enhancements are attributed to improved light absorption, efficient charge separation, and strong interfacial interaction, highlighting its potential for environmental remediation applications.

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Oral Presentation – OP-15

Tunable Dielectric Behavior of β -SiAlON-Based Composites Using BN and Graphene Nanoplatelets for High-Speed Aerospace SystemsShreyasee Nath^P, B. Haldar, Shirshendu Chakraborty*

CSIR-Central Glass and Ceramic Research Institute, Kolkata, India

Presenter: shreyaseenath1998@gmail.com

INTRODUCTION

SiAlON ceramics, derived from silicon nitride, exhibit excellent high-temperature stability, oxidation resistance, and mechanical strength for demanding applications.¹ They exist mainly as α -SiAlON and β -SiAlON, with β -SiAlON offering compositional flexibility through the substitution parameter z for tuning properties.² Modern aerospace and electronic systems require materials with combined electromagnetic (EM), thermal, and mechanical performance. SiAlON ceramics are promising for EM-transparent applications due to their low dielectric loss and high thermal stability. Incorporating hexagonal boron nitride and graphene nanoplatelets enables tailoring for EM transparency, thermal conductivity, and EMI shielding.³ This study develops β -SiAlON–BN and β -SiAlON–GNP composites via SPS to achieve tunable multifunctional properties for advanced aerospace applications.

MATERIALS AND METHODS

Si₃N₄, AlN, and Al₂O₃ powders were used to synthesize β -SiAlON, with h-BN and GNPs added as reinforcements. The base powders were mixed with acetone for 4 h to obtain a homogeneous mixture. h-BN (10–30 wt%) and GNPs (0.25–1 wt%, pre-sonicated in acetone) were separately incorporated and mixed for 3h. The suspensions were dried by evaporating acetone under stirring and then oven-dried at 80–120 °C. Finally, the powders were sintered at 1800 °C under a nitrogen atmosphere using spark plasma sintering (SPS).

RESULTS AND DISCUSSION

With increasing boron nitride content, bulk density decreases while relative density remains nearly constant, whereas graphene nanoplatelets reduce relative density. GNP addition reduces hardness but enhances fracture toughness and flexural strength up to an optimum, while BN decreases hardness and strength but improves toughness.(Table 1.)

Sample ID	Relative density	Flexural strength (MPa)	Dielectric Constant	Dielectric Loss
SN	99.30	190±11	7.4751±0.0253	0.0052±0.003
SBN30	98.96	124.17±5	5.9608±0.021	0.0012±0.0038
SG0.25	97.88	210.80±29	12.0595±0.620	0.0202±0.0275

From a dielectric perspective, BN lowers dielectric constant and maintains low loss, indicating good insulating behavior. In contrast, GNP increases dielectric constant due to interfacial polarization but also raises dielectric loss, especially at higher loadings, due to conductive pathway formation.

CONCLUSION

- Boron nitride lowers dielectric constant and loss, improving EM transparency but reducing hardness and strength.
- graphene nanoplatelets improve mechanical properties and increase dielectric constant, with optimal overall



performance achieved at intermediate content despite higher dielectric loss at higher loadings.

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Oral Presentation – OP-16

Paper-Based Metal Oxide – Carbon Hybrid Materials For Energy Storage Applications

Sumit Adak, Ranit Barman, Ranajit Pramanik, Pradip Bera, Raushan Khan

Department of Electronics and Communication Engineering,

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,

540, Dum Dum, Surer Math, Kolkata - 700074

E-mail: adaksumit106@gmail.com

INTRODUCTION

With the growing need for energy storage systems, researchers are always looking for new materials to improve performance. Traditional batteries and capacitors have limitations so they are exploring options. Supercapacitors are one technology that has gained attention. They can charge quickly a long time and store a lot of power. However, supercapacitors have a drawback. They do not store much energy. To solve this problem, researchers have developed materials, such as metal oxide and carbon hybrids. These hybrid materials combine the conductivity of carbon with the high energy storage of metal oxides. This results in performance overall. This report looks at how these materials improve energy storage in supercapacitors.

WORKING PRINCIPLE

The hybrid material works by using a combination of things. It has Electric Double Layer Capacitance from carbon and Pseudocapacitance from metal oxides. The hybrid material uses these two things together: Electric Double Layer Capacitance from carbon, Pseudocapacitance from metal oxides. This helps the hybrid material store a lot more energy than if it were just used carbon or metal oxides. The hybrid material really improves energy storage capacity because it uses both carbon and metal oxides together.

METHODOLOGY

The general steps to make this work include: We have to prepare the carbon substrate. Then we put a layer of metal oxide on the carbon surface. After that, we put everything together to make a supercapacitor. We test the supercapacitor by charging and discharging it times. We look at how well the supercapacitor works by checking things like capacitance and efficiency of the supercapacitor, the metal oxide and the carbon substrate.

RESULTS AND DISCUSSION

The use of metal oxide–carbon hybrid materials shows a noticeable improvement in supercapacitor performance. Due to combined EDLC and pseudocapacitance, carbon ensures efficient electron transport, compared to pure carbon-based supercapacitors. However, some challenges include: Stability issues of certain metal oxides, Higher cost for some materials like RuO₂, and complexity in fabrication methods. Despite these limitations, hybrid materials are considered a promising direction for next-generation energy storage systems[1], [2].

CONCLUSION

At present, Metal oxide and carbon hybrids are very important for supercapacitors. When we combine metal oxide and carbon hybrid materials, they do a better job than old energy storage devices because metal oxide and carbon hybrid materials use the good things about both metal oxide and carbon. People are still. Working on metal oxide and carbon hybrid materials. We think metal oxide and carbon hybrid materials will really help us store energy in a good way, for the earth and work well in the future with metal oxide and carbon hybrid materials.

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Oral Presentation – OP-17

Structural Evolution and Controlled Synthesis of Amorphous Carbon Nanotubes: Role of Doping and Hybridization

Piyush Mondal, Muskan Kumar, Sahil Chauhan, Shivanshu Raj, MD Shoaib Ansari

Department of Computer Science & Engineering,

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,

540, Dum Dum, Surer Math, Kolkata – 700074

Email: piyushraj7617@gmail.com

INTRODUCTION

In the landscape of carbonaceous nanomaterials, Amorphous Carbon Nanotubes (a-CNTs) have emerged as a significant area of study due to their unique structural disorder compared to their crystalline counterparts. Unlike the perfectly hexagonal lattice of multi-walled carbon nanotubes, a-CNTs consist of a mix of sp^2 and sp^3 hybridized carbon atoms, leading to a “long-range disorder” but “short-range order” configuration. This literature survey explores the structural evolution of these tubes during synthesis and examines how controlled doping—particularly with nitrogen or boron—and hybridization techniques can be utilized to tune their electronic and mechanical properties for applications in energy storage and sensing.

MATERIALS AND METHODS**Materials**

The synthesis and study of a-CNTs involve several precursor materials and catalysts:

- **Carbon Sources:** Hydrocarbons such as methane (CH_4), acetylene (C_2H_2), or solid-state precursors like ferrocene and polymers.
- **Dopants:** Nitrogen-rich compounds (urea, pyridine) and Boron sources (boric acid) are commonly identified in literature for heteroatom doping.
- **Catalysts:** Transition metal nanoparticles, primarily Iron (Fe), Nickel (Ni), and Cobalt (Co), often supported on alumina (Al_2O_3) or silica (SiO_2).

Methods

The fundamental working principle of a-CNT synthesis lies in Chemical Vapor Deposition (CVD) at relatively lower temperatures ($400^\circ C$ to $700^\circ C$) compared to crystalline tubes. At these temperatures, the carbon diffusion rate through the catalyst nanoparticle is insufficient to form perfectly graphenic layers, resulting in the “structural evolution” of an amorphous wall. Hybridization mechanisms involve the transition between sp^2 (graphitic-like) and sp^3 (diamond-like) carbon bonds, which dictates the tube’s flexibility and conductivity.

RESULTS AND DISCUSSION

A review of current literature indicates that the structural integrity of a-CNTs is highly dependent on the sp^2/sp^3 ratio. Controlled synthesis allows for the modification of this ratio through doping. Nitrogen doping, for instance, introduces chemically active sites and increases the metallic character of the nanotubes.

Table 1. Comparative Analysis of a-CNT Properties Based on Doping

Dopant Type	Hybridization Shift	Structural Impact	Key Parameter (Conductivity)
Undoped	Balanced sp^2/sp^3	High Disorder	Moderate (10^{-1} S/cm)
Nitrogen (N)	Increased sp^2	Pyridinic/Pyrrole sites	High (10^1 S/cm)
Boron (B)	Stable sp^3	Enhanced Stiffness	P-type behavior



The structural evolution is often visualized through Transmission Electron Microscopy (TEM), where the walls appear as “fuzzy” or disordered layers rather than distinct concentric circles. Discussion in various papers suggests that hybridization is the primary factor in determining the “long-range disorder”. Furthermore, the inclusion of dopants acts as a catalyst for “controlled synthesis,” allowing researchers to predict the electronic bandgap of the resulting material.

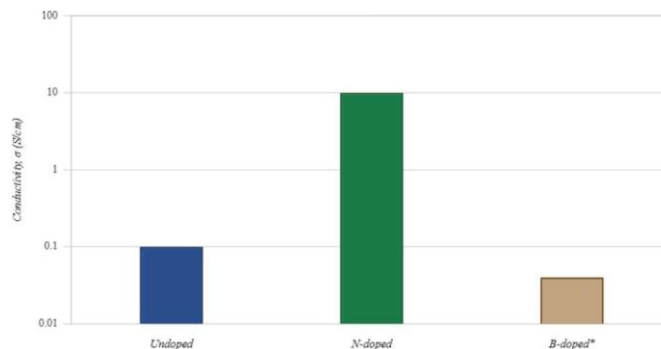


Fig. 1. Comparative conductivity of a-CNT by dopant type

Logarithmic scale; Boron (B) denotes p-type qualitative behaviour

CONCLUSION

The survey of current research on a-CNTs reveals that (1) the structural evolution is a temperature-dependent process governed by carbon diffusion kinetics, (2) sp^2 and sp^3 hybridization ratios can be effectively manipulated to alter mechanical properties, and (3) doping remains the most viable method for tailoring electronic states. Future work should focus on the practical implications of these tubes in flexible electronics where crystalline brittle-nature is a disadvantage.

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Oral Presentation – OP-18

Study of prey-predator model in Smith growth population dynamics with refuge and hunting cooperation

Neha Saha

1 Department of Basic Science and Humanities,
Dr. Sudhir Chandra Sur Institute of Technology & Sports Complex,
Kolkata, West Bengal 700074, India
E-mail: neha.saha2000@gmail.com (corresponding author)

INTRODUCTION

Predator–prey interactions are fundamental to understanding ecological dynamics, with classical models like the Lotka–Volterra model describing oscillatory behavior but often oversimplifying real systems [1]. To improve realism, nonlinear growth such as the Smith growth function is used to account for resource limitations [2]. Additional food for predators enhances their survival and growth, significantly influencing the stability and persistence of the predator–prey system [3].

MODEL FORMULATION AND ANALYSIS

We consider a predator–prey system where prey follows the Smith growth function and predation is described by a Holling type III functional response.

$$\frac{dx}{dt} = rx \left(\frac{\beta - x}{\beta + cx} \right) - \frac{\alpha x^2 y}{1 + \epsilon x^2}, \quad \frac{dy}{dt} = \frac{\alpha_1 \alpha x^2 y}{1 + \epsilon x^2} + \frac{sy}{1 + qy} - ny,$$

With positive initial conditions $x(0)=x_0 \geq 0$, $y(0)=y_0 \geq 0$, where r : prey growth rate; β : carrying capacity; c : crowding effect; α : predation rate; ϵ : handling time; α_1 : conversion efficiency; s : predator growth rate; q : density effect; n : predator death rate. The model describes prey growth under limited resources and predator dynamics governed by predation, alternative food sources, and natural mortality.

Equilibria

Trivial equilibrium: $E_0 = (0, 0)$

Prey-only equilibrium: $E_1 = (\beta, 0)$

Predator free $E_2 = (0, (s-n)/nq)$

Interior (coexistence) equilibrium: $E^* = (x^*, y^*)$, where $x^* > 0$, $y^* > 0$ satisfy:

$$r(\beta - x)/(\beta + cx) = \alpha xy/(1 + \epsilon x^2)$$

$$\alpha_1 \alpha x^2/(1 + \epsilon x^2) + s/(1 + qy) = n.$$



RESULTS AND DISCUSSION

We analyze the nullclines graphically. We observed that system exhibit one interior equilibrium points

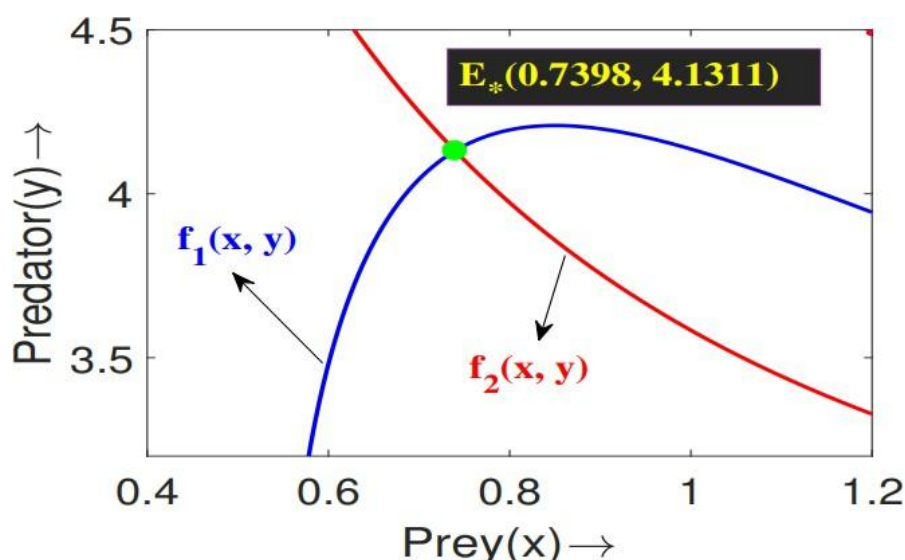


Figure 1. Nullclines of the given system: blue and red represent the prey and predator nullcline, respectively.

Green dot indicates the coexistence equilibrium point at their intersections.

CONCLUSION

In conclusion, the prey–predator model with Smith growth function and additional food for predators exhibits rich dynamical behavior, including stability changes and bifurcations. The results show that prey growth and predator support through alternative food sources play a crucial role in determining system stability and species persistence.

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Oral Presentation – OP-19

22 nm PTM based Digital Designs: Interfacing Single-threshold Ultra-low Power Circuits with Long Interconnects

Sagnik Mukherjee¹, Samagata Das¹, Samadrita Das¹, Amarnath Samanta¹, Arun KP², Jehan Taraporewalla³, Abhijit Ghosh¹, and Dipankar Saha¹

¹Department of Electronics and Communication Engineering, Narula Institute of Technology, Agarpara, Kolkata, 700109, India

²Department of Electronics and Telecommunication Engineering, Indian Institute of Engineering Science and Technology Shibpur, Howrah-711103, India

³Department of Electrical Engineering, Indian Institute of Technology Delhi, New Delhi-110016, India

INTRODUCTION

An accurate predictive MOSFET model is essential for early-stage circuit design, as it enables reliable forecasting of nanoscale transistor behavior. Precise prediction of device characteristics requires the inclusion of emerging physical effects, such as process variations and correlations among model parameters. To address these challenges, a new generation of predictive technology models (PTMs) has been reported in the literature [1-4]. Across technology nodes ranging from 180 nm to 45 nm, the Berkeley Predictive Technology Model (BPTM) models include more physical parameters during prediction than the Berkeley Short-Channel IGFET Model 4 (BSIM4) [3-5]. However, in the case of BPTM, since the model file for each technology node is independently fitted, the overall scaling trend is not smooth [3, 5]. Although BPTM performs adequately for technology nodes between 180 nm and 45 nm, its empirical nature constrains further scalability [3, 5]. In [5], a new generation of PTMs is reported to overcome these limitations, where advanced physical models are integrated into the predictive methodology to capture correlations among parameters more accurately. These models incorporate the dependence of V_{th0} on N_{ch} , along with mobility degradation and velocity overshoot [5, 6]. Nonetheless, these models can be further extended to include strained silicon, high-k dielectrics, and metal gates, enabling a broader impact on future design [5, 6]. In this work, we employ a 22 nm PTM [5] to model the interfacing of long interconnects with ultra-low power digital circuits. To obtain the total capacitance and resistance, the 100 μm interconnect length is multiplied by the capacitance and resistance per unit length (i.e., 140 aF/ μm and 62.1 $\Omega/\mu\text{m}$, respectively). This yields a total resistance of 6210 Ω and a total capacitance of 14 fF, which are then employed in the π -model of [7].

METHODOLOGY

All simulations are conducted in SPICE [8] using the 22 nm predictive technology model (PTM) [9] at an operating frequency of 100 MHz. Furthermore, NMOS and PMOS threshold voltages are taken as 0.503 V and 0.460 V, respectively, with the higher supply voltage (V_{ddH}) fixed at 0.8 V for the 22 nm technology node [5, 9]. However, the lower supply voltage (V_{ddL}) is 0.6 V unless otherwise mentioned. The widths of NMOS and PMOS transistors are set to default values of 200 nm and 500 nm, respectively. Besides, the default length of all transistors is 40 nm. In order to design an interconnect, the selection of an accurate model and interconnect parameters associated with the corresponding technology node is crucial. Thus, the π -model reported in [7, 10] is adopted in this work, with resistance and capacitance per unit length of 62.1 $\Omega/\mu\text{m}$ and 140 aF/ μm , respectively (considering the 22 nm technology node) [11, 12]. To estimate the interconnect length,



a digital circuit with multiple functional blocks implemented in 22 nm trigate CMOS technology [13] is considered, whereas the layout size of the circuit is $\sim 310 \mu\text{m} \times 130 \mu\text{m}$. Therefore, from the layout dimension, we can calculate the length of an average long interconnect using the thumb rule given by $(\sqrt{\text{ChipArea}})/2$ [12, 14]. The value of the interconnect length thus obtained is $100 \mu\text{m}$.

RESULTS AND DISCUSSION

In this work, ultra-low-power digital circuits are designed in which CMOS inverter-inverter circuits are interfaced with a 12T (twelve-transistor) static CMOS 2-input XOR gate and an 8T (eight-transistor) mixed-style 2-input XOR gate through long interconnects (modeled using π -networks). In the case of the 12T static CMOS 2-input XOR gate, four RC network paths are employed owing to the use of complementary input signals. In contrast, the 8T mixed-style 2-input XOR gate requires only two RC network paths (Figure 1 and Figure 2). Furthermore, the outputs of both XOR architectures are routed to static CMOS inverter-inverter stages using similar long interconnects. We refer to these architectures as Interface 1 and Interface 2, respectively. The corresponding output waveforms of Interface 1 and Interface 2 exhibit error-free logic.

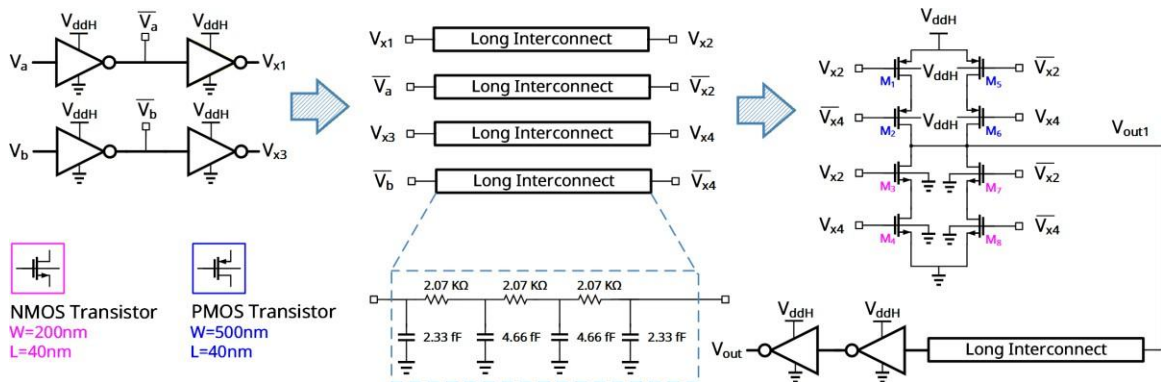
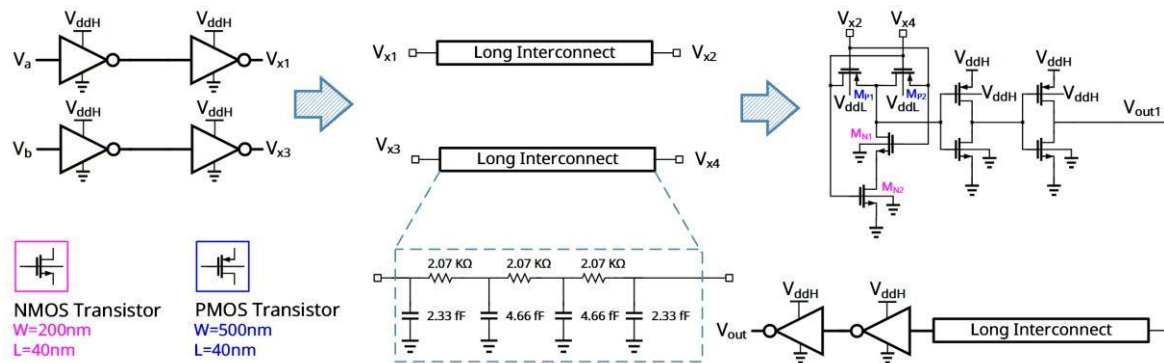


Figure 1: Circuit diagram illustrating Interface 1

Figure 2: Circuit diagram illustrating Interface 2



Besides, Table 1 presents a comparison of the energy efficiency and performance of the two interfaces.



Table 1: Comparison of energy efficiency and performance

Architecture	Supply Voltage	$V_{out-min}$	$V_{out-max}$	P_{avg}	T_{dmax}	PDP
Interface 1	$V_{ddH} = 0.8 \text{ V}$	0.006 mV	799.99 mV	3.3248 micro W	0.529 ns	1.758 fJ
Interface 2	$V_{ddH} = 0.8 \text{ V}, V_{ddL} = 0.6 \text{ V}$	0.002 mv	799.99 mV	2.2467 micro W	1.123 ns	2.523 fJ

CONCLUSION

In this study, CMOS inverter–inverter configurations are interfaced with both 12T static CMOS and 8T mixed-style 2-input XOR gates through long interconnects. Interface 2, which employs an 8T mixed-style XOR gate, offers advantages such as lower energy consumption and reduced silicon area while maintaining robust output.

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Oral Presentation – OP-20

Engineering MXene-Integrated Bi₂O₂Se Nanosheets for Enhanced Solar-Driven Ammonia Synthesis

Jishu Pramanik^{1,2}, Soumita Samajdar^{1,2}, Maitrayee Biswas^{1,2}, Pallab Bhattacharya^{3,2}, Swarup Ghosh⁴, and Srabanti Ghosh^{*1,2}

¹Energy Materials & Devices Division (EMDD), CSIR - Central Glass and Ceramic Research Institute, Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, India

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

³Functional Materials Group, Advanced Materials & Processes (AMP) Division, CSIR-National Metallurgical Laboratory (NML), Jamshedpur, Jharkhand 831007, India

⁴School of Computer Science and Artificial Intelligence, SR University, Warangal, Telangana 506371, India
(*Corresponding author), E-mail: ghosh.srabanti@gmail.com, srabanti.cgcric@csir.res.in

INTRODUCTION

Ammonia (NH₃) is not only an essential chemical feedstock but also a promising carbon-free hydrogen carrier. However, its conventional production via the Haber-Bosch process is highly energy-intensive and associated with CO₂ emissions.¹ In this context, photocatalytic nitrogen fixation offers a sustainable route for ammonia production under ambient conditions, though it remains limited by sluggish kinetics and competing hydrogen evolution reactions.² Herein, a Bi₂O₂Se/Ti₃C₂ MXene composite is rationally constructed via a simple co-precipitation method to enhance photocatalytic nitrogen reduction. The coupling of narrow band gap Bi₂O₂Se with highly conductive Ti₃C₂ MXene facilitates efficient charge separation, rapid electron transport, and improved N₂ adsorption through interfacial charge transfer, as supported by density functional theory (DFT) calculations.³ The optimised composite demonstrates ~152 μmol g⁻¹ NH₃ yield than pristine materials, attributed to synergistic interfacial effects that suppress charge recombination and enhance catalytic activity, offering a promising strategy for solar-driven ammonia synthesis.

MATERIALS AND METHODS:

Bi₂O₂Se nanosheets were synthesised via a room-temperature precipitation method by reacting Bi(NO₃)₃·5H₂O with selenourea in the presence of EDTA, followed by alkaline treatment (KOH/NaOH) to form a dark precipitate, which was collected and dried at 50 °C. Ti₃C₂ MXene was obtained through a modified alkaline reflux process, where the material was treated in 0.3 M KOH at 100 °C for 48 h, then centrifuged and dried. For composite formation, MXene was first dispersed by probe sonication, after which the Bi₂O₂Se precursor was introduced to enable in-situ nucleation on the MXene surface. The resulting product was washed, dried, and denoted as MBS50, MBS25, and MBS12 based on decreasing Bi₂O₂Se precursor concentrations while keeping MXene content constant.

Photocatalytic nitrogen fixation was performed under ambient conditions in a sealed quartz reactor using a 300 W xenon lamp. A suspension of 50 mg catalyst in 50 mL deionized water with methanol was purged with Ar and then N₂ to ensure an oxygen-free, N₂-saturated environment before irradiation for 6 h. Ammonia formation was monitored at regular intervals, with quantification carried out using the indophenol blue method via UV-vis spectroscopy after centrifugation.

1. RESULTS AND DISCUSSION: X-ray diffraction patterns confirm the successful integration of Bi₂O₂Se with MXene without impurity phases (Figure 1a), while Field Emission Scanning Electron Microscopy analysis reveals Bi₂O₂Se nanosheets uniformly anchored on MXene layered structure (Figure 1b), ensuring intimate interfacial contact. The increased photocurrent under N₂ atmosphere further suggests improved N₂ adsorption and activation (Figure 1c). Consistently, the photocatalytic results show that the composites outperform the pristine materials, with MBS25 achieving the highest NH₃ yield of ~152 μmol g⁻¹ after 6 h

reaction, along with excellent stability over repeated cycles (Figure 1d). Charge density analysis reveals electron accumulation at Bi₂O₂Se and depletion at Ti₃C₂O₂, establishing a built-in electric field that drives efficient charge separation across the vdW interface (Figure 1e). This interfacial field, combined with the high conductivity of Ti₃C₂



and strong light absorption of Bi₂O₂Se, enables rapid carrier transport and suppressed recombination, leading to enhanced photoelectrochemical performance.

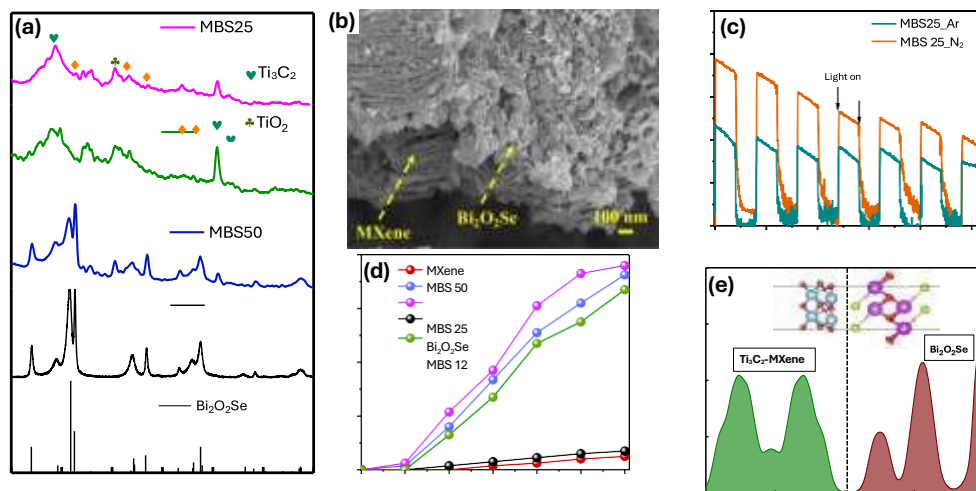


Figure 1: (a) XRD profile of Bi₂O₂Se, MBS50, MBS25, MBS12, (b) FESEM image of MBS25 composite, (c) Photocurrent density in Ar and N₂ medium of MBS25 composite, (d) NH₃ production of pristine materials and composites, (e) Charge density of MXene and Bi₂O₂Se.

CONCLUSION:

In summary, Bi₂O₂Se nanosheets were synthesized via a co-precipitation method and integrated with MXene to form a strongly coupled composite, where nanosheets are uniformly anchored on the conductive layered network. Structural and spectroscopic analyses confirm high surface area, abundant defects, and significant interfacial electronic interaction, including charge redistribution and electron transfer from MXene to Bi₂O₂Se. Among the samples, MBS25 exhibits the best performance with an NH₃ production rate of

~25.3 $\mu\text{mol g}^{-1} \text{h}^{-1}$. Optical, electrochemical, and DFT results collectively demonstrate that MXene acts as a conductive cocatalyst forming a Schottky junction, facilitating rapid electron transport, suppressing recombination, and providing active sites for N₂ reduction, thereby significantly boosting photocatalytic efficiency.

ACKNOWLEDGMENT:

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Oral Presentation – OP-21

Graphene Oxide-Coupled Copper Ferrite as a Photoanode for Efficient Photoelectrochemical Water Splitting**Sankar Samanta¹, Prof. Nikolai V Tarasenko², Dr. Alena A. Nevar² and Srabanti Ghosh^{*1,3}**¹Energy Materials & Devices Division (EMDD), CSIR - Central Glass and Ceramic Research Institute, Raja S. C. Mullick Road, Jadavpur, Kolkata, 700032, India² Plasma Physics Centre at B.I. Stepanov Institute of Physics, National Academy of Sciences of Belarus, Belarus³Academy of Scientific & Innovative Research (AcSIR), Ghaziabad, 201002, India*Corresponding author, E-mail: ghosh.srabanti@gmail.com, srabanti.cgcri@csir.res.in**INTRODUCTION:**

The growing demand for sustainable and clean energy technologies has intensified research into solar-driven photoelectrochemical (PEC) systems for efficient light-to-electricity and light-to-chemical energy conversion.¹ PEC efficiency is often limited by rapid charge recombination, weak light absorption, and poor charge transport, necessitating the rational design of advanced photoelectrodes with improved charge separation and transport properties.² Graphene Oxide (GO) enhances electron transport and suppresses recombination, while Copper Ferrite (CFO), despite its visible-light activity, is limited by poor charge mobility and fast electron-hole recombination.³

To overcome these limitations, constructing a CFO/GO composite provides an effective strategy. The incorporation of GO into CFO creates a conductive network that facilitates rapid electron extraction and transport, thereby improving charge separation efficiency. Additionally, the intimate interfacial contact between GO and CFO promotes electronic coupling, enhances light absorption, and increases the availability of active surface sites. Such synergistic effects are crucial for achieving improved photocurrent response and long-term stability in PEC systems. In this work, A CFO/GO nanocomposite synthesized via a hydrothermal route exhibit significantly enhanced photoelectrochemical performance with 200 $\mu\text{A}/\text{cm}^2$ current at 0.8 V vs Ag/AgCl, compared to pristine materials. This study highlights the importance of carbon-semiconductor hybrid structures in advancing high-performance PEC materials.

MATERIALS AND METHODS:

Graphene oxide (75 mg) was dispersed in 75 mL of deionized water and ultrasonicated for 2 h to obtain a uniform suspension. Pre-synthesized copper ferrite (CFO) was then added and sonicated to ensure homogeneous mixing. The mixture was transferred to a Teflon-lined autoclave and subjected to hydrothermal treatment at 160 °C for 8 h. After cooling, the product was collected by centrifugation, washed with deionized water and isopropanol, and dried to obtain the CFO/GO composite.

Photoelectrochemical (PEC) measurements were performed in a three-electrode configuration using 0.1 M Na₂SO₄ as the electrolyte. The as-synthesized CFO/GO coated FTO was used as the working electrode, with a Pt wire as the counter electrode and Ag/AgCl as the reference electrode. A 300 W xenon lamp was employed as the light source, and LSV, transient photocurrent, and EIS analyses were conducted to evaluate PEC performance.

RESULTS AND DISCUSSION:

The CFO/GO composite exhibits a well-integrated composite, where CFO nanoparticles are uniformly anchored on GO nanosheets (Figure 1a) providing high surface area and intimate interfacial contact. Photoelectrochemical measurements reveal a significantly enhanced photocurrent response with 200 $\mu\text{A}/\text{cm}^2$ current density at 0.8 V vs Ag/AgCl, compared to pristine CFO, indicating improved charge separation and transport (Figure 1b). The transient photocurrent shows stable and reproducible signals with negligible decay, confirming efficient suppression of recombination and good photostability (Figure 1c). Additionally, the impedance spectroscopy analysis demonstrates



reduced charge-transfer resistance for the composite, evidencing faster interfacial electron transport (Figure 1d). This enhanced PEC performance is attributed to the conductive GO network, which facilitates rapid electron extraction and promotes efficient photo-electrochemical hydrogen evolution.

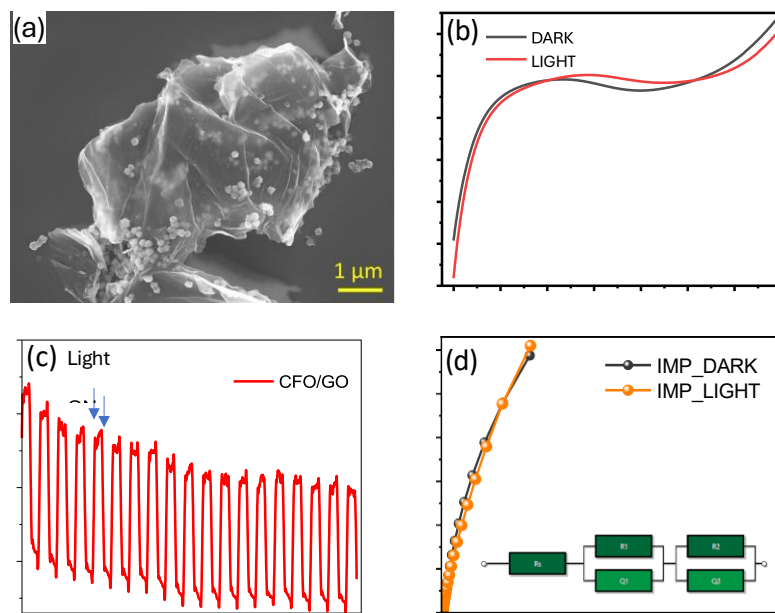


Figure 1. (a) FESEM (b) Linear sweep voltammogram (c) Chronoamperometry (d) Impedance spectroscopy of CFO/GO composite

CONCLUSION:

The CFO/GO nanocomposite synthesized via a hydrothermal route exhibit significantly enhanced photoelectrochemical performance compared to pristine CFO, owing to improved charge separation and accelerated electron transport through the conductive GO network. The strong interfacial interaction between CFO and GO effectively suppresses charge recombination and provides abundant active sites. The composite delivers a high photocurrent density of $200 \mu\text{A}/\text{cm}^2$ @ 0.8 V vs Ag/AgCl with excellent stability under repeated cycles. Furthermore, reduced charge-transfer resistance confirms improved interfacial kinetics. Overall, this work demonstrates that hydrothermally engineered carbon-semiconductor hybrids are promising for efficient PEC hydrogen generation.

ACKNOWLEDGMENT:

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Synergy of Materials Science and Antenna Technology: Recent Developments

Souvik Dinda¹, Rupsa Kar², Mayukh Saha³, Arpita Santra⁴, Abhijit Ghosh⁵, Soumen Pal⁶

¹⁻³B.Tech Student, Department of ECE, Narula Institute of Technology, Kolkata

⁴⁻⁶Faculty Member, Department of ECE, Narula Institute of Technology, Kolkata

E.MAIL : ¹souvikdinda505@gmail.com

souvikdinda505@gmail.com

Abstract

Materials science and engineering are rapidly evolving fields that underpin innovations across communication, healthcare, aerospace, and energy. Recent advances in nanocomposites, graphene, and photonic crystals have enabled devices with unprecedented efficiency, miniaturization, and multifunctionality. A prominent example is the microstrip patch antenna, which has become a testbed for integrating advanced materials into practical communication systems. This paper reviews recent developments in materials science, highlights their applications, and explores how patch antennas exemplify the synergy between material innovation and engineering design.

Keywords: nanocomposites, graphene, photonic crystals, smart and biodegradable materials, terahertz communication.

Introduction

Materials science is the foundation of modern engineering, shaping technologies from semiconductors to biomaterials. The discipline has expanded beyond traditional metallurgy and ceramics into nanotechnology, smart materials, and bio-inspired composites. These innovations are not only enhancing structural and functional properties but also enabling new applications in wireless communication, biomedical sensing, and aerospace systems. Patch antennas[1], known for their compactness and ease of fabrication, are increasingly designed with advanced materials to meet the demands of 5G, 6G, and terahertz (THz) communication systems[2]. Their integration demonstrates how materials science directly influences engineering performance[3]. This paper examines recent developments in materials science and engineering, with patch antennas as a case study of applied innovation[4].

Advances in Materials Science

1.1 Nanocomposites: Nanocomposites, formed by combining polymers, ceramics, or metals with nanoscale fillers, offer superior mechanical strength, enhanced dielectric properties, and tunable electromagnetic responses[5]. These features make them ideal for compact patch antennas, enabling miniaturization without loss of gain or bandwidth, particularly in C and X bands for satellite and radar systems[6]. They also improve thermal stability and resilience, paving the way for flexible, wearable, and biodegradable antenna[7] designs that support sustainable communication technologies.

1.2 Graphene and 2D Materials: Graphene's exceptional conductivity, flexibility, and tunability make it ideal for patch antennas, enabling THz operation, real-time reconfigurability, and wearable designs for beyond-6G, radar, IoT, and biomedical systems. Complementary 2D materials like MoS₂ enhance efficiency, while TMDs and h-BN support multi-band operation and reduced losses. Together, they drive compact, high-frequency, and sustainable communication technologies.

1.3 Photonic Crystals: Photonic crystals are periodic dielectric structures that create bandgaps to control electromagnetic waves, making them valuable in patch antennas. They enable multi-band resonance, reduce return loss, and improve gain and efficiency, supporting compact devices across multiple standards. Applications range from biomedical imaging and satellite communication to IoT, where triple-band designs offer lightweight, high-performance solutions. Looking ahead, hybrid integration with graphene and nanocomposites could yield reconfigurable, terahertz-



capable antennas, positioning photonic crystals as a cornerstone of next-generation communication systems. **Smart and Biodegradable Materials:** Smart materials like shape-memory alloys, piezoelectrics, and magnetostrictive compounds enable reconfigurable antennas that adapt frequency, polarization, or radiation patterns in real time, supporting applications in adaptive radar, cognitive radio, and next-gen wireless systems. Biodegradable polymers such as cellulose and PLA provide eco-friendly substrates for wearable and biomedical antennas, ensuring flexibility, sustainability, and safe degradation. Together, smart and biodegradable materials drive antennas that are efficient, adaptable, and environmentally responsible, with patch antennas offering lightweight, low-profile, and easily fabricated designs suitable for mobile, IoT, aerospace, and biomedical applications.

Future Directions

Materials science is driving antenna engineering toward transformative directions. AI-driven design accelerates performance prediction and prototyping, while flexible and biodegradable substrates support sustainable, wearable electronics. Advanced materials may enable quantum- frequency patch antennas for ultra-secure communication, and energy-harvesting smart materials could power IoT devices autonomously. Together, these innovations point to adaptable, sustainable, and intelligent communication systems of the future.

Conclusion

Recent advances in materials science—nanocomposites, graphene, and photonic crystals—are revolutionizing patch antennas with efficiency, miniaturization, and multifunctionality. Nanocomposites enhance dielectric properties for compact aerospace-ready designs, graphene enables THz operation and reconfigurability for beyond-6G and biomedical wearables, and photonic crystals deliver multi-band resonance and improved directivity for satellite and IoT systems. Together, these innovations drive sustainable, adaptable communication technologies, with future directions including AI-driven predictive design, quantum materials, and eco- friendly substrates.

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Defect Luminescence of Semiconductor Nanocrystals- A Single Particle Spectroscopic Perspective

Arunasish Layek¹, Subhasree Banerjee,² and Arindam Chowdhury³

¹Department of Chemistry, Adamas University, Barasat-Barrackpore Road, Kolkata 700126 ²Department of Chemistry, Panchmura Mahavidyalaya, Panchmura, Bankura-722156 ³Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076

E-mail: arunasis@gmail.com

INTRODUCTION

The particle size dependent optical properties of semiconductor are largely a result of internal structure of the NCs. However, for small NCs (<10 nm in size), surface states become very important as the size of a structure reduces; the ratio of the number of surface to bulk atoms, which increases with reducing particle size.¹ Therefore surface property plays a critical role in determining the optical properties of the NCs. The atoms on the surface of crystal are incompletely coordinated within the crystal lattice. These surface atoms give rise to energetically different electronic levels from those of the bulk levels.^{1,2} These surface states can act as traps for charge carriers and are often responsible for a large Stokes shifted broad defect luminescence and hence comprehensive understanding of the surface mediated photophysical dynamics is very important.²

To address this issue, optical spectroscopy has prevailed as one of the most important and versatile tools available to the experimentalist. While ensemble-averaged results are important, however, they often devoid of detailed information because of averaging effect which can obscure the discrete behaviour of individual particles. Single molecule fluorescence microscopy has emerged as one the most versatile tool to the scientists. Observations at single particle level removes the usual ensemble average, allowing the exploration of hidden heterogeneity in condensed phases as well as direct observation of complex photophysics without synchronization.

Here, we explore the luminescence properties of chemically grown ZnCdS and CdS nanocrystals systems which display broad visible luminescence. However, it is difficult to characterize the linewidths of the defect luminescence using ensemble photoluminescence (PL) measurements. Conversely, if photophysical properties of NCs can be probed at single-particle level, it is possible to decouple such homogeneous broadening effects arising from particle-size distributions. Herein, we demonstrate that the defect PL, irrespective of their transition energies, almost all single-particle emission profiles are found to have large spectral line-width (FWHM~400 meV). We also observe a small variation in the transition energies of individual NCs and this may be assigned to the particle size distribution as revealed by transmission electron microscopy image (data not shown). To further confirm our findings, we also recorded single particle PL spectroscopy of CdS NCs. This study conclusively establishes that defect luminescence semiconductor NCs are inherently broad due to distribution of multiple defects.

MATERIALS AND METHODS

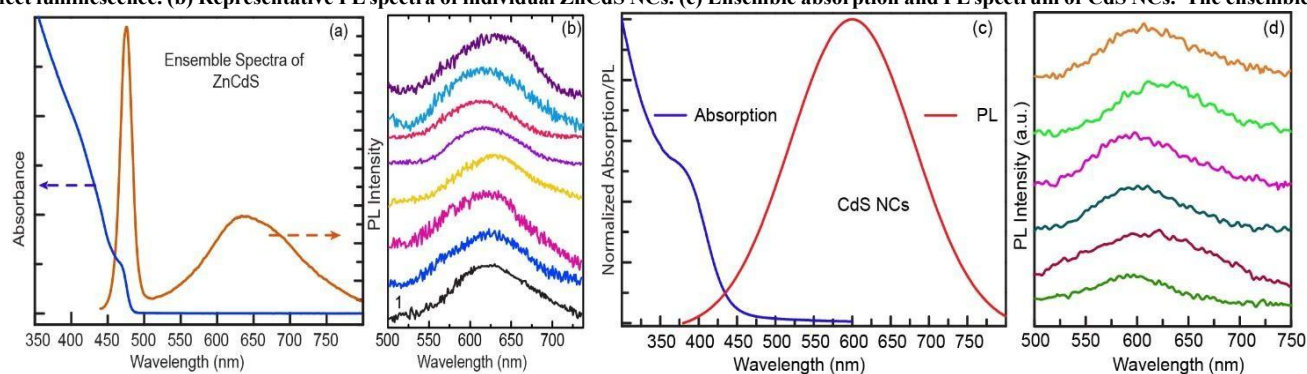
The synthesis of ZnCdS was carried out following the procedure reported elsewhere.³ CdS NCs were prepared by reverse micelle microemulsion method as prescribed in the literatures with few modifications.⁴ Single particle fluorescence microscopic experiments (detail procedures are given reference 5) were performed by appropriate dilution of the colloidal NCs solution and thereafter drop casting on a freshly cleaned fused silica coverslip. For the excitation of ZnCdS we have used 457 nm Ar ion laser while 405 nm diode laser was used for CdS sample. All the experiments were performed at room temperature



RESULTS AND DISCUSSION

The absorption and PL spectrum of ZnCdS solution recorded at room temperature is shown in Figure 1 (a). The absorption spectrum shows sharp excitonic feature at 460 nm. The ensemble PL spectrum shows a narrow band edge luminescence at 480 nm along with a broad defect luminescence band centered around 630 nm. The single particle spectrum of individual NCs shown in Figure 1 (b) are distinctly broad in nature. The line width of single particle spectrum is very large >400 meV as observed in ensemble spectrum. The observed large spectral width of defect luminescence is due to the presence homogeneously distributed large number of closely spaced defect states within individual NCs. It is worth mentioning that slight variation in the PL emission maxima of individual NCs may be assigned to effect of size distribution. The single particle spectroscopic study further corroborates our proposition that large spectral line-widths of defect luminescence in semiconductor NCs originates primarily from the multiple low lying defect distribution while size distribution may also contribute to a small extent.

Figure 1. (a) Ensemble absorption and PL spectrum of ZnCdS NCs. The ensemble PL spectrum displays sharp excitonic emission along with a large Stokes shifted broad defect luminescence. (b) Representative PL spectra of individual ZnCdS NCs. (c) Ensemble absorption and PL spectrum of CdS NCs. The ensemble PL spectrum



shows only a large Stokes shifted broad defect luminescence. (d) Representative PL spectra of individual CdS NCs. The single particle defect PL spectra shown in (b) and (d) clearly indicate that defect luminescence of single NCs are inherently broad.

CONCLUSION

Single particle PL spectroscopy study reveals that the large spectral line-width of the defect luminescence of semiconductor NCs is primarily due to presence of multiple closely spaced defects within individual NCs. The small variation in the single PL maxima for individual NCs may be assigned to the sample size inhomogeneity. Therefore, our proposition is quite general that defect luminescence of semiconductor NCs is inherently broad and is independent of materials and synthesis processes.

ACKNOWLEDGMENT

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Zirconium-Coordinated Multivariate Metal–Organic Framework (Zr-Adipic-2ata) For Electrochemical Energy Storage Applications

Soumi Patra^{1*}, Kausik Sardar², Basudeb Dutta³, Indrajit Bhattacharyya¹, Vemele Hiese Vadeo², Dipankar Das², Ratan Mandal⁴, Biswajit Das²

¹Department of Applied Science and Humanities, Guru Nanak Institute of Technology, Sodepur, Panihati; Kolkata-700114, India

²Nanoelectronics for Energy and Smart Technologies (NEST) Lab, Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer math, Kolkata - 700074, India

³Department of Chemistry, School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT) Deemed to be University, Bhubaneswar-751024, Odisha, India.

⁴School of Energy Studies, Jadavpur University, Kolkata- 700032, India
E-mail (soumi.patra@gnit.ac.in)

INTRODUCTION

Zirconium-coordinated multivariate metal–organic frameworks (MTV MOFs) represent an emerging class of crystalline porous materials built upon robust zirconium oxide clusters. These hybrid frameworks incorporate multiple organic linkers within a single structure, enabling tunable chemical functionality while maintaining structural integrity. Typically, Zr-MOFs are constructed from $\text{Zr}_6\text{O}_4(\text{OH})_4$ nodes interconnected with dicarboxylate ligands and their derivatives, offering exceptional thermal and chemical stability. The incorporation of diverse linkers in MTV MOFs provides a versatile platform for designing advanced materials for energy-related applications.

In this work, we report the synthesis and electrochemical investigation of a novel zirconium-based MTV MOF, Zr-Adipic-2ATA, designed for energy storage applications.

MATERIALS AND METHODS

Zr-Adipic-2ATA was synthesized via a solvothermal method using adipic acid and 2-aminoterephthalic acid as mixed organic linkers. The synthesis was carried out under controlled temperature and pressure conditions to ensure the formation of a crystalline framework.

The as-prepared material was characterized using Scanning Electron Microscopy (SEM) for morphological analysis, Single Crystal X-ray Diffraction (SCXRD) for structural confirmation, Thermogravimetric Analysis (TGA) for thermal stability, and Brunauer–Emmett–Teller (BET) analysis for porosity evaluation.

Electrochemical properties were investigated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) in a 1 M KOH electrolyte solution.

RESULTS AND DISCUSSION

The structural characterization confirms the successful formation of a zirconium-based multivariate framework with high crystallinity and porosity. SEM images reveal a well-defined morphology, while BET analysis indicates a high surface area suitable for electrochemical applications. TGA results demonstrate excellent thermal stability of the framework.

Electrochemical studies show that the Zr-Adipic-2ATA electrode exhibits distinct redox peaks in cyclic voltammetry, indicating a battery-type faradaic charge storage mechanism. The presence of multiple functional linkers enhances the electrochemical activity by providing diverse active sites.



Electrochemical impedance spectroscopy reveals low internal resistance and efficient charge transport within the framework, suggesting improved conductivity and ion diffusion pathways. The synergistic effect of mixed organic linkers and stable zirconium clusters contributes to enhanced electrochemical performance.

These findings highlight the potential of Zr-Adipic-2ATA as a promising electrode material for next-generation energy storage devices.

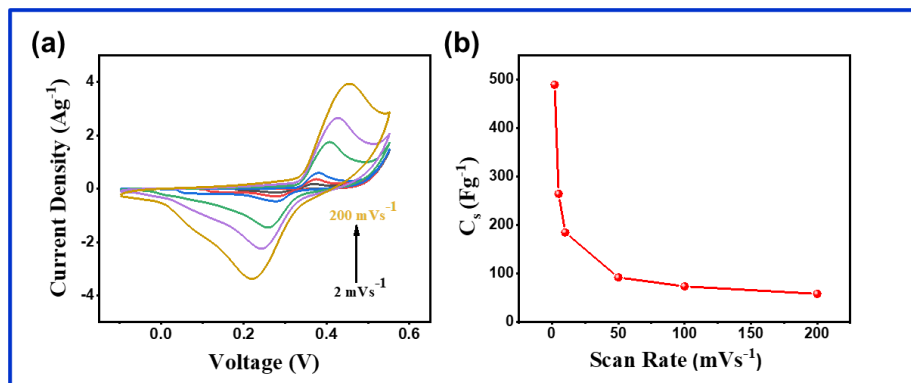


Figure 1: Cyclic Voltammetry Profiles at Different Scan Rates and Variation of Specific Capacitance with Scan Rate for Zr-Adipic-2ATA Electrode

The electrochemical performance of the Zr-Adipic-2ATA electrode was evaluated using cyclic voltammetry at various scan rates. The CV curves exhibit well-defined redox peaks, confirming a faradaic charge storage mechanism characteristic of battery-type behavior. It is observed that at a low scan rate of 2 mV s⁻¹, the electrode delivers the highest specific capacitance of 489.25 F g⁻¹, indicating efficient ion diffusion and maximum utilization of active sites within the porous framework. As the scan rate increases, the specific capacitance gradually decreases, which can be attributed to limited ion accessibility and reduced interaction time between electrolyte ions and electrode material. These results demonstrate the excellent electrochemical capability of the synthesized Zr-Adipic-2ATA and its suitability for high-performance energy storage applications.

CONCLUSION

A novel zirconium-based multivariate MOF, Zr-Adipic-2ATA, has been successfully synthesized and evaluated for electrochemical energy storage applications. The material exhibits high porosity, excellent thermal stability, and efficient charge transport properties. The observed faradaic behavior confirms its suitability for battery-type energy storage systems. The study demonstrates that multivariate linker engineering is an effective strategy for enhancing the electrochemical performance of MOFs.

ACKNOWLEDGMENT

The authors would like to acknowledge the support of the ANRF PE ECRG Grant (No. ANRF/ECRG/2024/002117/PMS) for providing financial assistance and experimental facilities to carry out this work. The authors also sincerely thank the JIS Group for providing the necessary facilities to conduct this research.

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Oral Presentation – OP-25

Nonlinear Optical Properties of MoS₂ Nanoflakes Using SSPM Technique

**Souvik Ghosh^{1*}, Vemele Hiese Vadeo¹, Krishnendu Jana¹, Subhajit Saha², Dipankar Das¹,
and Biswajit Das¹**

¹Nanoelectronics for Energy and Smart Technologies (NEST) Lab, Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer math, Kolkata - 700074, India

²Department of Renewable Energy Engineering, Maulana Abul Kalam Azad University of Technology, West Bengal, Haringhata-741249, West Bengal, India
Email: souvikghosh3012@gmail.com

INTRODUCTION

Two-dimensional transition metal dichalcogenides (TMDs) have attracted significant attention due to their excellent optical and electronic properties. Among them, molybdenum disulfide (MoS₂) exhibits strong light–matter interaction and promising nonlinear optical behaviour, making it suitable for photonic applications.

Spatial Self-Phase Modulation (SSPM) is an effective technique for studying third-order nonlinear optical properties through self-diffraction ring formation under laser excitation. In this work, SSPM experiments were performed on MoS₂ nanoflakes to investigate their nonlinear optical response. The nonlinear refractive index (n_2) and third-order nonlinear susceptibility ($\chi^{(3)}$) were estimated from the variation of diffraction ring number with laser intensity.

MATERIALS AND METHODS

MoS₂ nanoflakes were dispersed in NMP to prepare a stable colloidal suspension. The prepared solution was placed inside a quartz cuvette of fixed path length. A continuous wave laser beam was used as the excitation source and focused onto the sample using a convex lens. The transmitted beam produced self-diffraction ring patterns on a screen placed at a certain distance from the sample.

The number of diffraction rings was recorded at different laser intensities. The nonlinear refractive index was calculated using: $n_2 = \frac{\lambda}{2n_0 L_{eff}} \left(\frac{dN}{dI} \right)$... (1) where: λ = wavelength of incident laser, n_0 = linear

refractive index of MoS₂, L_{eff} = effective optical path length, $\frac{dN}{dI}$ = slope of ring number vs intensity graph

The third-order nonlinear susceptibility was determined using:

$$\chi^{(3)} = \frac{cn_0^2}{12\pi^2} \times 10^{-7} n_2 \quad \dots (2)$$

where c is the velocity of light.

RESULTS AND DISCUSSION

Under laser illumination, MoS₂ exhibited clear concentric diffraction rings due to SSPM. The number of rings increased linearly with increasing laser intensity, indicating strong nonlinear optical behaviour. The formation of diffraction rings confirms phase modulation caused by intensity-dependent refractive index variation. The slope of ring number versus laser intensity was extracted from experimental data and used to calculate n_2 . The obtained nonlinear refractive index was found to be of the order of $10^{-6} \text{ cm}^2/\text{W}$, while the total third-order susceptibility was estimated in the order of 10^{-2} esu , indicating good third-order nonlinear response in MoS₂. These results suggest that MoS₂ can be utilized for



optical switching, modulation, and photonic device applications.

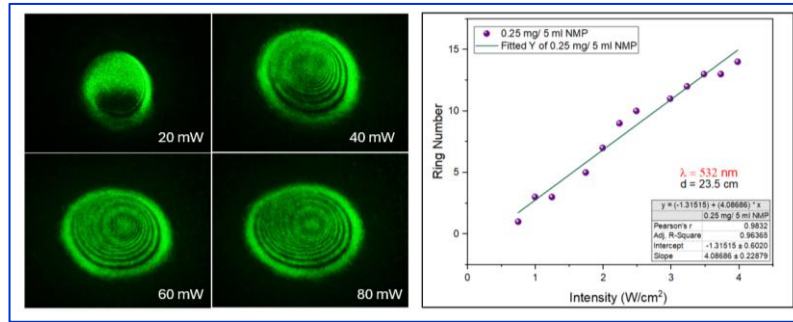


Figure 1. Intensity vs Ring number graph (0.25 mg MoS₂/ 5 mL NMP)

Table 1. Determination of $\chi^{(3)}$ and n_2 for MoS₂

λ [nm]	L [mm]	C [mg mL ⁻¹]	dN/dI [cm ² W ⁻¹]	n_2 [cm ² W ⁻¹]	$\chi^{(3)}$ total [esu]
532	10	0.2	5.32	3.4×10^{-6}	0.0151
532	10	0.1	4.88	3.1×10^{-6}	0.0139
532	10	0.05	4.09	2.6×10^{-6}	0.0116

CONCLUSION

SSPM experiments were successfully performed on MoS₂ nanoflakes to study their nonlinear optical properties. The diffraction ring analysis confirmed strong optical Kerr nonlinearity. The calculated n_2 and $\chi^{(3)}$ values demonstrate that MoS₂ is a promising material for nonlinear photonic applications. $n_2 = 3.4 \times 10^{-6}$ cm² W⁻¹ and $\chi^{(3)} = 0.0151$ esu is found for the 1 mg/mL concentration.

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Oral Presentation – OP-26

Optimizing Cow Urine as a Potential Electrolyte in MoS₂ based Catalyst for Hydrogen Evolution Reaction

Vemele Hiese Vadeo^{1*}, Souvik Ghosh¹, Krishnendu Jana¹, Subhajit Saha², Dipankar Das¹, and Biswajit Das¹

¹Nanoelectronics for Energy and Smart Technologies (NEST) Lab, Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer math, Kolkata - 700074, India

²Department of Renewable Energy Engineering, Maulana Abul Kalam Azad University of Technology, West Bengal, Haringhata-741249, West Bengal, India

Email: melhvadeo@gmail.com

INTRODUCTION

The search for sustainable and cost-effective electrolytes in hydrogen evolution reaction (HER) compared to conventional acidic media such as sulfuric acid (H₂SO₄) has led us to look for alternatives as well as promote circular economy principles. In this study, cow urine is investigated as a potential natural electrolyte, paired with molybdenum disulfide (MoS₂) as a catalyst, and compared against the benchmark H₂SO₄ system. Cow urine, rich in urea, salts, and organic compounds, offers ionic conductivity and eco-friendly availability, while MoS₂ provides high catalytic activity due to its layered structure and abundant active sites. In order to increase the ionic mobility, DI water was added at a 50:50 ratio which was observed to be the optimum condition for ionic mobility.

MATERIALS AND METHODS

MoS₂ Synthesis: MoS₂ was synthesized via Hydrothermal Process. Sodium Molybdate (Na₂MoO₄) precursor was mixed well in DI water. Thiourea as Sulphur precursor was added and stirred till a homogeneous solution was obtained. Then, the entire solution was transferred to an autoclave and kept in a Hot Air Oven at 180°C for 12-24 hours and cooled down naturally. The solution was then washed with DI water and dried to extract MoS₂ nanoflakes.

Cow Urine sample was obtained from a local Dairy and then a 50:50 ratio DI water solution was prepared. MoS₂ was drop casted on a Glassy Carbon Electrode and dipped into the solution as a catalyst. The entire experiment was conducted via a Potentiostat and compared with a 1M H₂SO₄ Electrolyte solution.

RESULTS AND DISCUSSION

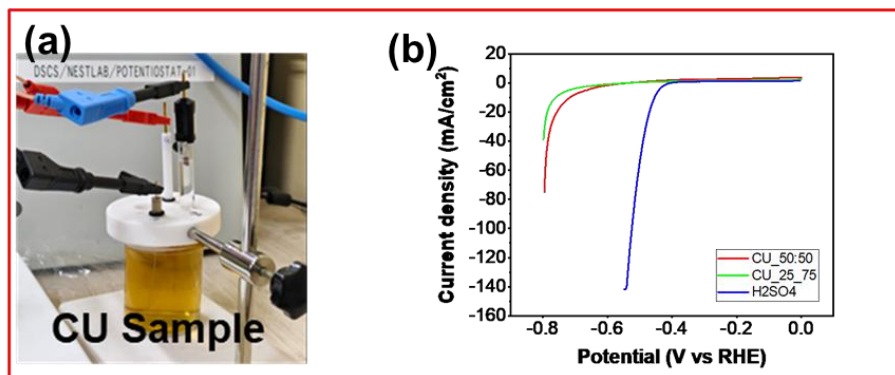


Figure 1. (a) Experimental Setup. three electrode Potentiostat dipped in Cow Urine sample. (b) Linear Sweep for H₂SO₄, CU 50:50 and CU 25:75 electrolyte solution.

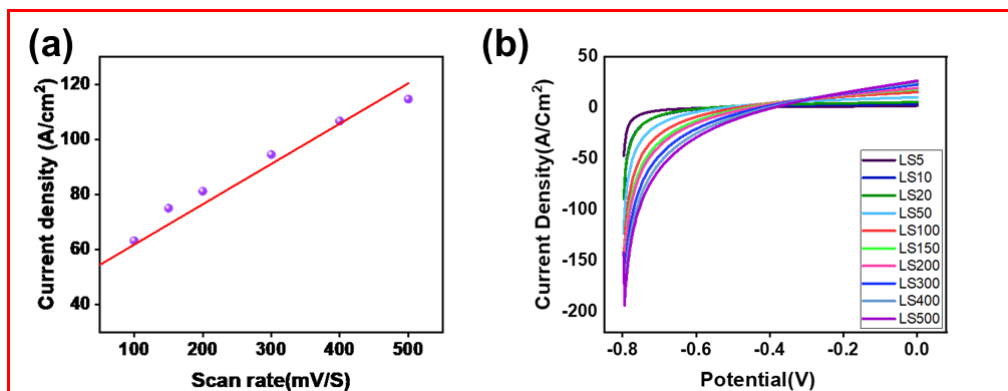


Figure 2. (a) Linear fit for CU 50:50 ratio. (b) Linear Sweep for CU 50:50 at different scan rates.

CONCLUSION

Despite the presence of organic compounds in Cow urine, we can observe an improvement in HER by optimum dilution with DI water as compared to CU_25:75. However, further study and optimizing different Catalyst variation is needed for HER using Cow Urine as an electrolyte.

ACKNOWLEDGMENT

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Oral Presentation – OP-27

Probing Third-Order Nonlinear Refractive Index and Susceptibility of V₂O₅ using SSPM-Based Self-Diffraction Technique

Indrajit Bhattacharyya^{1*}, Kausik Sardar², Soumi Patra¹, Vemele Hiese Vadeo², Dipankar Das², Biswajit Das²

¹Department of Applied Science and Humanities, Guru Nanak Institute of Technology, Sodepur, Panihati; Kolkata-700114, India

²Nanoelectronics for Energy and Smart Technologies (NEST) Lab, Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer math, Kolkata - 700074, India

E-mail (indrajit.bhattacharjee@gnit.ac.in)

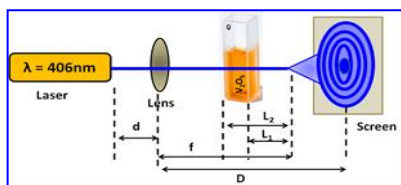
INTRODUCTION

Measurement of nonlinear optical (NLO) parameters of materials with strong dielectric response under the illumination of an intense laser beam has received significant attention in the field of potential applications and fabrications of photonic devices. When an intense coherent laser beam with a finite cross-section is allowed to pass through materials, a unique phase modulation is induced in the spatial profile of the incident beam. The present paper attempts to explore the third-order optical nonlinear response of V₂O₅ in N-methyl-2-pyrrolidone (NMP) at the exciting wavelength of 406nm. The simple optical setup involving a CW diode laser evaluates the nonlinear refractive index (n_2) and the third order non-linear susceptibility ($\chi^{(3)}$) of the sample by analyzing the modulation of SSPM¹ signals resulting from the laser power dependent expansion and deformation of self-diffraction rings generated inside the sample with the help of “Wind Chime” model². Our study thus attempts to provide valuable insights on the nonlinear optical properties of V₂O₅ from the study on self diffraction of light that may have potential applications on the advancement of all-optical future devices.

MATERIALS AND METHODS

V₂O₅ nanorods were synthesized using hydrothermal method³. Initially, 0.36 g of V₂O₅ was dissolved in 30 mL of deionized water, followed by the dropwise addition of 5 mL of 30% H₂O₂ under continuous stirring for 30 minutes. The resulting solution was transferred to a 40 mL Teflon-lined autoclave and heated at 190 °C for 24 hours. After natural cooling, the precipitate was collected, washed with deionized water, and dried at 70 °C. Finally, the product was annealed at 450 °C for 1 hour to obtain well-defined V₂O₅ nanorods.

Here we investigate the third order nonlinear optical susceptibility ($\chi^{(3)}$) of V₂O₅ in N-methyl-2-pyrrolidone (NMP) induced by strong Kerr nonlinear effect at 406nm where the refractive index of the material shows a strong dependence on the intensity of the incident laser light (figure 1). A CW blue diode laser with a maximum power of 40 mW is focused inside the sample in the quartz cuvette with a lens ($f=20\text{cm}$) which induces a strong self-focusing effect and consequently results in the formation of concentric diffraction rings on a white screen in the far field. A digital





camera placed behind the screen enables to capture the continuous evolution and deformation of the self-diffraction rings resulting from the thermal blooming with a change in the intensity of the incident laser light.

Figure 1. The schematic of the experimental setup for measuring SSPM signal from samples

RESULTS AND DISCUSSION

The nonlinear refractive index (n_2) of V_2O_5 can be determined from the following formula:

$$n_2 = (\lambda / 2n_0 L_{\text{eff}}) \times dN/dI \quad (1)$$

where n_0 is the linear refractive index of the sample, L_{eff} is the effective propagation path passing through the sample dispersion and dN/dI is the slope of the N (number of the concentric rings captured on the far field) vs I (intensity of the incident laser light in Wcm^{-2}) plot. The third order nonlinear susceptibility $\chi^{(3)}$ of the sample is further determined by:

$$\chi^{(3)} = (cn_0^2/12\pi^2) \times 10^{-7} n_2 \text{ (esu)} \quad (2)$$

where c is the velocity of light in sapce. Figure 2 shows the vriation of the diffraction ring numbers as a function of the intensity of the incident laser beam at 406nm. Each data is collected after a sufficient duration of the exposure of the laser beam on the sample. The result clearly shows that the number of rings and their diameters increase with the increase of the laser beam intensity which results from the strong nonlinear response of V_2O_5 at the incident wavelength at 406nm. The solid points reperesent our experiemntal data and the straight line reperesnts the fitted linearity based on the experiemntal data (figure 2). The corresponding slope (dN/dI) at 406 nm evaluates the total third order nonlinear susceptibility from the equation (2).

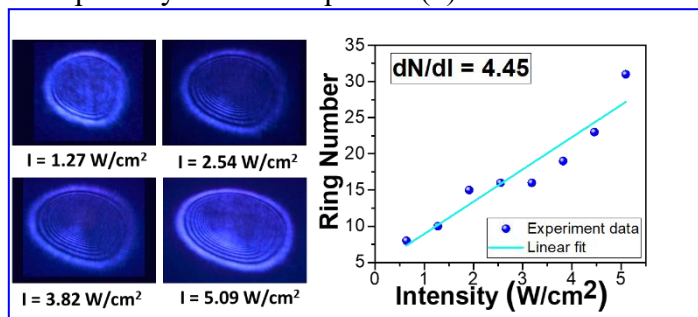


Figure 2. Evolution of rings with the change of laser intensity and the plot of diffraction ring numbers vs laser intensity for V_2O_5 at 406nm using NMP as the solvent

CONCLUSION

In summary, we have investigated the third order optical response of V_2O_5 in NMP using SSPM method at 406nm. The whole coherent light-matter interaction in the sample has been analyzed using the Wind-Chime model that offers significant explanation for the underlying mechanism behind the observed NLO behavior and thus offers innovative insights on all-optical device applications using such nonlinear optical materials.

ACKNOWLEDGMENT

The authors would like to acknowledge the support of the ANRF PE ECRG Grant (No. ANRF/ECRG/2024/002117/PMS) for providing financial assistance and experimental facilities to carry out this work. The authors also sincerely thank the JIS Group for providing the necessary facilities to conduct this research.

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Oral Presentation – OP-28

Resistive Switching Characteristics of Hydrothermally Synthesized TiO₂ for Memristor-Based MIM Devices

Krishnendu Jana^{1*}, Souvik Ghosh¹, Vemele Hiese Vadeo¹, Dipankar Das¹, and Biswajit Das¹

¹Nanoelectronics for Energy and Smart Technologies (NEST) Lab, Department of Basic Science & Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer math, Kolkata - 700074, India

E-mail (krishnendujana474@gmail.com)

INTRODUCTION

With the rapid growth of data intensive technologies such as artificial intelligence, data analytics and internet of things (IOT) the global demand for large scale data storage and energy efficient data processing has increased exponentially. Under such circumstances, Parallel computing has emerged as a prominent solution. However, the traditional von Neumann architecture inherently suffers from von Neumann bottleneck due to its physical separation of the memory and processing units.

In this context, memristors have emerged as a promising solution. These are two terminal devices that predominantly work on the phenomenon called, “Resistive Switching”. Resistive switching (RS) devices encode information through programmable changes in resistance, which means the resistance across the layer of an RS device depends upon the applied voltage across the layer. Their low energy consumption during operation and excellent data retention makes them an attractive candidate for a wide range of applications (such as non-volatile storage, logic, radiofrequency communication). A typical RS device is a metal-insulator-metal (MIM) stack, with insulating layers consisting of oxide materials or chalcogenides. In this study we have considered Titanium dioxide (TiO₂) synthesised through hydrothermal process as the main functional layer for the MIM structure.

MATERIALS AND METHODS

The synthesis of TiO₂ thin film layer on fluorine-doped tin oxide (FTO) substrate was done through hydrothermal process. 1st the FTO samples were cleaned using a cleaning solution prepared by mixing acetone, 2-propanol and DI water in 1:1:2 ratio. Then the FTOs were dried. For the hydrothermal process, 30ml of DI water and 30ml of HCl was mixed very slowly for 30 minutes using magnetic stirrer. Then 1ml of Titanium (IV) butoxide (Ti(OBu)₄) is added drop by drop and mixed for another 5 minutes. The whole solution was then transferred to a teflon autoclave. After that the FTO was submerged inside the solution using glass slides and sealed. The autoclave was heated gradually to a 180°C inside an hot air oven for one hour and gradually cooled down.

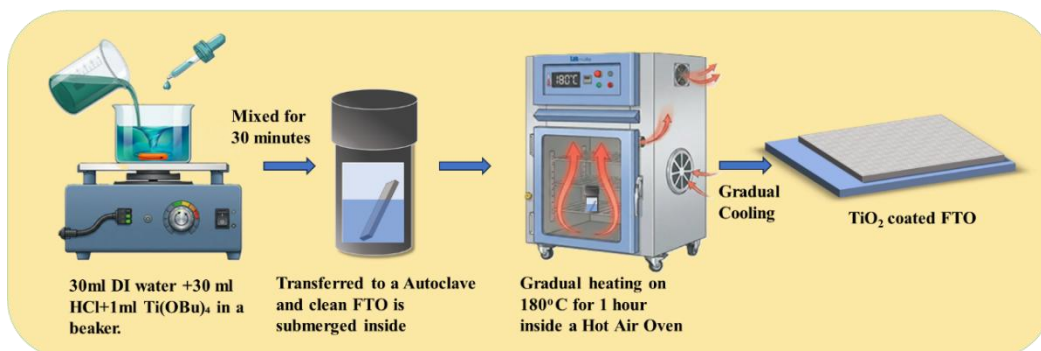


Fig-1: Schematic representation for Hydrothermal synthesis of TiO₂ film on FTO



RESULTS AND DISCUSSION

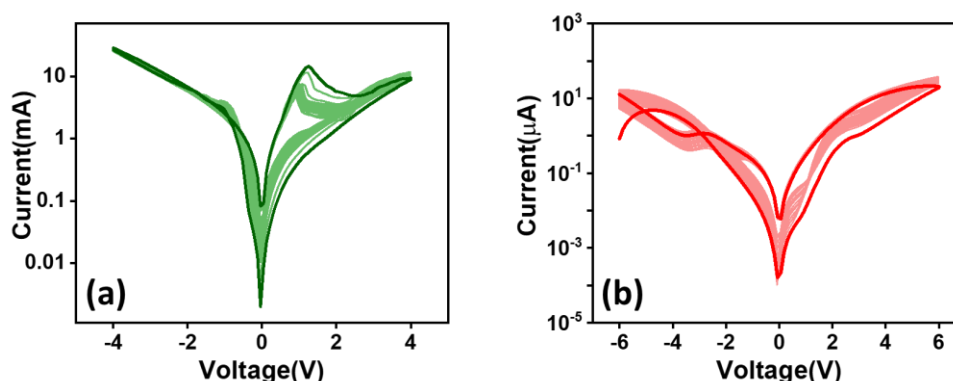


Fig-2: V vs log I curve for (a) unannealed TiO₂, (b) Annealed TiO₂

The resistive switching characteristics of the TiO₂ based device were systematically tested through current-voltage (logI vs V) measurements. The device exhibits clear RS behavior between +4V and -4V with a switching ratio of 10², shown in [fig-2(a)]. The set process corresponding to low resistive state (LRS) is around -2V and the reset process corresponding to high resistive state (HRS) is around +4V. LRS indicates the formation of conducting path through TiO₂ layer conversly the HRS indicates the rupture of conducting path. The formation of conducting path is facilitated by the intrinsic oxygen vacancies of TiO₂ layer. When the device was annealed at 400°C for 30minutes the intrinsic vacancies were removed and the switching almost vanishes decreasing the ration to almost 10, shown in [fig-2(b)].

CONCLUSION

TiO₂ demonstrates reliable resistive switching, making it suitable for memristor applications. The switching mechanism is governed by oxygen vacancy migration and filament formation. Annealing reduces oxygen vacancies, leading to the disappearance of resistive switching behavior

ACKNOWLEDGMENT

The authors would like to acknowledge the support of the ANRF PE ECRG Grant (No. ANRF/ECRG/2024/002117/PMS) for providing financial assistance and experimental facilities to carry out this work. The authors also sincerely thank the JIS Group for providing the necessary facilities to conduct this research.

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Oral Presentation – OP-29

Enhanced Electrochemical Performance of MnWO₄-aCNT Hybrid for Supercapacitor ApplicationsKausik Sardar^{1,3}, Subhasish Thakur¹, Kalyan Kumar Chattopadhyay²¹School of Materials Science and Nanotechnology, Jadavpur University, India²Department of Physics, Jadavpur University, India³Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, JIS Group, India

E-mail: (kausik.sardar@dsec.ac.in)

INTRODUCTION

The increasing demand for sustainable energy storage has accelerated research on electrochemical supercapacitors (SCs), known for high power density, fast charge-discharge rates, and long cycle life. SCs are classified into electrochemical double-layer capacitors (EDLCs) and pseudocapacitors. While carbon-based EDLCs offer excellent power performance, their low specific capacitance limits energy storage. In contrast, transition metal oxide (TMO)-based pseudocapacitors provide higher energy density but suffer from poor electrical conductivity.

To overcome these limitations, hybrid materials combining TMOs with conductive carbon frameworks have emerged as an effective strategy. In this work, a MnWO₄-amorphous carbon nanotube (aCNT) hybrid is developed via a cost-effective approach, enhancing electron transport, surface area, and electrolyte accessibility.

The MnWO₄-aCNT electrode delivers a high specific capacitance of **764 F g⁻¹** with excellent cycling stability (~100% retention after 10,000 cycles). A solid-state asymmetric device further exhibits an energy density of **8.4 Wh kg⁻¹** and a power density of **560 W kg⁻¹**, highlighting its potential for advanced energy storage applications.

MATERIALS AND METHODS

Amorphous carbon nanotubes (aCNTs) were synthesized via a low-temperature solid-state method using ferrocene and NH₄Cl. MnWO₄ nanorods were prepared hydrothermally from manganese acetate and sodium tungstate at 200 °C. The MnWO₄-aCNT hybrid was obtained by in situ hydrothermal growth of MnWO₄ on aCNTs.

Electrochemical performance was evaluated in 1 M KOH using a three-electrode setup with nickel foam as the working electrode. Cyclic voltammetry, charge-discharge, and impedance analyses were employed.

RESULTS AND DISCUSSION

Structural and morphological analyses confirm the formation of MnWO₄ nanorods uniformly anchored on a 1D aCNT network, resulting in enhanced surface area and porosity. The hybrid electrode exhibits superior electrochemical performance compared to individual components, achieving a high specific capacitance of **764 F g⁻¹** at 2 mV s⁻¹ with excellent rate capability. GCD and EIS results indicate improved charge transfer, reduced resistance, and faster ion diffusion. The electrode also demonstrates outstanding cycling stability with ~100% capacitance retention and coulombic efficiency after 10,000 cycles. Furthermore, a solid-state asymmetric supercapacitor device delivers an energy density of **8.4 Wh kg⁻¹** and a power density of **560 W kg⁻¹**, attributed to the synergistic interaction between conductive aCNTs and redox-active MnWO₄.

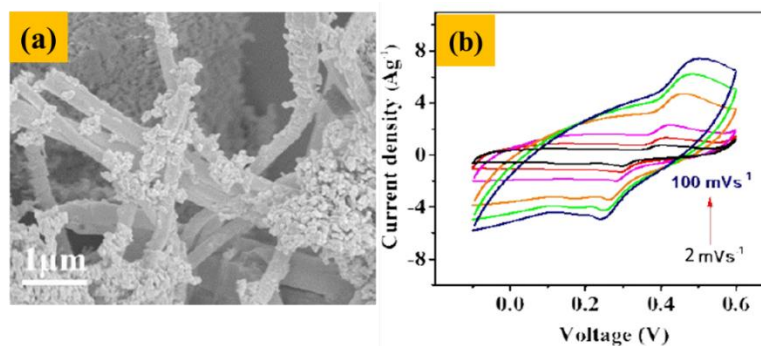


Figure (a) FESEM image of the hybrid, (b) CV curves of MnWO₄-aCNT electrodes at different scan rates.

CONCLUSION

A MnWO₄-aCNT hybrid electrode was successfully developed via a simple and scalable synthesis route. The hybrid structure significantly enhances electrochemical performance through improved conductivity, higher surface area, and synergistic redox activity.

The fabricated device exhibits high capacitance, excellent cycling stability, and competitive energy and power densities. This study provides a promising pathway for designing efficient, stable, and cost-effective hybrid electrode materials for next-generation supercapacitor applications.

ACKNOWLEDGMENT

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**Oral Presentation – OP-30****Light-Induced [2 + 2] Cycloaddition Triggers Photosalient Behaviour with Structural Transformation, and detection of Fe³⁺ in aqueous solvent by Zn(II) Crystals**

Koushik Saha, 1 Mohammad Hedayetullah Mir*2 and Chittaranjan Sinha*1

1 Department of Chemistry, Jadavpur University, Kolkata 700032, West Bengal, India.

2 Department of Chemistry, Aliah University, Kolkata 700156, West Bengal, India.)

INTRODUCTION

Recently, solid-state [2+2]-photocycloaddition reactions have gained significant attention because of the stimulating post-synthetic structural modification and photosalient effect. This property makes them promising candidates for wireless actuators for positioning of research applications in flexible electronics, sensors, photoactuators, photoswitches, and artificial muscles. Various mechanical motions, including bending, twisting, expansion, jumping, crawling, peeling, and wiggling can be generated through structural transformation via partially or completely dimerized structure. The photoreaction may not proceed uniformly throughout the entire crystal due to high molecular absorbance or competing side reactions. Following a violent photosalient effect, maintaining structural integrity sufficient to enable SCSC transformation is particularly challenging. Consequently, green and hazard-free synthetic pathway to achieve such transformations remains difficult. A clear boundary between the mechanical motion and SCSC transformation is difficult to define, and such transformations remain challenging. Photosalient behaviour originates from stress generated by uneven, light-induced structural changes, typically involving anisotropic expansion or contraction of the crystal unit cell, arising from processes, such as azobenzene isomerization, diarylethene cyclization, and other topochemical reactions.

MATERIALS AND METHODS

All reagents, including 4-(1-naphthylvinyl) pyridine (4-NVP), 1H-pyrrole-3-carboxylic acid (HPy3CA), and zinc nitrate hexahydrate [Zn(NO₃)₂·6H₂O] were purchased from Sigma-Aldrich and used as without further purification. Deionized (DI) water was employed throughout all experimental procedures. 1H NMR spectra were recorded using a JEOL JNM-ECZ400S/L1 spectrometer operating at 400 MHz, with DMSO-d₆ as the solvent and tetramethylsilane (TMS) as the internal reference. FT-IR spectra were acquired using a PerkinElmer RX1 Fourier-transform infrared spectrophotometer. Single-crystal X-ray diffraction (SCXRD) data for all compounds were collected at low temperature using an Oxford Diffraction Supernova diffractometer equipped with an INCOATEC microfocus Mo-K α X-ray source ($\lambda = 0.71073 \text{ \AA}$) and multilayer optics. Powder X-ray diffraction (PXRD) patterns were recorded at ambient temperature using a Bruker D8 ADVANCE diffractometer with Cu K α radiation ($\lambda = 1.548 \text{ \AA}$), operated at 40 kV and 40 mA, over a 2θ range of 5–55°.

RESULTS AND DISCUSSION

Photosalient molecular crystals offer a powerful platform for converting light into mechanical motion. Here, we report a discrete Zn(II) complex, [Zn(4-NVP)₂(Py3CA)₂] (1) [HPy3CA = 1H-pyrrole-3-carboxylic acid; 4-NVP = 4-(1-naphthylvinyl) pyridine], which exhibits “photosalient effect” under UV-light manifested as rapid bending, delamination, cracking, hopping, and popping. A stereoselective [2+2] photo-dimerization forms 1,3-bis(4'-pyridyl)-2,4-bis(naphthyl)cyclobutane moiety, leading to one-dimensional coordination polymer [Zn₂(4-NVP)₄(Py3CA)₄]_n (2) through single crystal to single crystal (SCSC) structural transformation. For the first time, the SCSC alteration of 1 to



2 via anisotropic distortion is investigated via stepwise intermediate formation with time-dependent quasi in-situ single-crystal XRD. Interestingly, photosalient behaviour of 1 is retained in 1-polyvinyl alcohol composite, which displays light-induced bending, walking, and swimming like photomechanical motions, highlighting its potential for flexible and soft photo-responsive devices.

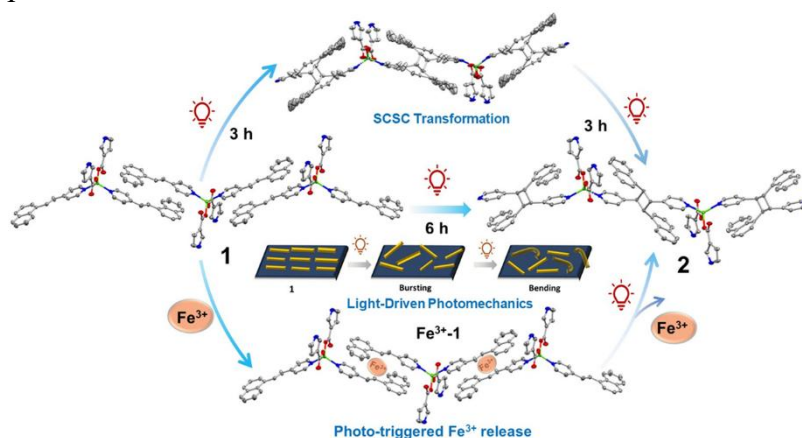


Figure: Schematic illustration of stepwise photodimerization-induced phase transition, photosalient behaviour.

CONCLUSION

In summary, this study demonstrates facile synthesis of a Zn(II)-based single crystal (1) that efficiently converts light into mechanical motion through a photosalient response driven by [2+2] cycloaddition. The 1 undergoes single-crystal-to-single-crystal (SCSC) transformation (2) via anisotropic distortion, characterized through time-resolved quasi in situ X-ray diffraction, supported by powder XRD, ¹H/ ¹³C NMR, UV-Vis, fluorescence, and DFT/ TD-DFT-computational studies providing mechanistic insight into anisotropic distortion and structural transformation. The retention of photomechanical activity in 1-PVA composite permits diverse motions, such as bending, walking, and swimming, emphasizing its applicability in flexible smart materials. This work lays the foundation for the design of photo-responsive crystalline materials endow potential applications in photomechanical actuation with stimuli-responsive ion delivery, opening opportunities in soft robotics, flexible sensor.

ACKNOWLEDGMENT

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Poster Presentation





Production of Hydrogen and Biofuels from Algal Biomass using Aqueous phase reforming process

^{1*}Taanisha Mukhopadhyay, ²Dr.Gourisankar Roy Mahapatra

¹Department of Chemical Engineering,

²Department of Applied Science and Humanities

Haldia Institute of Technology (Autonomy), Haldia 721657, West Bengal, India.

* To whom correspondence should be addressed: E-mail: *grm.chem@gmail.com

ABSTRACT

With the growth of the human population, the need for sustainable resources of energy has increased a lot. Large scale utilisation of fossil fuels would lead to absence of viable energy resources for our future progeny, so, for that we need renewable and clean sources of energy which are called Green Energy Resources.

Biological hydrogen (H₂) production (BHP) enhancement through the use of nanoparticle (NPs) supplements in the media is being recognized in recent times as an encouraging approach. The NPs, including those of metal and metal oxides, have shown a significant improvement in the BHP. A number of organisms as pure or mixed cultures can produce H₂ in presence of NPs from pure sugars and biowaste as a feed. However, their H₂ production efficiencies have been found to vary significantly with the type of NPs and their concentration.

Therefore, Suitable bacteria like *C. butyric* as inoculum and AuNPs provided a suitable approach for efficient H₂ production from sucrose. Also, *Kapahulu's alvarezii* and sludge was processed for bio-hydrogen production.

As a result, Reforming of aqueous phase with 7.5 wt% Au It is found that, with synthetic wastewater containing sucrose as a feed, anaerobic culture resulted in 62.3% higher yield than those to the control applying the minimum amount of AuNPs, remarkably, the H₂ production, overall catalyst showed 61.25% of bio-hydrogen. Maximum bio-hydrogen yield was 36.1% for 2:1 (sludge: algae) at 360°C. The high ratio of acetate to butyrate and low production of ethanol in the presence of AuNPs is associated with a significant increase in H₂ production.

Aqueous phase reforming produces hydrogen from biomass-derived oxygenated compounds such as glycerol, sugars, and sugar alcohols. APR is unique in that reforming is done in the liquid phase. The process generates Biohydrogen without volatilizing water, which represents a major energy saving and therefore produces emission-free Hydrogen from biofuel with the use of macroalgae *Kapahulu's alvarezii* to With the purpose of expanding applications in the field of production of Hydrogen with the help of Bio nanotechnology, the Biosynthesis of Au NPs by aqueous reforming of a synthetic compound (brewery wastewater) is supported on activated Carbon. It is observed that AuNPs has the catalytic performance for the degradation of pollutants at the industrial level.

Therefore, Gold nanoparticles exhibit excellent catalytic degradation and decomposition of pollutants making the environment cleaner and sustainable.



Thus, Hydrothermal gasification (APR) resulted in syngas, biochar and higher H₂ production by liquid phase formation and Anaerobic Digestion of cyanobacterium lead to the breakdown of complex Inorganic and organic compounds in the Industrial Wastewater that led to easy Reforming process. Recent Research with Certain Limitations and Recommendations are also to be taken care of for the Aqueous Phase Reforming Process. It can be used at domestic sectors and small scale Industrial operations for synthetic wastewater treatment and production of biofuels and Biohydrogen since the procedure is costly than the normal established SMR or CFR (Steam Methane Reforming & Catalytic Reforming).

The process including the Bioreactor and Pyrolysis Incineration Plant should be more cost-effective for synthesising Au and H₂ production.

Keywords: Hydrothermal gasification, Macroalgae, Microbial sludge, Bio-hydrogen production (BHP), Aqueous phase reforming (APR), Gold nanoparticles (AuNPs), Anaerobic Digestion

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Cr-doped ZnO nanomaterial-based highly sensitive trace acetone sensor: A potential diabetic breath sensor

Swarnabha Mallik, Srijia De Biswas, Sagnik Das and Debdulal Saha*
CSIR-Central Glass and Ceramic Research Institute, Kolkata, W.B., India
Corresponding Author's E-mail: debdulal.cgcri@csir.res.in

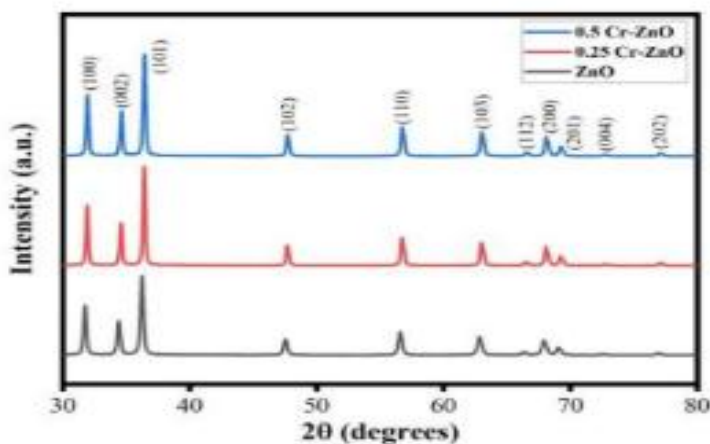
INTRODUCTION

Detection of trace acetone is critical for environmental monitoring and non-invasive health diagnostics. Acetone is the breath biomarker of diabetes. ZnO, a wide bandgap semiconductor, is widely used in Chemi resistive gas sensors due to its stability and sensitivity. However, pristine ZnO suffers from limited selectivity. Cr doping enhances defect chemistry and surface reactivity, improving acetone sensing performance at low concentrations.

MATERIALS AND METHODS

Cr doped ZnO nano powder was synthesized via co-precipitation method using $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ and $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$. NH_4OH was added dropwise (pH 10–12) to precipitate hydroxides of $\text{Zn}(\text{OH})_2$ and $\text{Cr}(\text{OH})_3$. The mixture was aged (12–24 h), centrifuged, washed to neutral pH, dried at 120 °C, and calcined at 400 °C for 2 h [1], yielding crystalline nano powder suitable for gas sensing.

RESULTS AND DISCUSSION



1. XRD

Figure. 1 X Ray Diffraction pattern for the three compositions of ZnO nano powders

The XRD patterns of pure ZnO and Cr co-doped ZnO (0.25 and 0.5 wt%) exhibit well-defined peaks corresponding to the hexagonal wurtzite structure, indicating high crystallinity. No secondary phases are observed, confirming successful Cr incorporation. Slight peak broadening suggests reduced crystallite size. The patterns match the standard JCPDS card no. 36-1451 [2] for ZnO.



2. FESEM

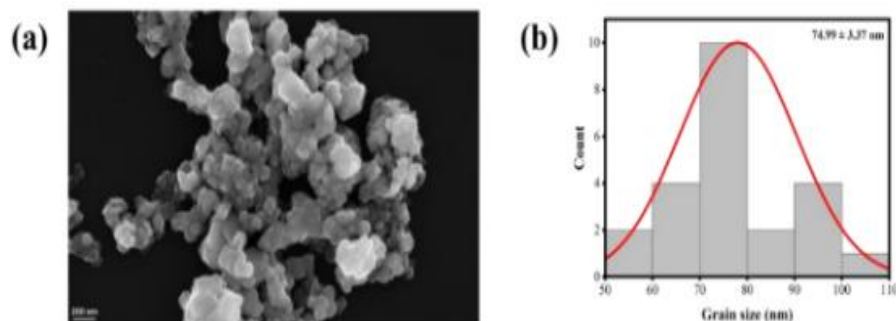


Figure 2. (a) Micrograph of 0.25 wt% Cr co-doped ZnO (b) Histogram with calculated grain size

The FESEM image shows agglomerated, quasi-spherical Cr-doped ZnO nanoparticles with a porous morphology, favourable for gas adsorption. Particle clustering is evident due to high surface energy. The grain size distribution histogram indicates an average particle size of $\sim 74.99 \pm 3.37$ nm, confirming nanoscale dimensions with relatively uniform size distribution.

3. BET

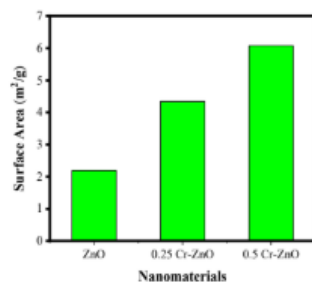


Figure 3. Surface area of the three compositions

We can observe that with increase in dopant concentration the surface area of the ZnO nanoparticles increases at a phenomenal rate, thereby increasing the sensitivity towards the target gas, Acetone. It is shown in Fig. 3(a)

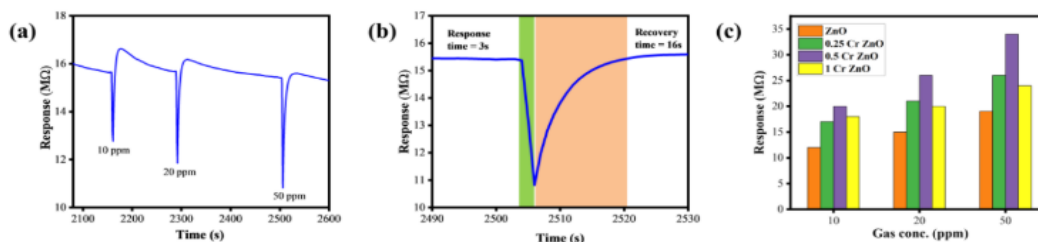


Figure 4. (a) Dynamic Response of 0.5 wt % Cr-ZnO towards diff. conc. of Acetone (b) Response recovery curve (c) Sensitivity comparison among the sensors

0.5 wt% Cr-ZnO has given highest sensitivity (20%) towards 10 ppm Acetone at 350° C among the gas sensors. It has also shown excellent response recovery time towards 50 ppm Acetone. Sensitivity drops for 1 wt% Cr-ZnO as shown in Fig 4 (c).

CONCLUSION: We can infer that Cr-doped ZnO nano powder exhibited enhanced structural and surface properties, as confirmed by XRD, FESEM, and BET analyses. The sensor exhibited n-type sensing characteristics and demonstrated rapid response (3 s) and recovery (16 s) towards 50 ppm acetone, indicating improved sensitivity and kinetics. These results highlight its potential for efficient, fast, and reliable Chemi resistive gas sensing applications.

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Transition Metal Based Electrocatalysts For Green Hydrogen Production

Soumyajit R., Aniruddha R., Mohit K. O., Aditya M., Mayank G., Md Irfan S.

Department of Computer Science and Engineering, Dr. Sudhir Chandra Sur Institute of Technology
and Sports Complex, 540, Dum Dum, Surer math, Kolkata - 700074

E-mail: soumyajitrakshit040@gmail.com

INTRODUCTION

Green hydrogen currently accounts for <1% of global hydrogen production (~95 Mt yr⁻¹ total), yet it is projected to supply ~10–25% of global energy demand by 2050 due to its carbon-neutral nature. Compared to fossil fuel-based hydrogen (SMR efficiency ~65–75%, ~9–12 kg CO₂ per kg H₂), alkaline water electrolysis (AWE) enables zero-emission H₂ generation with system efficiencies of ~60–80% under practical conditions. AWE employs an aqueous KOH/NaOH electrolyte (20–30 wt%), porous Ni-based electrodes, and a diaphragm separator, operating typically at 60–90 °C. The half-reactions are: Hydrogen Evolution Reaction or HER (cathodic half): $2\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + 2\text{OH}^-$ Oxygen Evolution Reaction or OER (anodic half): $4\text{OH}^- \rightarrow \text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^-$ Noble metal catalysts like platinum (Pt) for HER and iridium/ruthenium oxides (IrO₂/RuO₂) for OER have near-zero overpotentials and low Tafel slopes (~30 mV dec⁻¹), suggesting that they are highly efficient. However, their high costs, scarcity and poor long-term economic viability limit large-scale deployment. This has made transition metals-based catalysts promising alternatives with their abundance, tunable electronic structure and competitive catalytic activity in alkaline medium. This review critically covers the development and performance of such catalysts.

2. MATERIALS AND METHODS

This literature review of transition metal-based electrocatalysts for alkaline water electrolysis was conducted using recent research and review articles. Materials include oxides, hydroxides, phosphides, nitrides, carbides, and alloys of Ni, Fe, Co, and Mo. Performance metrics analyzed were overpotential (η @ 10 mA cm⁻²), Tafel slope, exchange current density, and stability (50–100 h). Electronic structure effects, including d-band center and adsorption energies, were also evaluated.

RESULTS AND DISCUSSION

The Oxygen Evolution Reaction (OER), involving a sluggish four-electron transfer pathway, dominates the overall overpotential (η_{total}), often contributing over 70% of energy losses in alkaline electrolysis systems. Typical noble metal catalysts exhibit $\eta \approx 20\text{--}50$ mV (HER, Pt) and 200–300 mV (OER, IrO₂/RuO₂) at 10 mA cm⁻², with Tafel slopes ~30–40 mV dec⁻¹. A comparative summary of representative transition metal-based electrocatalysts is given in Table 1

Table 1



Catalyst Material	Reaction	Overpotential (η @10 mA cm ⁻²)	Tafel slope	Stability
NiFe LDH	OER	~220 mV	~45 mV dec ⁻¹	100 h
Co ₃ O ₄	OER	~300 mV	~60 mV dec ⁻¹	50 h
Ni ₂ P	HER	~120 mV	~50 mV dec ⁻¹	50 h
CoP	HER	~100 mV	~45 mV dec ⁻¹	60 h
NiMo alloy	HER	~80 mV	~40 mV dec ⁻¹	80 h

NiFe-based layered double hydroxides (LDH) demonstrate superior OER activity due to synergistic Ni–Fe electronic coupling, which optimizes adsorption free energies ($\Delta G \approx 1.6$ – 1.8 eV) for intermediates (*OH, *O, *OOH). For HER, transition metal phosphides, nitrides, and alloys exhibit near-optimal hydrogen adsorption ($\Delta G_H \approx \pm 0.1$ eV), facilitating Volmer–Heyrovsky/Tafel pathways and accelerating water dissociation kinetics. Transition metal catalysts can be systematically enhanced via four primary modification strategies:

- Elemental doping (heteroatom incorporation) $\rightarrow$ shifts d-band center ($\Delta \epsilon_d \approx 0.1$ – 0.3 eV), improving adsorption energetics
- Heterostructure/interface engineering $\rightarrow$ induces charge redistribution and interfacial electric fields, lowering kinetic barriers
- Defect engineering (vacancies, dislocations) $\rightarrow$ increases active site density by ~ 2 – $5\times$ and enhances intermediate binding
- Nano structuring/morphology control $\rightarrow$ increases electrochemically active surface area (ECSA) by up to $\sim 10\times$ and improves mass transport.

These strategies collectively:

- Reduce overpotential by ~ 50 – 150 mV
- Lower Tafel slopes to ~ 40 – 60 mV dec⁻¹
- Increase exchange current density (j_0 up to 10^{-3} – 10^{-2} mA cm⁻²)
- Enhance durability to 50–100 h under alkaline conditions

For instance, Co- or Mo-doped NiFe LDH systems achieve Tafel slopes of ~ 40 – 55 mV dec⁻¹ and $\eta \approx 180$ – 220 mV, approaching noble metal benchmarks. Similarly, NiMo alloys outperform most non-noble HER catalysts due to optimized hydrogen binding and enhanced conductivity. Despite these advances, challenges persist in achieving industrially relevant current densities (>500 mA cm⁻²) and long-term stability (>1000 h), along with precise atomic-level understanding of catalytic active sites.

CONCLUSION

Transition metal-based electrocatalysts demonstrate competitive activity in alkaline water electrolysis, achieving $\eta \approx 80$ – 300 mV and Tafel slopes ~ 40 – 60 mV dec⁻¹, approaching noble metal benchmarks. Electronic structure engineering (d-band tuning, defect and interface control) has been key to optimizing adsorption energetics and catalytic kinetics.



However, performance gaps persist at industrial conditions, particularly at high current densities ($>500 \text{ mA cm}^{-2}$) and long-term stability ($>1000 \text{ h}$). Bridging these limitations requires precise control of active sites and standardized evaluation protocols. Advances in transition metal based catalyst design are expected to enable scalable, cost-effective hydrogen production, making them critical for future gigawatt-scale hydrogen systems.

ACKNOWLEDGMENT

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NiO Hollow Nanospheres for High-Performance Supercapacitors

Subhodeep Roy, ^{A1}, Shreya Mukherjee, ^{B2}, Subhadip Karmakar, ^{C3}, Debmalya Maji, ^{D4}, Sayon Modak, ^{E5},
Sushmita Bera, ^{F6}, E-mail: -subhadeep21@gmail.com

INTRODUCTION

Supercapacitors are advanced energy storage devices known for high power density, rapid charge– discharge, and long cycle life. They store energy through electrostatic charge accumulation and fast surface redox reactions, making them more efficient than conventional batteries for quick energy delivery. Nickel oxide (NiO) is a promising electrode material due to its low cost, environmental friendliness, and high theoretical capacitance. However, its practical performance is limited by poor electrical conductivity and low surface area. To overcome these limitations, NiO is designed into hollow and multihulled nanostructures, which provide larger surface area, shorter ion diffusion paths, and better structural stability. Among these, double-shelled NiO structures show superior performance due to an optimal balance between porosity and conductivity. Therefore, NiO hollow nanospheres are highly suitable for high-performance supercapacitor applications.

MATERIALS AND METHODS

Materials: Nickel salts (NiCl₂), carbon spheres (template), urea, KOH electrolyte, and nickel foam were used.

Methods: NiO hollow nanospheres were prepared using a layer-by-layer method with carbon templates, followed by heat treatment. The device works on pseudo capacitance through reversible redox reactions of NiO

RESULTS AND DISCUSSION

NiO hollow nanospheres with single-, double-, and triple-shelled structures were successfully synthesized using the layer-by-layer method. XRD confirmed pure cubic NiO, while SEM and TEM showed clear hollow structures. The double-shelled NiO exhibited the best morphology with a porous structure and highest surface area (~92.99 m²/g). Electrochemical studies revealed pseudocapacitive behaviour, with double-shelled NiO showing the highest performance. It achieved a maximum capacitance of 612.5 F/g and retained about 90% capacity after 1000 cycles, along with low internal resistance. Overall, double-shelled NiO demonstrated superior performance due to its high surface area and efficient ion transport.

TABLE AND FIGURES

Sample	Oxidation Peak Current (A)	Reduction Peak Current (A)	Peak Potential (V)
S-NiO	~0.08	~ -0.07	~0.55
D-NiO	~0.15	~ -0.14	~0.55
T-NiO	~0.05	~ -0.05	~0.55

The table shows that D-NiO has the highest oxidation and reduction peak currents, indicating stronger redox activity and better pseudocapacitive performance compared to S-NiO and T-NiO.

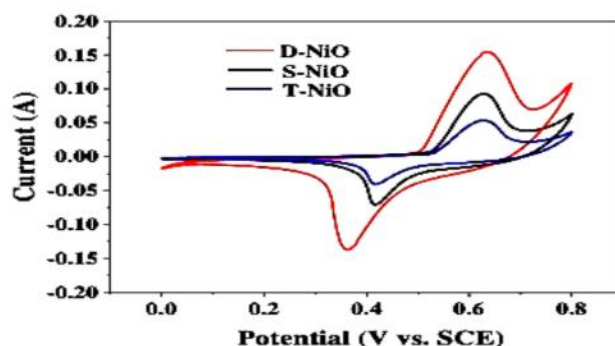


Fig. 6. Cyclic voltammograms of S-NiO, D-NiO and T-NiO at a scan rate of 5 mV s⁻¹.

cyclic voltammetry (CV) graph shows the electrochemical behaviour of S-NiO, D-NiO, and T-NiO at a scan rate of 5 mV/s. All curves exhibit distinct oxidation and reduction peaks, confirming pseudocapacitive redox reactions of NiO. Among the samples, D-NiO displays the highest current response and largest enclosed area, indicating superior capacitance and faster charge transfer. S-NiO shows moderate performance, while T-NiO has the lowest current response. The improved performance of D-NiO is due to its optimized double-shelled structure, which enhances surface area and ion diffusion.

CONCLUSION

NiO hollow nanospheres are promising materials for supercapacitor applications due to their high theoretical capacitance and low cost. The study shows that structural design plays a crucial role in performance. Among the different structures, double-shelled NiO (D-NiO) exhibits the best electrochemical performance, with high specific capacitance, good cycling stability, and low internal resistance. This is mainly due to its higher surface area and efficient ion transport. Therefore, optimizing the nanostructure of NiO is an effective way to enhance supercapacitor performance, making it suitable for future energy storage applications.

ACKNOWLEDGMENT

I would like to express my sincere gratitude to my teacher for their valuable guidance and support in completing this literature survey. I also extend my heartfelt thanks to the Department of Basic Sciences and Humanities, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, for providing the necessary academic support and resources.

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3D Printable Anthropomorphic Prosthetic Finger For Digit Amputation Assistance

Partha Sarathi Ghosh¹, Debjit Misra¹, and Sugato Ghosh^{1*}

¹JIS Institute of Advanced Studies and Research, JIS University, Kolkata

E-mail: drsugato.ghosh@gmail.com

INTRODUCTION

Finger amputations greatly reduce fine motor skills and overall quality of life. Most workplace-related limb loss involves traumatic finger amputations. Traditional prosthetic devices are often very expensive [1]. However, 3D printing has made it easier and more affordable to create customized assistive devices [2]. A review by Ten Kate et al. also suggests that 3D-printed upper limb prostheses can offer better functionality and a more natural, human-like appearance [3]. For limb prostheses, many research groups prefer ABS over PLA because it offers better impact resistance, higher heat tolerance, and greater durability under repeated use [4]. In the present study, focuses on the development of a robust, cost effective, and customizable prosthetic finger design and fabricated through 3D printing process. The proposed design is intended to restore essential hand function and enhance grip strength.

MATERIALS AND METHODS

In the current study, a biomimetic, human-like architecture is used. Model developed using SolidWorks 2025. For the 3D printing process, a fused deposition modeling (FDM) printer, the Reality Ender 3 V2 (Figure 1), was used. The components were fabricated entirely from Acrylonitrile Butadiene Styrene (ABS) plastic using TESSER/CT 1.75mm ABS filament as shown in Figure 1.

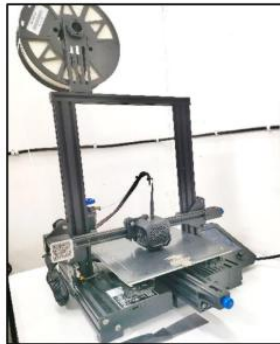


Figure 1. FDM 3D printer with ABS Filament

The fabrication procedure involves pre drying the ABS filament at 80 °C for 4-5 hours to remove moisture. During the printing process, the cooling fan kept at minimum (0-10%) to prevent rapid cooling that leads to warping. Table 1 shows the optimized recommended Values for the 3D Printer Slicing parameters.



Table 1. Slicing Parameters and Recommended Values

Slicing Parameter	Recommended Value	Reason
Infill Density	40%	Balance of weight and compression strength
Infill Pattern	Gyroid	Maximum isotropic strength and impact absorption
Wall Perimeter	3 Layers	Thicker walls significantly reduce breakage
Layer Height	0.08 mm	High resolution improves joint fit and surface finish
Nozzle Temp	260 °C	Ensures optimal melt flow and interlayer bonding
Bed Temperature	110 °C	Prevents warping and improves first-layer adhesion

RESULTS AND DISCUSSION

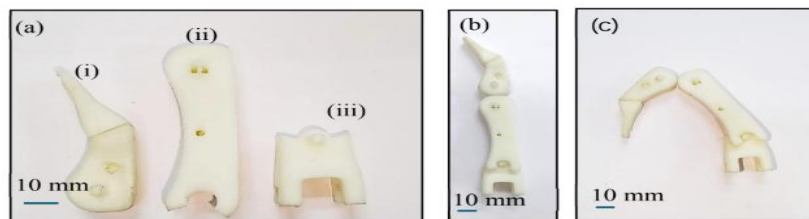


Figure 2. The right-hand index finger is shown in (a) parts, (b) extended and (c) flexed configurations.

CONCLUSION

3D printing offers strong potential for customization, including personalized socket design, as well as adjustments in color, shape, and size. Using ABS plastic provides a highly durable, functional, and low-cost solution. Designing a biomimetic, anthropomorphic prosthetic architecture provides better functionality and grip control. The current approach reduces the cost and complexity of obtaining functional assistive devices for patients with partial hand amputations. Future work will focus on movement and motion control along with clinical validation of grip force.

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Application of an Arsenic Hyper-tolerant Soil Bacterium in Arsenic Bioremediation and Plant Growth Promotion

Apurba Mandal, Nandan Sinha, Saraswat Majumdar, Debjani Mandal, Abhishek Basu*

Department of Molecular Biology and Biotechnology, Sripat Singh College, Murshidabad 742123, India

*Corresponding Author: Dr. Abhishek Basu

E-mail: abasu@sripatsinghcollege.edu.in

INTRODUCTION

The soil and groundwater of the Bhagabangola I block of Murshidabad district, West Bengal, India is severely arsenic contaminated, posing major environmental and agricultural challenges. An indigenous bacterial strain was isolated from the garden soil of the Mahishasthali village, which can tolerate 36.49 mM arsenic (III) and 280.44 mM arsenic (V) making it an arsenic (III and V) hyper-tolerant bacterium. Its growth pattern remains largely unaffected in the presence of 10 mM arsenic (III), emphasizing its strong adaptability in arsenic-stressed environments. Scanning electron microscopic analysis depicted this bacterium to be rod-shaped with a size of $\sim 1.45\mu\text{m}$. 16S rDNA sequencing, followed by subsequent phylogenetic analysis established the identity of the bacterium as *Microbacterium paraoxydans* and further, whole-genome sequencing and analysis of the bacterium confirmed the strain to be *Microbacterium paraoxydans* strain DSM 15019. This bacterium is capable of bioremediation of arsenic due to several arsenic tolerance genes like *arsR*, *arsB*, *arsC* (*ars* operon) and *acr* genes (*acr1*, *acr2*, *acr3*) showing 30.8% and 35.2% bioremediation for 1mM arsenic (III) and 22.6%, and 30.5% of bioremediation for 4mM arsenic (III), over a period of 24 and 48h, respectively. The strain also exhibited multiple plant growth-promoting traits, like atmospheric nitrogen fixation, phosphate solubilization, indole-3-acetic acid (IAA) production and siderophore production. These observations were corroborated by the whole-genome analysis where we can see many plant-growth promoting genes. This plant growth promoting potential of the isolated bacterium was confirmed through pot experiments with chilli seeds, where chilli seedlings were treated with the bacterial suspension (1% of 108 cfu/ml) and resulted in increase of the dry weight of roots and shoots, the length and the number of branches in the plants. The treated plants also showed increase in height, weight, chlorophyll content and yield (fruit weight). Overall, this bacterium demonstrates strong potential for arsenic bioremediation and as a biofertilizer for sustainable agriculture.

Keywords: arsenic hyper-tolerant bacterium; 16S rDNA sequencing; phylogenetic analysis; whole-genome sequencing; scanning electron microscopy; *Microbacterium paraoxydans*; arsenic bioremediation; plant growth promotion; sustainable agriculture



Agentic AI in Materials Science: A Stateful Multi-Agent Consensus for Sustainable High-Entropy Alloy Discovery

Ankita Kanjilal¹, Mandril Sircar², Arkaprabha Chakraborty³, Roopkatha Majumdar⁴, Sounak Sarkar⁵, Sanjoy Bhattacharjee⁶

¹⁻⁵ Department of CSE AIML, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer Math, Kolkata – 700074

⁶ Department of CSE, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer Math, Kolkata – 700074
E-mail: ankitakanjilal2004@gmail.com

INTRODUCTION

The proposed work addresses the urgent need for sustainable practices in materials science. The discovery of novel materials, and in particular, High Entropy Alloys (HEAs), has always been slowed down by the robust compositional search space. While generative machine learning models have boosted the field of property prediction but existing systems often suffer from “error amplification” in single pipeline and also a lack of integrated multi-objective constraints that deals with the sustainability factor and raw material ethics. The proposed work presents a novel Stateful Multi-Agent Consensus Framework designed to automate the discovery of stable, high-performance and sustainable alloys. Through this transition from a single-model based prediction to an orchestrated and decentralized framework, where several specialized AI agent debate – this work aims to reduce hallucinated physical properties while enforcing green engineering standards.

MATERIALS AND METHODS

The methodology involves a Centralized Supervisor AI Agent architecture to orchestrate a debate between three specialized sub-agents. The proposed work is developed using Lang Graph Framework that is dedicated to build Agentic AI systems. It implements a stateful feedback loop (Directed Acyclic Graph), managing agent memory and error correction. The detailed methodology is as follows:

1. **The Researcher Agent:** This agent is responsible for data collection and structure of materials and compounds from the Materials Project (MP) API and Pymatgen for crystallographic data processing.
2. **The Physicist Agent:** Utilizes Graph Neural Networks (M3Gnet) to evaluate thermodynamic stability
3. **The Sustainability Agent:** Initiates life-cycle assessments and audits for the critical raw materials (CRMs)
4. **The Consensus Mechanism** is mathematically drawn to assess both structural necessity and also ecological impact.



RESULTS AND DISCUSSION: The proposed work was evaluated by benchmarking the agent-proposed HEAs against known experimental datasets. The stateful multi-agent approach significantly outperformed traditional linear AI models.

Metric	Single-Agent Baseline	Multi-Agent Consensus
Inference Accuracy	72.4%	91.8%
Hallucination Rate	28.1%	4.2%
Sustainability Index	Low (Ignored)	High (Enforced)

Table 1. Comparison of Single vs. Multi-Agent Architecture Performance.

The multi-agent consensus model reduced the "hallucination rate" of unstable chemical compositions by nearly 25% compared to standard sequential AI chains.

CONCLUSION

By implementing the autonomous multi-agent consensus framework, error amplification in AI-driven materials discovery is significantly mitigated. By enforcing a stateful feedback loop, both theoretical and practical implications of the proposed work prove that AI can reliably adhere to both physical and environmental concerns with ethical sourcing constraints. The conclusion drawn suggests that Agentic Governance is essential for creating reliable, explainable, and sustainable AI systems in materials science, laying the basis for next generation of autonomous "self-driven" laboratories.

ACKNOWLEDGMENT

We express our profound gratitude and appreciation to the Machine Learning Laboratory of Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex for providing the essential computing infrastructure for the training and assessment of our models and also to the Basic Science and Humanities Department for giving us this opportunity through the RDAMSE 2nd Conference 2026.

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Nanostructured Metal Oxide Based Pressure Sensors for Smart Electronic Applications

SUDIPTA MAJUMDER, SWARNAB DAS, SINDHUJA TRIPATHI, AYANTIKA TRIPATHI,
ANUSHKA SETH, SANKHASIS ROY

Department of Computer Science & Engineering
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex
540, Dum Dum, Surer Math, Kolkata – 700074

INTRODUCTION

Flexible pressure sensors are an essential component in modern smart electronic systems, let it be wearable devices or healthcare monitoring, robotics or human-machine interfaces, compared to conventional rigid sensors, flexible sensors offer better adaptability to curved surfaces and dynamic environments. In recent years, nanostructured metal oxides such as ZnO, TiO₂, SnO₂, CuO etc. have gained attention due to high sensitivity, mechanical stability, and enhanced surface properties. At the nanoscale, these materials show improved electromechanical behavior, making them highly suitable for pressure sensing applications. This work presents a literature survey focusing on the commonly used materials and their performance comparison, sensing mechanism for smart electronic applications.

MATERIALS AND METHODS: Flexible pressure sensors generally consist of three main components: electrodes, dielectric/sensing layer, and substrate.

Metal Oxide Nanomaterials: Zinc Oxide (ZnO) nanowires/nanorods, Titanium Dioxide (TiO₂) nanofibers, Tin Oxide (SnO₂) nanoparticles, Copper Oxide (CuO) nanostructures

Flexible Substrates: Polydimethylsiloxane (PDMS), Polyurethane (PU), Polyethylene terephthalate (PET)

Electrode Materials: Gold (Au), Silver (Ag), Copper (Cu), Conductive polymers (PEDOT: PSS), Carbon-based materials (CNTs, graphene)

These materials are selected based on flexibility, conductivity, mechanical strength, and biocompatibility.

WORKING PRINCIPLE: Flexible pressure sensors operate based on different sensing mechanisms such as piezoresistive, capacitive, and piezoelectric effects. For capacitive-type sensors, the working principle is based on

change in capacitance: $C = \epsilon \frac{A}{d}$

[C = Capacitance, ϵ = Permittivity, A = Area of electrodes, d = Distance between electrodes]

When, external pressure is applied the dielectric layer compresses, distance between electrodes decreases and the capacitance increases. In nanostructured metal oxide sensors, micro/nano-scale deformation significantly enhances sensitivity. For piezoresistive sensors, Resistance changes due to deformation of conductive pathways. For piezoelectric sensors, Mechanical stress generates electrical voltage.



RESULTS AND DISCUSSION: The performance of nanostructured metal oxide pressure sensors depends on material type, nanostructure, and sensing mechanism.

Table 1: Comparative Analysis of Metal Oxide Pressure Sensors

Material	Structure	Mechanism	Sensitivity	Range	Key Advantage
ZnO	Nanorods	Piezoelectric	High	Low–Medium	Self-powered
TiO ₂	Nanofibers	Capacitive	Moderate	Wide	Stable
SnO ₂	Nanoparticles	Piezoresistive	High	Medium	Conductive
CuO	Thin film	Piezoresistive	Moderate	Medium	Low cost

Nanostructured materials enhance sensor performance due to their high surface-to-volume ratio and improved mechanical response. Structures like nanorods, nanofibers, and porous networks increase compressibility, leading to higher sensitivity. Among these, ZnO nanostructures exhibit strong piezoelectric behavior, enabling self-powered sensing. TiO₂-based sensors provide better stability and wider detection range in capacitive systems, while SnO₂ and CuO show good sensitivity in piezoresistive sensors but are more affected by environmental conditions. Flexible substrates such as PDMS and polyurethane improve adaptability for wearable applications, and micro structured designs further enhance sensitivity and response. However, challenges remain, including trade-offs between sensitivity and durability, environmental effects, and fabrication complexity.

CONCLUSION: Nanostructured metal oxides enhance pressure sensing through improved surface interaction and flexibility. However, stability and fabrication complexity limit performance. These sensors show strong potential for wearable and smart applications. Future work should focus on improving durability, environmental stability, and scalable fabrication for reliable real-world implementation.

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Chalcogenide-Based Smarty Materials For Supercapacitor Application

Sagnik Guha Roy, ^{A1}, Soumodeep Dutta, ^{B2}, Bikram Pal, ^{C3}, Baisakhi Mondal, ^{D4}, Saniya Parvin, ^{E5}
Plabani Dutta, ^{F6},

Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex
Maulana Abul Kalam Azad University of Technology
Email: - deepsoumo83@gmail.com

INTRODUCTION

In conjunction with the increasing popularity of portable electronic devices, electric cars, and renewable energy sources, there is growing demand for efficient energy storage technologies. The latter is characterized by such properties as a high power-to-weight ratio, high energy density, fast charging, and long service life. Despite the benefits that capacitors possess, the main disadvantage of this type of energy storage is its low energy density compared to batteries.

MATERIALS AND METHODS

Materials: Transition metal salts(Nickel Nitrate, Cobalt Nitrate), Chalcogen Sources(Selenium powder, tellurium compounds), Solvents(Ethanol, Distilled Water), Electrolyte(KOH, Na₂SO₄).

Methods: The transition metal salt and chalcogen source are dissolved in a solvent to form a homogeneous solution. The mixture is then subjected to a synthesis technique such as hydrothermal or solvothermal method at elevated temperature and pressure. This process leads to the formation of metal chalcogenide nanostructures (e.g., NiS, CoSe, MoS₂). The synthesized chalcogenide material is mixed with a binder (like PVDF) and a conductive additive (if required). This mixture is coated onto a conductive substrate such as nickel foam or carbon cloth. The prepared electrode is combined with a suitable electrolyte (e.g., KOH solution). A separator may be used to prevent short circuit between electrodes. The system is assembled into a test cell for electrochemical analysis. The performance of the electrode is evaluated using techniques such as:

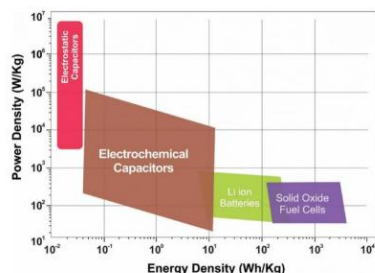
- Cyclic Voltammetry (CV)
- Galvanostatic Charge–Discharge (GCD)
- Electrochemical Impedance Spectroscopy (EIS)

RESULTS AND DISCUSSION

It was observed that the synthesized chalcogenide electrode material displayed promising electrochemical properties upon testing within a supercapacitor configuration. The obtained CV profiles were characterized by a quasi-rectangular form with well-defined redox peaks, which implied that the process involves the electric double layer capacitance and pseudo capacitance. As per GCD analysis, the obtained profiles were almost symmetrical, which implies that the process is highly reversible and exhibits high coulombic efficiency. The computed specific capacitance is quite high when compared to traditional carbonaceous materials. The enhanced performance of chalcogenide-based smart materials involves a number of important contributors. First, the chalcogen elements



(sulfur or selenium) when combined with transition metals create many different oxidation states, which lead to strong redox reactions and higher charge storage capabilities.



1) Cyclic Voltammetry Data Table

Scan Rate (mV/s)	Peak Current (A)	Specific Capacitance (F/g)
5	0.012	420
10	0.021	390
20	0.038	350
50	0.082	300

As scan rate increases, capacitance slightly decreases.

based smart materials involves a number of important contributors. First, the chalcogen elements (sulfur or selenium) when combined with transition.

CONCLUSION

Smart chalcogenide materials exhibit great prospects in developing future supercapacitors owing to their exceptional electrical conductivity, redox activities, and adjustable nanostructures. From the test results, there has been an observed improvement in specific capacitance as well as acceptable cycling stability. This is because these materials can utilize both double-layer and pseudocapacitive reactions for better results. Despite having some challenges, especially concerning scalability and durability, these smart materials are likely to play a vital role in creating highly efficient energy storage devices.

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Synthesis–Structure–Property Relationship in Doped Amorphous Carbon Nanotubes for Electrochemical Devices

Rishikesh Shaw, Md Faiz Ahmed, Raj Shaw, Ricky Pandit, Prem Pratap Singh, Prince Kumar
Department of Computer Science Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports
Complex, Kolkata – 700074E-mail: godrishi61@gmail.com

INTRODUCTION

Amorphous Carbon Nanotubes (a-CNTs) are a class of nanostructured carbon materials characterized by their disordered atomic arrangement and high defect density. Unlike crystalline CNTs, a-CNTs contain mixed sp² and sp³ bonding, leading to irregular tubular structures. This disorder enhances surface reactivity, making them suitable for electrochemical applications. Heteroatom doping (N, B, S, metals) further improves conductivity and catalytic activity. The performance of these materials depends on the Synthesis–Structure–Property (SSP) relationship.

DIFFERENT METHODS OF a-CNT SYNTHESIS:

Bottom-up chemical methods involve chemical reactions that form carbon nanotubes (CNTs) from precursors. There are several approaches: Chemical Vapor Deposition (CVD): Hydrocarbon gases decompose over catalysts like Fe, Co, or Ni. Low temperatures often lead to amorphous CNTs. Pyrolysis: Ferrocene-based decomposition produces highly defective amorphous CNTs. Hydrothermal Methods: Liquid-phase synthesis produces CNT-like amorphous structures. These methods rely on chemical reactions to build CNTs from molecular precursors, often resulting in varying degrees of structural order depending on the process conditions. Top-down physical methods create CNTs by breaking down larger carbon structures. Two key approaches are:

Arc Discharge: CNTs form via an electric arc, but amorphous carbon is a common impurity. Laser Ablation: Graphite is vaporized by a laser, potentially forming amorphous CNTs if cooling is too rapid. These methods rely on physical processes to generate CNTs, often requiring careful control to minimize defects and impurities.

RESULTS AND DISCUSSION:

3.1 Synthesis–Structure Relationship Low temperature and rapid growth produce defect-rich, amorphous structures. Doping introduces more active sites.

3.2 Structure–Property Relationship Defects increase reactivity and surface area. Doping enhances conductivity and electrochemical activity.

3.3 Electrochemical Performance a-CNTs show improved performance in supercapacitors, batteries, and fuel cells.



Aspect	Bottom-Up (Chemical Methods)	Top-Down (Physical Methods)
<u>Approach</u>	Build from atoms/molecules	Break bulk material
<u>Structural Control</u>	High control over structure	Limited control
<u>Defect Engineering</u>	Controlled and tunable	Mostly uncontrolled
<u>Doping Capability</u>	Easy and efficient	Difficult
<u>Temperature Requirement</u>	Moderate	Very high
<u>Product Type</u>	Amorphous CNTs (targeted)	Mostly crystalline CNTs
<u>Cost & Scalability</u>	Cost-effective, scalable	Expensive, less scalable
<u>Suitability</u>	Best for electrochemical applications	Less suitable

CONCLUSION:

Therefore, it can be concluded that controlled chemical synthesis (bottom-up approach) plays a dominant role in establishing the optimal Synthesis–Structure–Property relationship, making it the preferred strategy for designing high-performance amorphous CNT-based electrochemical devices.

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Waste-To-Sensor Conversion of Biomass Process Liquors Into Organic Chemi-Resistive Sensors

Prasun Majumder, , Rupkatha Patra, , Partha Pratim Chakraborty, , Averi Banerjee,
Techno International New Town
Email: - majumderprasun6@gmail.com

INTRODUCTION

Abstract

The residual process streams generated during biomass-to-biofuel conversion are usually treated like low-value waste despite their accumulation of chemically rich organic matter. The study transformed a previously unused residual liquid fraction that was obtained during the in-situ distillation step in *Parthenium hysterophorus* processing into a functional chemi-resistive sensing organic material. It involved the combination of yellow-colored liquid filtrates of lignin separation and hemicellulose extraction products before direct distillation for alcohol recovery. Volatile alcohol was removed in the distillation process, and the non-volatile organic constituents in process liquors were concentrated and subsequently subjected to an alkali treatment. As such, they were concentrated and were then subjected to controlled alkaline treatment. The brown organic fraction, containing mostly humic- and phenolic-like compounds, rich in oxygen, was the result of the concentration process. The organic material as received was converted into a semi-viscous form, which was the active layer of the sensing material grown using pencil graphite electrodes on vero-board substrate for chemi-resistive sensor construction by the researchers. This sensor experience a change in resistance value upon exposure to moisture, which is the cause of the presence of ionic and protonic conduction within the organic matrix. This work represents a novel way by which waste becomes the sensor, thus getting both value and substance-transforming biomass beyond just fuels and solid products into functional electronic materials.

Keywords:

Organic chemi-resistive sensor; humic substances; phenolic compounds; biomass-derived materials; *Parthenium hysterophorus*; residual process valorization.



AI/ML-Based Drug Repurposing for Rare Diseases: A Critical Analysis of Data-Driven Prediction and Translational Limitations

Sukanya Kar And Debabrata Ghosh Dastidar*

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Panihati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Rare diseases constitute a major global healthcare challenge, marked by low prevalence, limited clinical trial data, and insufficient investment in dedicated drug development; although more than 7,000 rare diseases have been identified affecting nearly 300 million people worldwide, only about 5–7% [1][2] have approved treatments, underscoring the economic and scientific limitations of traditional drug discovery approaches. Drug repurposing has therefore emerged as a practical alternative, offering reduced development time, lower costs, and improved safety by utilizing existing pharmacological knowledge [1]. In parallel, artificial Intelligence (AI) and machine learning (ML) have increasingly been applied to this field, enabling large-scale analysis of drug–target interactions, gene–disease associations, and biological pathways to identify potential therapeutic candidates. However, despite significant technological progress, the clinical success of AI-driven drug repurposing in rare diseases remains limited, suggesting that the primary barriers are not algorithmic shortcomings but constraints related to data availability, quality, and underlying biological complexity.

MATERIALS AND METHODS: This study was conducted as a systematic review following a PRISMA-based analytical framework to ensure structured literature selection and reproducibility. Comprehensive searches were performed across PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using keywords such as “AI drug repurposing rare diseases,” “machine learning drug discovery data limitations,” and “network-based drug repurposing rare diseases.” The search was limited to peer-reviewed articles published in English between 2020 and 2025. Studies were included if they focused on AI/ML-based drug repurposing, computational prediction models, and applications in rare diseases, while unrelated computational methods, incomplete datasets, and duplicate studies were excluded. Articles were screened through title, abstract, and full-text evaluation, and relevant data on model type, dataset characteristics, prediction methods, and validation strategies were extracted. critical synthesis approach was then applied to identify mechanistic limitations, inconsistencies, and translational gaps.

RESULTS AND DISCUSSION: AI/ML-based drug repurposing functions as a data-driven predictive system that analyzes large-scale biomedical datasets to uncover hidden drug–disease relationships using approaches such as similarity-based models, network-based methods, and knowledge graph or deep learning frameworks. These models integrate diverse sources like genomic data, clinical records, and scientific literature to generate predictive hypotheses, but their performance is highly dependent on data completeness and quality rather than algorithmic sophistication alone. In the context of rare diseases, a major limitation is data scarcity, as these conditions typically lack large patient cohorts, comprehensive clinical datasets, and well-defined biological pathways, leading to sparse networks and reduced predictive power. highlighting that AI cannot infer beyond available data. Additionally, dataset bias creates acknowledge imbalance, with overrepresentation of well-studied diseases and underrepresentation of rare conditions, causing models to reinforce existing knowledge instead of identifying novel therapeutic targets.



Another critical issue is that AI predictions are largely correlation-based rather than causal, meaning they may suggest associations without explaining mechanisms of action, biological relevance, or clinical efficacy, thereby limiting interpretability. Furthermore, a significant translational gap exists, as many computational predictions fail to progress to clinical application due to inadequate experimental validation, poor integration with biological systems, and lack of standardized evaluation frameworks. Altogether, these challenges reflect a multi-level limitation spanning data scarcity and bias, model-level reliance on correlations, and translational barriers, indicating that improving algorithms alone is insufficient without parallel advancements in data quality, biological validation, and clinical integration.

Table 1.

Level	Limitation	Impact on Prediction
Data	Sparse and incomplete datasets	Reduced predictive accuracy
Data	Bias toward well-studied diseases	Limited novelty
Model	Correlation-based predictions	Lack of mechanistic insight
Validation	Lack of experimental confirmation	Poor translation
Clinical	Limited patient data	Restricted applicability

Limitations in AI-Based Drug Repurposing for Rare Diseases

CONCLUSION: This review demonstrates that AI/ML-based drug repurposing for rare diseases operates as a fundamentally data-dependent predictive system, where performance is constrained more by data availability and quality than by computational capability. The analysis highlights that data scarcity and bias significantly reduce predictive accuracy, while AI models predominantly capture correlations rather than true causal mechanisms, limiting biological interpretability. Additionally, the lack of robust validation frameworks hinders the translation of computational predictions into clinical applications, revealing multi-level limitations across the entire pipeline, from data to model to real-world implementation. Therefore, AI-driven drug repurposing should be reframed as a hypothesis-generating approach constrained by data quality and biological complexity, requiring strong integration with experimental validation and multi-source data to enable reliable and clinically meaningful outcomes.

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Poster Presentation – PP-13



Artificial Intelligence in Cancer Drug Repurposing: A Critical Analysis of Predictive Modelling, Biological Complexity, and Translational Challenges

Arup Aich, And Debabrata Ghosh Dastidar*

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Panihati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Cancer drug discovery remains constrained by high development costs, long timelines, and high attrition rates, limiting the efficient translation of therapeutic candidates into clinical practice. Despite advances in molecular oncology, drug development continues to suffer from low success rates, particularly in late-stage clinical trials, highlighting a fundamental inefficiency in conventional discovery paradigms [2]. Drug repurposing has emerged as a promising alternative strategy, enabling the identification of new therapeutic uses for existing drugs, thereby reducing development time and cost. The integration of artificial intelligence (AI) and machine learning (ML) has further accelerated this approach by enabling large-scale analysis of drug–target interactions, genomic datasets, and clinical data [5]. However, despite rapid advancements in computational capability and increasing predictive power, the translation of AI-generated candidates into clinically effective cancer therapies remains limited.

MATERIALS AND METHODS: This study was conducted using a PRISMA-based systematic review framework to ensure structured literature identification, screening, and synthesis. Literature searches were carried out in PubMed, Scopus, Web of Science, and ScienceDirect using the keywords “AI drug repurposing cancer,” “machine learning oncology drug discovery,” and “tumor heterogeneity computational prediction.” The review was limited to peer-reviewed articles published between 2020 and 2025. Included studies focused on AI/ML-based drug repurposing in oncology, mechanistic and computational analyses, and research addressing validation or translational aspects. Excluded studies involved non-cancer applications or purely descriptive reports without analytical interpretation.

RESULT AND DISCUSSION: AI/ML models act as data-driven predictive systems by integrating genomic profiles, drug–target interactions, and clinical data to rapidly identify repurposable drug candidates using network-based modeling, deep learning, and multi-omics integration, thereby accelerating early-stage discovery [5]. However, these predictions are mainly correlation-based rather than mechanistic or causal, often lacking mechanistic interpretability, biological causation, and pathway-level validation, which limits reliability in biological systems [6]. This challenge is further increased by cancer complexity, including tumor heterogeneity, dynamic mutation profiles, and adaptive signaling pathways that are not fully captured by static AI training datasets [1]. A major prediction–validation gap also exists, as many AI-predicted, candidates lack experimental validation, clinical confirmation, and reproducibility, meaning prediction success does not always equal therapeutic success [1]. In addition, AI performance depends on data quality, and bias toward well-studied cancers, incomplete multi-omics datasets, and underrepresentation of diverse populations reduce generalizability and clinical applicability [6]. Beyond prediction, translational barriers such as lack of standardized validation pipelines, weak experimental integration, and regulatory challenges show that failure arises from multi-level system limitations rather than a single bottleneck.



Table 1. Key Determinants and Limitations of AI-Based Cancer Drug Repurposing

Level	Parameter	Limitation	Impact
Data	Multi-omics datasets	Incomplete and biased	Reduced accuracy
Model	AI prediction	Correlation-based	Limited causality
Biology	Tumor heterogeneity	Dynamic variability	Poor generalization
Validation	Experimental confirmation	Limited integration	Translation failure
Clinical	Implementation	Regulatory barriers	Low adoption

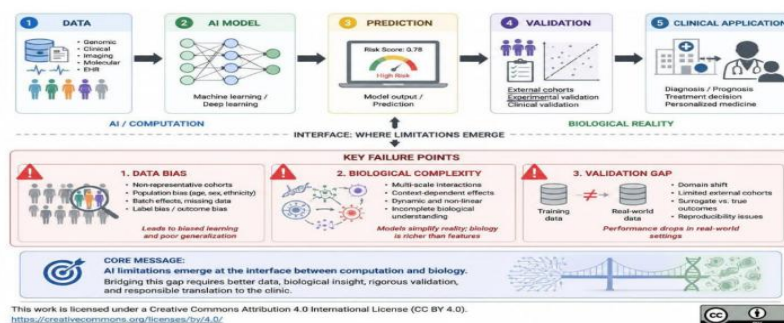


Fig 1: AI Prediction vs Biological Reality Framework

CONCLUSION: This review demonstrates that AI-driven cancer drug repurposing is a powerful but prediction-limited approach, where success is constrained by biological complexity and insufficient validation rather than computational capability. The analysis reveals that AI enables large-scale and rapid prediction of drug candidates, cancer heterogeneity fundamentally limits predictive accuracy, correlation-based models lack mechanistic depth, and validation and translation remain the primary bottlenecks. AI in cancer drug repurposing should be redefined as a hypothesis-generating tool, where effective therapeutic development requires integration of computational prediction with biological validation and clinical context rather than reliance on AI models alone.

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HYDROPHOBIC CARBON QUANTUM DOTS FOR NIR-II BIOIMAGING: A CRITICAL ANALYSIS OF STRUCTURE -ENERGY RELATIONSHIPS AND OPTICAL PERFORMANCE

Debanjan Bhattacharya, And Debabrata Ghosh Dastidar*
Guru Nanak Institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Fluorescence-based bioimaging is fundamentally constrained by the optical limitations of conventional fluorophores operating in the visible and near-infrared-I (NIR-I) regions, including strong photon scattering, limited tissue penetration, and high biological autofluorescence. These limitations significantly reduce imaging depth and resolution in vivo. The second near-infrared window (NIR-II, 1000–1700 nm) has emerged as a promising alternative, offering reduced scattering, deeper tissue penetration, and improved signal-to-noise ratios for biomedical imaging applications [2][9]. Carbon quantum dots (CQDs) have gained attention as potential NIR-II probes due to their tunable photoluminescence, high photostability, and biocompatibility [4][8]. Recent advances demonstrate CQDs with emission extending into the NIR-II region, enabling improved imaging performance. However, unlike conventional fluorophores, NIR-II emission in CQDs is not intrinsic but arises from engineered structural and electronic modifications, particularly involving surface chemistry and defect states [1]. Hydrophobic CQDs are frequently reported to exhibit enhanced emission efficiency and stability. However, this observation introduces a deeper mechanistic question: does hydrophobicity directly enhance emission, or does it merely modulate the environment of engineered electronic states responsible for NIR-II luminescence? This review critically evaluates recent literature (2020–2025) to position NIR-II CQDs as structure–energy engineered systems, where optical performance emerges from controlled electronic structure and surface-state interactions rather than intrinsic nanoscale size effects.

MATERIALS AND METHODS: This study was conducted as a systematic review using a PRISMA-based analytical framework, with literature collected from PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar. Search keywords included “NIR-II carbon quantum dots mechanism,” “CQDs surface states NIR emission,” and “hydrophobic CQDs photoluminescence,” and the review was restricted to peer-reviewed publications from 2020–2025. Inclusion criteria comprised studies addressing NIR/NIR-II carbon quantum dots, mechanistic insights into photoluminescence, and structure–property and surface-state analyses, while exclusion criteria included non-carbon nanomaterials and purely application-based reports lacking mechanistic discussion. A critical synthesis approach was applied to identify mechanistic trends, contradictions, and unresolved research gaps.

RESULTS AND DISCUSSION: Engineered Origin of NIR-II Emission: Unlike conventional semiconductor quantum dots, CQDs do not inherently emit in the NIR-II region; instead, NIR-II emission arises from engineered electronic



structures, including extended π -conjugation, heteroatom doping, and defect-state formation [1][6]. Recent studies demonstrate that CQDs can be tuned from visible to NIR-II emission (up to ~ 1265 nm) through controlled molecular design and precursor engineering [1], indicating that NIR-II emission is not intrinsic but an emergent property of engineered electronic states.

Core Size vs Surface-State Dominance: A fundamental debate in CQD photo physics concerns whether emission is governed by quantum confinement (core size) or by surface states and defect-induced energy levels; however, evidence increasingly supports surface-state dominance, particularly in red-shifted and NIR emission systems [3][9]. Surface defects, heteroatom doping (e.g., nitrogen), and molecular fragments introduce energy traps that facilitate low-energy (long-wavelength) emission, suggesting that NIR-II emission is primarily governed by surface-state engineering rather than core size alone.

Structure–Energy Relationship and Charge Transfer: NIR-II emission arises from nanoscale structure–energy relationships, where engineered electronic transitions enable bandgap narrowing, driven by π -conjugated domains, donor–acceptor interactions, surface defect states, and charge-transfer transitions. Recent reports highlight that donor–acceptor interactions between core and surface groups create new emissive states responsible for NIR-II fluorescence [6], establishing CQDs as energy-level engineered systems rather than size dependent emitters.

Role of Hydrophobicity: Intrinsic or Environmental Control? Hydrophobic CQDs are often reported to exhibit improved emission efficiency; however, mechanistic analysis suggests that this effect is largely indirect, as hydrophobic environments reduce interaction with polar solvents, suppress non-radiative decay pathways, and stabilize excited states. Studies show that emission intensity decreases significantly in aqueous environments due to quenching effects, highlighting the role of environmental interactions rather than intrinsic electronic modification, and indicating that hydrophobicity functions as an environmental stabilizer of emissive states rather than a primary origin of NIR-II emission.

Trade-Off: Optical Performance vs Biological Applicability Despite enhanced optical properties, hydrophobic CQDs present major limitations, including poor aqueous dispersibility, reduced biocompatibility, and challenges in systemic delivery, creating a critical trade-off between enhanced emission efficiency and reduced biological usability, which is particularly important for in vivo imaging applications where aqueous stability is essential.

Quantum Yield Limitation in NIR-II Region: A persistent challenge in NIR-II CQDs is low quantum yield, with studies reporting values typically below 5% in the NIR-II region and increased non-radiative decay at lower energy gaps, reflecting a fundamental physical limitation in which red-shifted emission inherently increases non-radiative loss pathways.

Critical Gap: Lack of Predictive Structure–Property Models A major limitation across studies is the absence of predictive frameworks linking precursor chemistry, surface functionalization, and electronic structure to emission wavelength and intensity, resulting in CQD design remaining largely empirical and lacking quantitative models for the rational tuning of NIR-II properties [6].

Table 1. Key Determinants of NIR-II Emission in CQDs

Parameter	Structural Role	Optical Impact
π -conjugated domains	Bandgap narrowing	Red-shifted emission
Surface defects	Trap-state formation	Enables NIR emission
Heteroatom doping	Modifies electronic states	Enhances emission efficiency
Hydrophobic environment	Reduces quenching	Improves intensity
Charge-transfer states	New emissive pathways	Enables NIR-II fluorescence

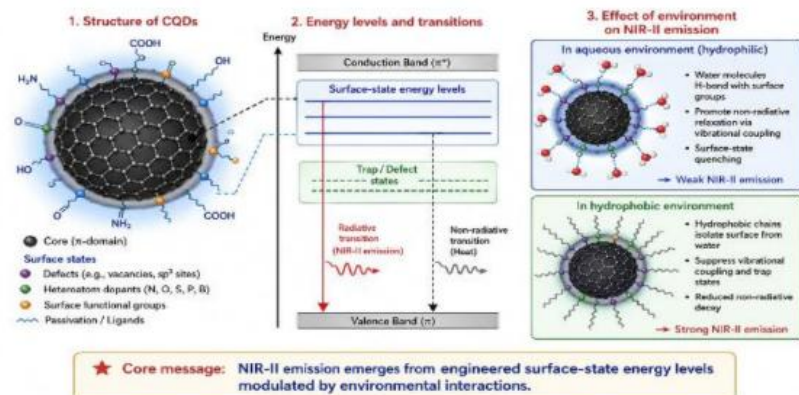


Figure 1: Structure–Energy–Emission Model for NIR-II CQDs

CONCLUSION:

This review demonstrates that hydrophobic carbon quantum dots for NIR-II bioimaging are best understood as structure–energy engineered photophysical systems, where emission behaviour arises from controlled electronic states rather than intrinsic material properties. The analysis reveals that NIR-II emission is an engineered outcome of surface-state and defect- level modification, with surface states dominating over quantum confinement in determining emission behaviour, while hydrophobicity enhances emission indirectly by suppressing non-radiative decay. However, trade-offs between optical performance and biological applicability limit practical use, and the lack of predictive models restricts the rational design of CQDs. Overall, NIR-II CQDs should be redefined as design-driven nanophotonic systems, where controlled manipulation of electronic structure, surface chemistry, and environmental interactions is essential for achieving high-performance bioimaging probes.

ACKNOWLEDGEMENT:

I sincerely express my gratitude to Guru Nanak Educational Trust for providing me with this valuable opportunity.

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7. Figure 1. Structure–Energy–Emission Model for NIR-II CQDs. Generated using artificial intelligence tools developed by OpenAI, based on author-defined prompts.



Cyp450 Genetic Polymorphisms and Drug Response Variability in The Indian Population: A Critical Analysis of Pharmacogenomic Translation

Deep Das, And Debabrata Ghosh Dastidar*

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Patients receiving the same drug often exhibit significant variability in therapeutic outcomes, including reduced efficacy and increased risk of adverse drug reactions, despite standardized dosing regimens, highlighting a fundamental limitation in current clinical practice where drug response is treated as uniform rather than individualized. Drug metabolism plays a central role in determining therapeutic outcomes, primarily mediated by cytochrome P450 (CYP450) enzymes, which are responsible for the metabolism of a large proportion of clinically used drugs, with key isoforms such as CYP2D6, CYP2C19, and CYP3A4 contributing significantly to drug biotransformation [4][6]. However, these enzymes are highly polymorphic, and genetic variations lead to substantial inter-individual differences in metabolic capacity. Recent studies in Indian populations demonstrate significant genetic diversity in CYP450 variants, with population-specific allele distributions that differ markedly from global patterns [1]. Notably, large-scale genomic analyses indicate that a substantial proportion of individuals may require dose adjustments based on CYP2D6 genotype alone [1]. This raises a critical mechanistic question: is variability in drug response a stochastic clinical phenomenon, or a predictable outcome of genetically encoded metabolic differences?

This review critically evaluates recent literature (2020–2025) to establish drug response variability as a genetically driven metabolic phenomenon, emphasizing the gap between pharmacogenomic knowledge and clinical implementation in the Indian context.

MATERIALS AND METHODS:

This study was conducted as a systematic review using a PRISMA-based analytical framework, with literature collected from PubMed, Scopus, Web of Science, Science Direct, and Google Scholar; search keywords included “CYP450 polymorphism India pharmacogenomics,” “CYP2D6 CYP2C19 drug metabolism variability, and “Pharmacogenomics Indian population drug response.” The review was restricted to peer-reviewed publications from 2020–2025, with inclusion criteria focusing on studies addressing CYP450 polymorphisms, population-specific pharmacogenomic data in India, and the clinical implications of metabolic variability, while exclusion criteria eliminated non-human studies and non-pharmacogenomic analyses. A critical synthesis approach was applied to identify mechanistic relationships, population-specific trends, and translational gaps.

RESULTS AND DISCUSSION:



CYP450 Polymorphism as a Determinant of Drug Metabolism: CYP450 enzymes exhibit genetic polymorphism, leading to variability in enzyme activity; isoforms like CYP2D6 and CYP2C19 metabolize many commonly prescribed drugs, including antidepressants and cardiovascular agents [6]. Genetic variations (SNPs, deletions, duplications) result in metabolizer phenotypes: poor (PM), intermediate (IM), and extensive/normal (EM). **Mechanistic Basis: Gene–Enzyme–Drug Interaction System** CYP450 polymorphisms alter enzyme activity, modifying metabolism: reduced enzyme activity → accumulation → toxicity; increased enzyme activity → rapid clearance → therapeutic failure, showing drug response depends on a gene–enzyme–drug system, not uniform pharmacokinetics [2]. Thus, clinical variability is mechanistically predictable from genetic variation. **Population-Specific Variability in the Indian Context:** India's genetic diversity leads to unique CYP2D6 alleles, variable frequencies, and high actionable variants; one and three may benefit from genotype-guided dosing [1], with many showing non-normal metabolizer phenotypes [6]. **Clinical Consequences of Metabolic Variability:** CYP450 polymorphisms cause higher adverse reactions (PM), reduced efficacy (ultra- rapid), and altered drug interactions, contributing to treatment failure and increased healthcare burden; variability reflects systematic genetic differences. **Translational Gap: From Genotype to Clinical Practice:** Pharmacogenomics remains underused in India due to lack of population-specific guidelines, limited testing, poor clinical integration, and underrepresentation in global models, with limited Indian data [6]. **Critical Gap: Absence of Population-Specific Predictive Frameworks:** Lack of integrated frameworks linking genetic variation, enzyme activity, drug response, and clinical decisions; most studies report allele frequencies without actionable guidelines.

Table 1. Impact of CYP450 Polymorphism on Drug Response

Parameter	Genetic Effect	Clinical Outcome
CYP2D6 variation	Altered enzyme activity	Changes in drug metabolism
CYP2C19 polymorphism	Variable metabolic rate	Dose adjustment required
Poor metabolizer phenotype	Reduced clearance	Increased toxicity risk
Ultra-rapid metabolizer	Increased clearance	Reduced drug efficacy

CONCLUSION:

This review demonstrates that variability in drug response is fundamentally a genetically driven metabolic phenomenon governed by CYP450 polymorphisms and population-specific genetic diversity, with analysis showing that CYP450 polymorphisms significantly influence drug metabolism and therapeutic outcomes. Indian populations exhibit distinct genetic variability with clear clinical relevance, and drug response variability is largely predictable rather than random; however, major gaps persist in translating pharmacogenomic knowledge into routine clinical practice, underscoring that effective personalized drug therapy requires the integration of population-specific genetic data into clinical decision-making and a shift from uniform dosing strategies to genotype-guided precision medicine.

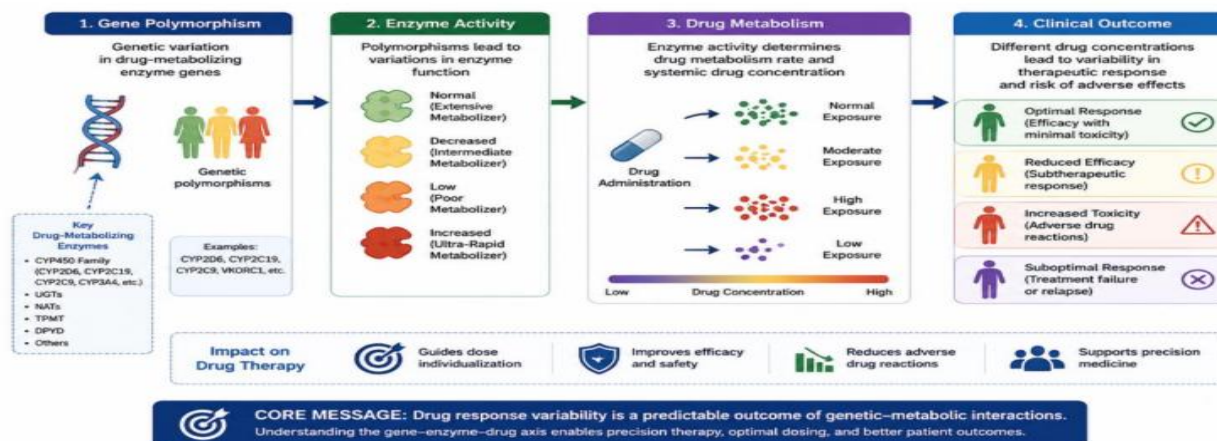


Figure 1: Gene-Enzyme-Drug Interaction model

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Hydrophobic Carbon Quantum Dots: A Critical Analysis of Surface-State Engineering and Photophysical Control Mechanisms

Chandranath Dey, And Debabrata Ghosh Dastidar*

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Conventional carbon quantum dots (CQDs) are mainly hydrophilic due to oxygen-containing surface groups, which improve water dispersibility but limit use in non-polar and optoelectronic systems. Although they exhibit tenable photoluminescence, high stability, and easy synthesis [1], their optical behaviour is driven more by surface chemistry than core size. Surface modification strategies—such as heteroatom doping, passivation, and ligand functionalization—can induce hydrophobicity while altering optical properties [2], expanding applications but complicating structure–property relationships. This leads to a critical mechanistic question: is the enhanced optical performance of hydrophobic CQDs a result of hydrophobicity itself, or a consequence of underlying surface-state engineering?

This review critically evaluates recent literature to position hydrophobic CQDs as surface-engineered photophysical systems, where emission behaviour is governed by engineered electronic states rather than intrinsic core properties.

MATERIALS AND METHODS:

This study was conducted as a systematic review using a PRISMA-based analytical framework, with literature searches performed across PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using keywords such as “hydrophobic carbon quantum dots photoluminescence,” “CQDs surface state emission mechanism,” and “surface passivation carbon dots optical properties.” The review was limited to peer-reviewed articles published between 2020 and 2025, including studies focused on CQD photoluminescence mechanisms, surface functionalization and hydrophobic modification, and structure–property relationships, while excluding non-CQD quantum dot systems and purely application-based studies without mechanistic insight. A critical synthesis approach was applied to identify mechanistic trends, contradictions, and unresolved gaps.

RESULTS AND DISCUSSION

1. CQD photoluminescence arises from quantum confinement, intrinsic core states, and surface/defect states, but surface states dominate emission, particularly in functionalized systems [1][3]. Emission results from radiative recombination at surface defect sites, governed by functional groups, heteroatom doping, and electronic energy levels, which explains the excitation-dependent and tunable fluorescence observed in CQDs [3]. 2. Hydrophobic CQDs are typically synthesized through organic ligand passivation, long-chain functionalization, and heteroatom doping, which alter the surface electronic structure by reducing defect density, modifying electron distribution, and



stabilizing excited states. These surface engineering strategies suppress non-radiative recombination pathways, enhancing photoluminescence efficiency [2][3], indicating that hydrophobicity reflects underlying surface-state modification rather than merely a solubility property. **3.** Hydrophobicity acts as a photophysical control parameter in CQDs by suppressing solvent-induced quenching; in hydrophilic systems, interactions with polar solvents promote non-radiative decay and reduce emission intensity, whereas hydrophobic passivation minimizes solvent interaction, reduces vibrational energy loss, and enhances radiative recombination, leading to improved emission efficiency and stability [2]. Thus, hydrophobicity indirectly governs photophysical behaviour through modification of surface-state interactions. **4.** The optical properties of CQDs are governed by the interplay of surface energy states, defect levels, and electronic transitions, with surface engineering altering the energy gap between emissive states to enable tunable emission across the visible and near-infrared regions [1]. CQDs exhibit both intrinsic (core-related) and surface-state emission, with the latter dominating in functionalized systems, highlighting the critical role of nanoscale structure–energy relationships. **5.** Hydrophobic CQDs, despite improved optical performance, face key limitations including reduced dispersibility in aqueous systems, limited biocompatibility, and difficulties in biological integration, creating a fundamental trade-off between enhanced emission and reduced applicability—an issue that remains insufficiently addressed in current literature. **6.** A major limitation in current CQD research is the lack of quantitative structure–property models linking surface functionalization, hydrophobicity, and electronic structure to photoluminescence behavior. Most studies remain qualitative, lacking clear correlations between surface chemistry and emission, reproducible synthesis strategies, and standardized characterization protocols, which ultimately restricts the rational design of CQDs for targeted applications.

Table 1. Influence of Surface Engineering on Optical Properties of CQDs

Parameter	Structural Effect	Impact on Photoluminescence
Surface functional groups	Modify electronic states	Tune emission wavelength
Defect density	Introduces trap states	Controls emission intensity
Hydrophobic passivation	Reduces solvent interaction	Enhances emission efficiency
Heteroatom doping	Alters energy levels	Improves quantum yield
Ligand environment	Controls recombination pathways	Affects stability and lifetime

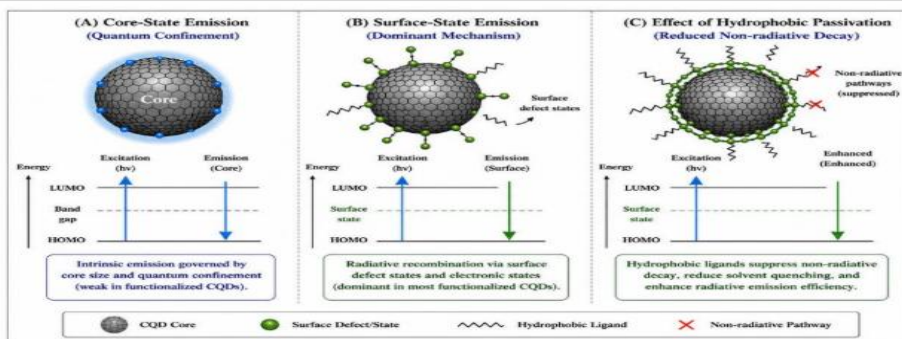


Figure 1. Surface-state vs core-state emission model in carbon quantum dots (CQDs). (A) Core-state emission



arises from quantum confinement within the CQD core, where radiative recombination occurs between HOMO and LUMO levels; this intrinsic emission is typically weak in functionalized CQDs. (B) Surface-state emission, the dominant mechanism in most functionalized CQDs, originates from surface defect states that introduce intermediate energy levels, enabling radiative recombination via electron trapping at the surface. (C) Hydrophobic passivation suppresses non-radiative decay pathways, reduces solvent-induced quenching, and enhances radiative emission efficiency by stabilizing surface states. Energy level diagrams illustrate excitation and emission pathways for each mechanism.

CONCLUSION: This review establishes that hydrophobic CQDs function as surface-engineered photophysical systems, where emission is dominated by surface-state dynamics rather than core properties. Hydrophobic modification enhances photoluminescence by reducing non-radiative pathways, but trade-offs with dispersibility limit applications. The lack of quantitative structure–property models remain a key limitation, highlighting the need for precise control of surface chemistry and electronic structure.

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Drying-Induced Structural Evolution in Chitosan Microparticles: A Critical Determinant of Porosity, Diffusion Pathways, And Drug Release

Arkadeep Mandal, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Chitosan-based microparticles prepared via ionic gelation are typically formed in a hydrated state and subsequently subjected to drying processes such as air drying, freeze drying, or spray drying to obtain stable formulations. While drying is often considered a post-processing step, emerging evidence indicates that it plays a critical role in defining the final microstructure and drug release behaviour of the system. During drying, solvent removal induces structural rearrangement within the polymer network, leading to changes in porosity, pore size distribution, and matrix density. Studies demonstrate that different drying methods produce significantly different structural outcomes, even when the initial wet microparticles are identical [1]. This suggests that drying is not a passive step but an active structural transformation process. Importantly, drying-induced changes directly influence drug release kinetics. For instance, highly porous structures formed during freeze drying often exhibit rapid release and burst effects, whereas dense structures formed during air drying show slower and more controlled release [1]. Despite this, most studies treat drying as a secondary factor, without integrating it into mechanistic understanding of release behaviour. This leads to a critical research question: Is drug release in chitosan microparticles governed by initial formulation, or by structural evolution induced during drying?

This review critically evaluates recent literature (2020–2025) to establish drying as a primary determinant of microstructure and diffusion behaviour, redefining it as a key design parameter in drug delivery systems.

MATERIALS AND METHODS:

This study was conducted as a systematic review using a PRISMA-based analytical framework to ensure reproducibility and structured literature selection. Literature searches were performed across PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using search terms such as “Chitosan microparticles drying effect drug release,” “freeze drying porosity chitosan microspheres,” and “spray drying structure drug release chitosan.” The search was limited to peer-reviewed articles published between 2020 and 2025 in English. Inclusion criteria comprised studies addressing drying methods, structural characterization, porosity, and drug release behaviour in chitosan systems, while exclusion criteria included unrelated materials, incomplete datasets, and duplicate studies. Articles were screened through title, abstract, and full-text analysis, and extracted data included drying methods, structural properties, porosity, and release profiles. A critical analytical synthesis approach was applied to identify process–structure–function relationships and mechanistic gaps.



RESULT AND CONCLUSION

1. Drying as a Structural Transformation Process Drying of chitosan microparticles involves solvent evaporation, capillary forces, and polymer chain rearrangement, leading to structural consolidation that can significantly alter the internal architecture. Different drying methods produce distinct structural outcomes, with air drying resulting in dense, collapsed structures, freeze drying generating porous, expanded networks, and spray drying producing smooth, compact particles. Experimental studies confirm that drying modifies particle diameter, porosity, and surface area, directly influencing drug loading and release behaviour [1]. Therefore, drying should be considered a structure-forming step rather than merely a stabilization step.

2. Influence of Drying Method on Porosity and Microstructure The most significant effect of drying is on porosity, which governs diffusion pathways. Freeze drying involves sublimation of ice crystals, resulting in the formation of large pores, high surface area, and interconnected networks. In contrast, air drying leads to solvent evaporation-driven collapse, reduced pore volume, and the formation of a dense matrix. Studies show that porosity increases progressively from air drying to slow freezing to rapid freezing conditions, directly correlating with increased swelling and drug release rates [1].

3. Impact on Drug Release Kinetics Drying-induced structural changes have a direct impact on drug release behaviour, where dense structures formed by air drying restrict diffusion and result in slow release, while highly porous structures produced by freeze drying enable rapid diffusion and lead to burst release. Experimental evidence demonstrates that fast freezing generates the highest porosity and the most pronounced burst release, whereas slow freezing yields moderate release, and air drying produces the slowest release profiles [1]. This indicates that drug release is not solely governed by formulation but is strongly influenced by structural modifications induced during post-processing.

4. Drying-Induced Heterogeneity and Instability A critical but often overlooked aspect is that drying introduces structural heterogeneity and defects such as pore size variation, surface irregularities, and micro-cracks, which arise due to non-uniform solvent removal and the development of internal stresses during the drying process. From a physical perspective, drying of porous systems involves complex phenomena such as capillary pressure-driven flow and structural collapse, leading to non-uniform architecture [2]. This heterogeneity results in uneven diffusion pathways, unpredictable drug release behaviour, and reduced reproducibility.

5. Drying vs Formulation: Which Dominates? A key insight emerging from recent studies is that drying can override formulation effects. Two systems with identical composition but different drying methods can exhibit completely different release profiles. This challenges the conventional formulation-centric view and suggests that: drying is not a secondary factor but a dominant determinant of functional performance

6. Critical Gap: Lack of Integrated Process–Structure–Function Models Despite clear evidence, current literature lacks predictive models linking:

- Drying conditions
- Structural evolution (porosity, density)
 - Drug release kinetics



Most studies treat drying as an isolated variable rather than integrating it into a unified mechanistic framework.

Table 1. Influence of Drying Methods on Structure and Drug Release

Drying Method	Structural Outcome	Porosity	Drug Release Behavior
Air drying	Dense, collapsed matrix	Low	Slow, sustained release
Slow freeze drying	Moderately porous	Medium	Controlled release
Rapid freeze drying	Highly porous	High	Fast release, burst effect
Spray drying	Smooth, compact particles	Low-moderate	Diffusion-controlled release

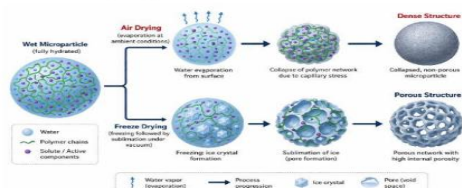


Figure 1: Drying-Induced Structural Evolution Model

CONCLUSION: This review demonstrates that drying is not merely a post-processing step but a critical determinant of structural and functional properties in chitosan microparticles. The analysis reveals that: • Drying induces significant structural transformation affecting porosity and density • Different drying methods produce fundamentally different release behaviors • Porosity and diffusion pathways are strongly governed by drying conditions • Structural heterogeneity introduced during drying affects reproducibility A major limitation in current research is the absence of predictive frameworks linking drying parameters to release kinetics. Drying should be redefined as a primary structural engineering step, where control over solvent removal dynamics is essential for designing predictable drug delivery systems.

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Molecular Docking Analysis of Ortataxel Against B-Tubulin Mutants And B-III Isotype: Insights Into Mutation-Dependent Binding Variation

Zubia Khan, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Microtubules are dynamic polymers formed by α/β -tubulin heterodimers and play a central role in mitotic spindle assembly and intracellular transport. Their dynamic instability is regulated by structural transitions in β -tubulin, particularly involving the M-loop, which mediates lateral interactions between protofilaments [1]. Ortataxel is a semi-synthetic taxane derivative structurally modified to enhance activity against resistant tubulin variants. Similar to other taxanes, it binds to the toxoid pocket of β -tubulin and stabilizes microtubules by promoting a polymerized conformation. However, resistance mechanisms such as β III-tubulin (TUBB3) isotype expression and point mutations in β -tubulin can significantly alter ligand binding and functional stabilization. Mutations including A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I are distributed across the binding pocket, M-loop, and allosteric regions, affecting ligand binding through steric, electrostatic, and conformational changes. The present study evaluates the binding affinity of ortataxel across wild-type β -tubulin, TUBB3 isotype, and multiple resistance-associated mutants using a multi-structure docking approach.

MATERIALS AND METHODS: Ortataxel was subjected to molecular docking against eleven β -tubulin structures, including wild-type, β III-tubulin (TUBB3), and nine mutant variants (A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I), using the SMINA docking engine as described in the report. Ligand 3D conformations were generated using RDK it and optimized with MMFF94 force field. Docking was performed against an ensemble of protein structures, and the best docking score for each variant was selected. The mean docking score was calculated across all structures. Binding affinity (kcal/mol) was used as the primary metric to evaluate ligand– protein interaction strength.

RESULTS AND DISCUSSION:

3. RESULTS AND DISCUSSION

Table1. Docking Score Distribution Across β -Tubulin Variants

Target	Docking Score (kcal/mol)
Wild-type β -tubulin	–8.57
TUBB3 (β III)	–6.80
Mutants (range)	–6.06 to –7.66



Table 1. Docking Score Distribution Across β -Tubulin Variants Target Docking Score (kcal/mol) Wild-type β -tubulin -8.57 TUBB3 (β III) -6.80 Mutants (range) -6.06 to -7.66 The results indicate a reduction in binding affinity from wild-type to mutated variants, with a moderate spread in docking values. The docking analysis demonstrated that ortataxel maintains interaction with multiple β -tubulin variants despite structural alterations associated with isotype expression and mutation-induced perturbations. A reduction in binding affinity was observed from -8.57 kcal/mol in wild-type β -tubulin to -6.80 kcal/mol in the β III-tubulin (TUBB3) isotype, reflecting structural differences within the taxoid binding pocket, including increased conformational flexibility and altered residue composition. However, the moderate reduction indicates that ortataxel retains partial binding capability despite isotype-associated structural variation. Mutation-specific analysis further revealed varying sensitivity of ortataxel toward alterations in the binding pocket, M-loop region, structural core, and allosteric interface residues. Binding pocket mutations such as A250V and F272V introduced steric constraints and loss of aromatic interactions, resulting in reduced ligand stabilization and weaker hydrophobic anchoring. Similarly, M-loop mutations T276I and R284N altered local flexibility, hydrogen bonding potential, and electrostatic interactions, leading to moderate reductions in binding affinity. Core structural mutations including A233T and D199N produced some of the lowest docking scores, suggesting that polarity changes and surface electrostatic modifications destabilize the binding pocket and indirectly influence ligand positioning. In addition, allosteric and interface mutations such as A187T, S174A, and R308C demonstrated variable effects on docking affinity, with A187T maintaining relatively strong interaction while other mutations moderately reduced structural stability and ligand binding. Overall, the docking profile suggests that ortataxel exhibits moderate sensitivity to structural perturbations within β -tubulin and relies on a combination of hydrophobic and polar interactions for stable binding. Structural alterations within the taxoid pocket significantly influence ligand orientation and binding affinity, indicating dependence on specific residue interactions for optimal stabilization.

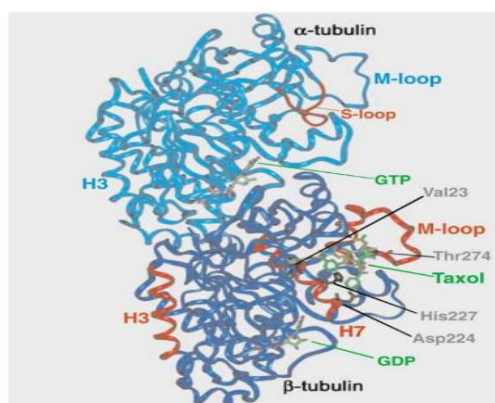


Figure 1. Structural representation of β -tubulin highlighting taxoid binding pocket and mutation sites

[Adapted From: doi: 10.1038/sj.onc.1206934]

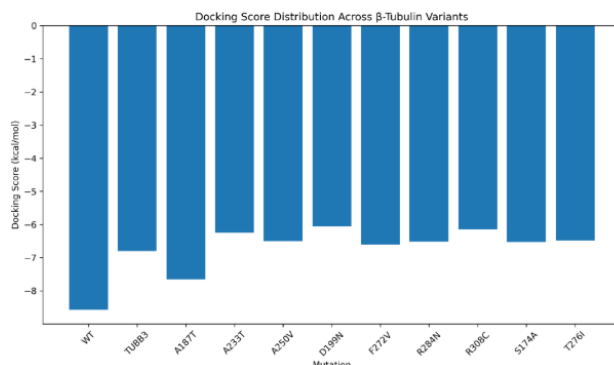


Figure 2. Docking score distribution of ortataxel across wild-type, TUBB3, and mutant variants.

CONCLUSION:

The present study demonstrates that ortataxel exhibits moderate binding affinity toward β -tubulin, with a reduction observed in β III-tubulin and mutation-bearing variants. Mutations affecting the binding pocket and M-loop region significantly influence ligand binding through steric and electrostatic perturbations. While ortataxel retains binding capability across all variants, its interaction profile indicates sensitivity to structural disruptions within the toxoid pocket. The results highlight the importance of local structural integrity in maintaining ligand– tubulin interactions and provide insights into mutation-dependent binding variation.

ACKNOWLEDGMENT

The authors acknowledge the support of institutional computational facilities and research infrastructure.

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Antimicrobial Peptides in Tuberculosis Therapy: A Multi-Scale Analysis of Host–Pathogen Interactions And Intracellular Targeting Mechanisms (2020–2025)

Rounak Bhattacharyya, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Despite being treated for more than half a century, Tuberculosis (TB) remains a major public health concern due to its prolonged therapy regimen, development of multi-drug-resistant organisms as well as the ability of the organism to persist in host macrophages. Unlike most extracellular bacterial pathogens, Mycobacterium tuberculosis infection occurs intracellularly, meaning that the bacteria will remain relatively protected from most forms of treatment due to the nature of their replication process. The class of antimicrobial peptides (AMPs), which has gained importance in drug discovery due to its unique mechanism of action, has been found to possess both direct and indirect antibacterial properties. Traditionally, AMPs have been described as microorganism-membrane damaging agents; however, the latest findings indicate that apart from destroying microorganisms, AMPs can also alter the functions of immune system through the regulation of specific pathways as well as stimulation of and cytokines [1][2]. In spite of the advances, the therapeutic translation of AMPs in TB remains very less. The question then arises: do AMPs primarily function as antimicrobial agents, or as modulators of host–pathogen interactions within the intracellular environment?

MATERIALS AND METHODS:

This is a PRISMA-driven systematic review of the literature reporting on literature retrieval and synthesis. Databases such as PubMed, Scopus, Web of Science, and ScienceDirect were explored for articles related to AMPs and TB, using search strings such as “antimicrobial peptides tuberculosis”, “intracellular macrophage AMP mechanism”, and “host-directed therapy TB peptides”. Only articles that have been reviewed by peers from 2020 to 2025 were considered in the review. The research covered studies on the mechanism of action of AMPs in TB, which includes studies related to intracellular, immunological, and delivery mechanisms. Studies involving extracellular mechanisms without mechanisms of action were not considered. Critical Synthesis Approach was used to assess the mechanisms of action, discrepancies between in vitro and in vivo results, and translational challenges.

RESULTS AND DISCUSSION

The problem with the use of AMPs as an anti-TB drug lies in the differential activity of AMPs in and out of cells. While many of the AMPs are potent activators for extracellular M. tuberculosis infections, their efficiency in intracellular M. tuberculosis is inconsistent. For example, host-defense protein such as lysozyme is a potent extracellular bactericide, while their effectiveness inside macrophages is compromised by poor cell penetration [2]. It can be inferred that antimicrobial activity of AMPs may not be the determining factor, and efficient cell entry is the primary determinant. AMPs have modulatory effects on both innate and adaptive immune systems. They activate macrophage functions and produce cytokines that facilitate bacterial clearance by immune cells [1]. In addition, in some bacteria, AMP-induced autophagy activates host cells' bactericidal functions, which indicate that



host-related functions of AMPs can be as important as their antibacterial activities [3]. In essence, AMPs' function changes from being an antibiotic to becoming modulators of host-pathogen interactions. The multifunctional activities of AMPs pose a mechanistic issue. The presence of granulomas and latent bacterial infection creates a barrier to the penetration of antibiotics into infected cells, where they are effective only when they can penetrate and destroy target cells. There is no literature on how efficiently AMPs penetrate the granuloma layer or work on latent bacteria. Additionally, while AMPs cause resistance in lower levels compared to conventional drugs due to the action mechanism, there have been claims by some researchers that resistance is not entirely prevented and may even be underestimated due to the lack of long-term studies [4]. Additionally, the stability of AMPs, their susceptibility to enzymatic degradation, and cellular uptake may present challenges for future treatment. The inconsistency between positive in vitro results of AMP action and negative in vivo results implies a need to develop a new set of in vitro tests that would reflect the actual conditions of infection.

Table 1. Multi-Scale Determinants of AMP Efficacy in Tuberculosis

Level	Mechanism	Limitation
Molecular	Membrane disruption	Limited intracellular relevance
Cellular	Immune modulation	Variable host response
Intracellular	Macrophage targeting	Poor penetration
Tissue	Granuloma structure	Restricted access
Systemic	Delivery & stability	Rapid degradation

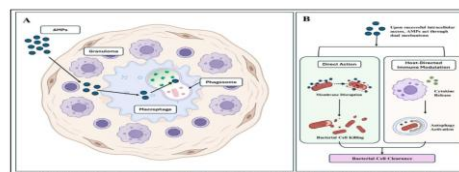


Figure 1. Multi-scale barriers and dual mechanisms of antimicrobial peptide (AMP) activity in tuberculosis. (A) AMPs encounter sequential barriers at the granuloma, macrophage, and intracellular levels, limiting access to *Mycobacterium tuberculosis*. (B) Upon intracellular entry, AMPs act via direct bactericidal effects and host-directed immune modulation, promoting bacterial clearance.

CONCLUSION: In summary, AMPs for tuberculosis treatment ought to be viewed as multi-scale

modulators of host-pathogen interactions, not classical antibiotics. The antibacterial action of AMPs is inherently limited in tuberculosis because of intra-cellular, immune, and tissue-level limitations. It is clear from the review that:

- Access is the critical variable determining AMPs' success
- Immunomodulation may be as significant as cell death
- Conventional models have exaggerated efficacy because of over-simplified biology
- Stability, specificity, and delivery pose major translation barriers

AMP-based TB therapy should shift from a molecule-centric approach to a system-level strategy that integrates intracellular targeting, immune modulation, and delivery optimization to achieve effective clinical translation.

ACKNOWLEDGEMENT

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Mutation-Specific Analysis Of Cabazitaxel Binding To β -Tubulin Using Multi-Target Molecular Docking

Barsha Bardhan, And Debabrata Ghosh Dastidar*
Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Microtubules are dynamic cytoskeletal polymers composed of α/β -tubulin heterodimers, essential for mitotic spindle formation and intracellular transport. Their functional behavior is governed by conformational transitions within β -tubulin, particularly involving the M-loop region, which plays a crucial role in lateral protofilament interactions. Cabazitaxel is a semi-synthetic taxane designed to interact with the taxoid binding pocket of β -tubulin and stabilize microtubules by promoting a polymerized state. Despite the effectiveness of taxane-based agents, resistance is frequently observed due to structural variations in β -tubulin. These include the expression of the β III-tubulin isotype (TUBB3), which exhibits altered binding characteristics, and point mutations that perturb the structural integrity of the taxoid pocket [1]. Mutations such as A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I are distributed across functional domains of β -tubulin, including the binding pocket, M-loop, and allosteric regions. These mutations can influence ligand binding through steric hindrance, electrostatic disruption, and conformational destabilization [1][2]. The present study aims to evaluate the effect of these mutations and isotype variation on cabazitaxel binding affinity using a multi-target molecular docking approach.

MATERIALS AND METHODS:

Cabazitaxel was subjected to molecular docking against eleven β -tubulin targets, including wild-type, β III-tubulin (TUBB3), and nine mutant variants (A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I), using the GIRL server multi-target docking platform. Ligand conformations were generated using ETKDGV3 followed by energy minimization with the UFF force field. Docking was performed using the SMINA engine with an exhaustiveness parameter of 8 and an energy window of 3 kcal/mol, generating multiple binding poses. An ensemble docking strategy was applied, where each ligand was docked against multiple conformations of each protein target. The best docking score for each target was selected for analysis. Binding affinity values (kcal/mol) were used as the primary metric for evaluating ligand–protein interactions.

RESULTS AND DISCUSSION:

Table1. Docking Score Distribution Across β -Tubulin Variants

Target	Docking Score (kcal/mol)
Wild-type β -tubulin	–8.57
TUBB3 (β III)	–6.80
Mutants (range)	–6.06 to –7.66

The results indicate a reduction in binding affinity from wild-type to mutated variants, with a moderate spread in docking values. The docking analysis demonstrated that cabazitaxel maintains relatively stable binding affinity



across multiple β -tubulin variants despite structural alterations associated with isotype expression and mutation-induced perturbations [1]. A reduction in binding affinity was observed from -9.27 kcal/mol in wild-type β -tubulin to -7.18 kcal/mol in the β III-tubulin (TUBB3) isotype, which may be attributed to increased conformational flexibility and altered hydrophobic topology within the toxoid binding pocket. However, the reduction remained moderate, indicating preserved ligand accommodation despite isotype-associated structural variation. Mutation-specific analysis further revealed limited sensitivity of cabazitaxel binding toward alterations in the binding pocket, M-loop region, structural core, and allosteric interface residues [2]. Binding pocket mutations such as A250V and F272V introduced steric and aromatic modifications while maintaining relatively stable affinities, suggesting reduced dependence on rigid steric alignment or π - π interactions. Similarly, M-loop mutations T276I and R284N produced minimal effects on docking affinity despite altering hydrogen bonding potential and electrostatic characteristics, indicating that cabazitaxel binding is not critically dependent on precise M-loop conformation. Core and structural mutations including A233T and D199N also showed negligible influence on ligand interaction, suggesting tolerance toward local pocket instability and electrostatic variation. In addition, allosteric and interface mutations such as A187T, S174A, and R308C demonstrated only modest changes in docking scores despite affecting structural stability and inter-dimer interactions [3]. Overall, the narrow range of docking scores across all variants suggests that cabazitaxel interacts with β -tubulin through a distributed interaction network rather than relying on a limited number of critical residues. This mechanistic adaptability enables the ligand to maintain stable binding despite mutation-induced structural perturbations within the toxoid binding pocket [2][3].

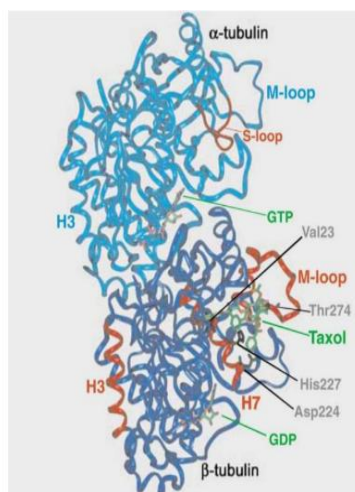


Figure 1. Structural representation of β -tubulin highlighting taxoid binding pocket and mutation sites.
[Adapted From: doi: [10.1038/sj.onc.1206934](https://doi.org/10.1038/sj.onc.1206934)]

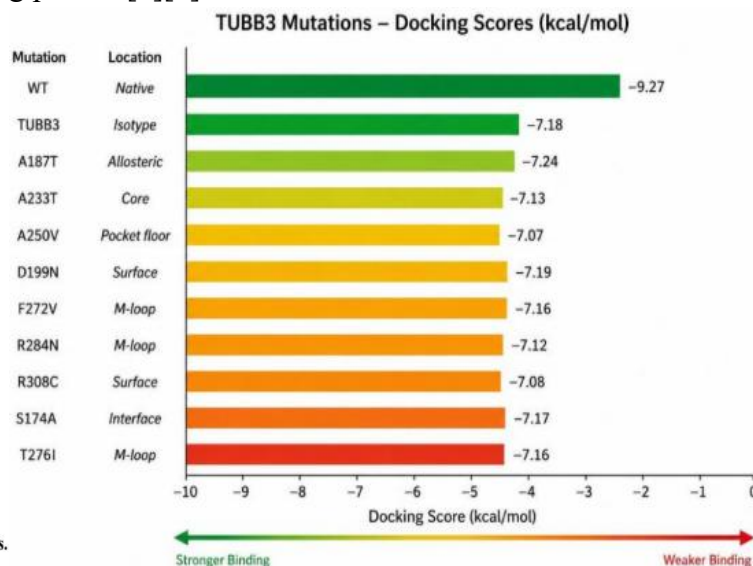


Figure 2. Docking score distribution of ortataxel across wild-type, TUBB3, and mutant variants.



CONCLUSION:

The present study demonstrates that cabazitaxel maintains consistent binding affinity across β -tubulin variants, including TUBB3 and multiple resistance-associated mutations. While a reduction in binding affinity is observed relative to wild-type, the variation across mutants remains minimal. Mutations affecting the binding pocket, M-loop, and allosteric regions do not significantly disrupt ligand binding, indicating that cabazitaxel exhibits structural adaptability within the toxoid pocket. This behavior suggests that ligand interaction is governed by a distributed network of interactions rather than dependence on specific residues. These findings highlight the importance of interaction flexibility in overcoming mutation-induced structural perturbations and provide insights for the design of next-generation microtubule-stabilizing agents.

ACKNOWLEDGMENT:

The authors acknowledge the support of institutional research facilities and computational resources used in this study.

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Molecular Docking Analysis of Milataxel Against β -Tubulin Mutants And Biii Isotype: Structural Insights Into Mutation-Dependent Binding Variation

Snehashree Roy, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Microtubules are essential cytoskeletal polymers composed of α/β -tubulin heterodimers and are involved in critical cellular processes including mitosis and intracellular transport. Their dynamic instability is governed by conformational transitions in β -tubulin, particularly within the M-loop, which facilitates lateral protofilament interactions. Milat axel is a semi-synthetic taxane derivative characterized by structural modifications in the oxetane

ring and side chain, designed to influence interaction dynamics within the toxoid binding pocket. Similar to other taxanes, Milat axel binds to β -tubulin and stabilizes microtubules by promoting a polymerized conformation. Resistance to taxanes arises due to β III-tubulin (TUBB3) isotype expression and mutations within the β -tubulin structure. These mutations, including A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I, are distributed across the binding pocket, M-loop, and allosteric regions, influencing ligand binding through steric, electrostatic, and conformational changes. The present study evaluates the binding affinity of milataxel across wild-type β -tubulin, TUBB3 isotype, and multiple resistance-associated mutants using a multi-structure molecular docking approach.

MATERIALS AND METHODS:

Milat axel was docked against eleven β -tubulin protein structures, including wild-type, β III-tubulin (TUBB3), and nine mutant variants (A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I), using the SMINA docking engine (GIRL Server for high throughput virtual screening developed by Dr. Debabrata Ghosh Dastidar et al.) Ligand conformations were generated using RDKit and optimized using the MMFF94 force field. Docking was performed against an ensemble of protein structures, and the best docking score for each variant was selected. Mean binding affinity values were calculated across all structures.

RESULTS AND DISCUSSION

3.1 Docking Score Distribution Across β -Tubulin Variants

Docking results (Page 2) show the following:

Target	Docking Score (kcal/mol)
Wild-type β -tubulin –	8.59
TUBB3 (β III) –	8.25
Mutants (range) –	5.86 to –6.93

The data indicate strong binding affinity toward both wild-type and TUBB3 isotype, with a significant reduction observed across mutant variants.

3.2 Effect of β III-Tubulin (TUBB3) Isotype



The docking score for TUBB3 (−8.25 kcal/mol) is comparable to the wild-type value (−8.59 kcal/mol), indicating minimal reduction in binding affinity. This suggests that Milat axel exhibits strong tolerance to isotype-driven structural variation. The comparable binding affinity implies that the ligand is capable of accommodating increased conformational flexibility and altered residue composition within the toxoid pocket.

3.3 Mutation-Specific Effects on Binding Affinity

3.3.1 Binding Pocket Mutations

- A250V (−5.93 kcal/mol): Introduction of steric bulk leads to displacement of the ligand from optimal orientation, resulting in reduced binding affinity.
- F272V (−6.10 kcal/mol): Loss of aromatic interaction reduces hydrophobic stabilization and weakens ligand anchoring.

3.3.2 M-Loop Region Mutations

- T276I (−6.04 kcal/mol): Alters hydrogen bonding potential and local flexibility, leading to moderate reduction in binding affinity.
- R284N (−5.88 kcal/mol): Loss of electrostatic interaction contributes to destabilization of ligand binding.

3.3.3 Core Structural Mutations

- A233T (−5.86 kcal/mol): Exhibits one of the lowest docking scores, indicating significant destabilization of the binding pocket due to polarity introduction.
- D199N (−6.11 kcal/mol): Surface electrostatic alteration moderately affects ligand positioning.

3.3.4 Allosteric and Interface Mutations

- A187T (−6.93 kcal/mol): Maintains relatively higher binding affinity, indicating limited direct disruption of the binding site.
- S174A (−6.08 kcal/mol) and R308C (−6.19 kcal/mol): Affect structural stability at the protein interface, resulting in moderate reduction in binding affinity.

3.4 Mechanistic Interpretation The docking profile indicates that Milat axel exhibits strong binding affinity toward structurally flexible β -tubulin variants such as TUBB3 but demonstrates sensitivity to mutations that directly disrupt the toxoid binding pocket and M-loop region. The significant reduction in binding affinity across multiple mutants suggests that ligand interaction is partially dependent on specific residue interactions and pocket geometry. Structural perturbations caused by mutations lead to loss of stabilizing interactions, resulting in decreased binding strength. The ability to retain high binding affinity in TUBB3 indicates that Milat axel can accommodate global conformational flexibility, while local structural disruptions within the binding pocket remain a limiting factor.

3.5 Figures and Tables

Table 1. Docking score summary across β -tubulin variants

Mutation	Location	Docking Score (kcal/mol)	Mutation	Location	Docking Score (kcal/mol)
WT	Native –	8.59	R284N	M-loop –	5.88
TUBB3	Isotype –	8.25	R308C	Surface –	6.19
A187T	Allosteric –	6.93	S174A	Interface –	6.08
A233T	Core –	5.86	T276I	M-loop –	6.04
A250V	Pocket floor –	5.93			
D199N	Surface –	6.11			
F272V	M-loop –	6.10			

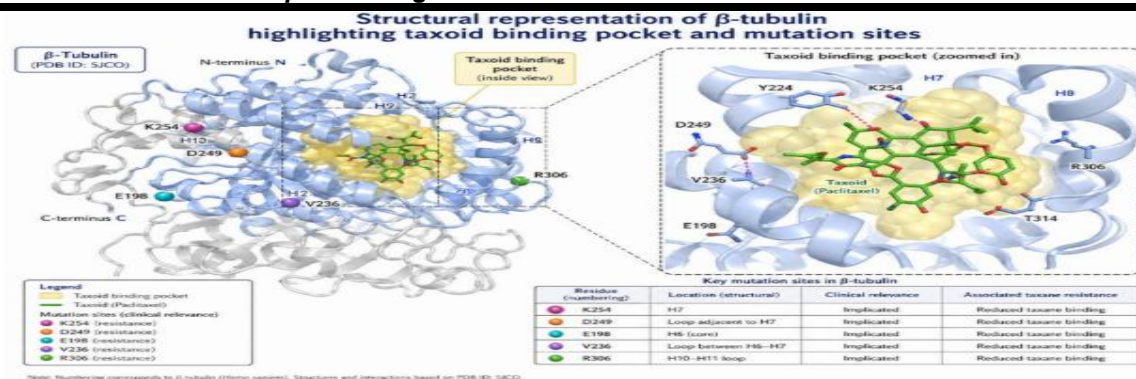


Figure 1. Structural representation of β -tubulin highlighting taxoid binding pocket and mutation sites.

Figure 2. Docking score distribution of milataxel across wild-type, TUBB3, and mutant variants.

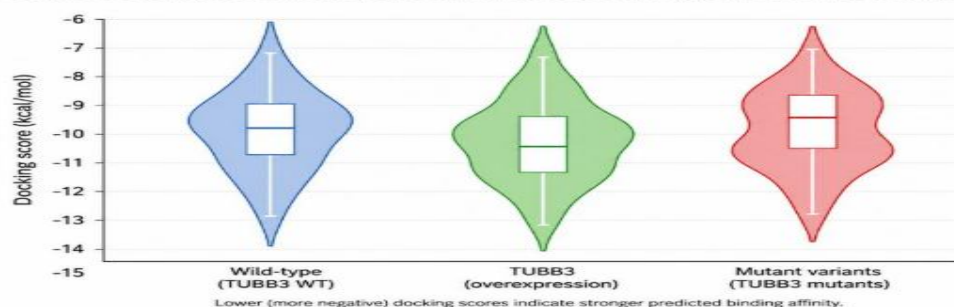


Figure 2. Docking score distribution of milataxel across wild-type, TUBB3, and mutant variants.

CONCLUSION

The present study demonstrates that Milat axel exhibits strong binding affinity toward both wild-type β -tubulin and the β III-tubulin isotype, indicating effective accommodation of isotype-induced structural variability. However, mutations affecting the binding pocket and M-loop region significantly reduce binding affinity through steric and electrostatic perturbations. The results suggest that while Milat axel can tolerate global conformational flexibility, it remains sensitive to local structural disruptions within the toxoid binding pocket. These findings provide insights into mutation-dependent binding behavior and may contribute to the rational design of taxane derivatives with improved resistance profiles.

ACKNOWLEDGMENT

The authors acknowledge the support of institutional computational facilities and research infrastructure.

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Pulmonary Deposition–Absorption–Clearance Coupling as A Determinant of Systemic Bioavailability in Inhalable Drug Delivery Systems

Sastik Kar, and Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Systemic drug delivery via conventional routes such as oral administration is often limited by degradation, poor permeability, and extensive first-pass metabolism. Inhalable drug delivery systems provide an alternative route by utilizing the pulmonary interface for systemic absorption. The lungs offer distinct physiological advantages, including a large surface area, thin alveolar epithelium, and extensive vascularization, which enable rapid drug uptake into systemic circulation [1]. However, achieving consistent systemic bioavailability through inhalation is not governed solely by access to the lung surface. Instead, drug delivery efficiency is constrained by competing physiological processes within the respiratory system. This raises a central mechanistic question: Is systemic bioavailability determined by lung deposition alone, or by the dynamic interplay between deposition, absorption, and clearance processes?

MATERIALS AND METHODS

This study was conducted using a PRISMA-based systematic review method. Literature was searched from PubMed, Scopus, Web of Science, and ScienceDirect using keywords such as “pulmonary drug delivery deposition absorption clearance,” “aerosol particle size lung deposition mechanism,” and “mucociliary clearance inhalation pharmacokinetics.” Only peer-reviewed articles published between 2020 and 2025 were included. Studies related to inhalable drug delivery systems, mechanisms of lung deposition and absorption, and pulmonary clearance processes were selected. Studies on non-inhalation drug delivery systems and descriptive studies without mechanistic explanation were excluded. Finally, a critical synthesis approach was used to analyze and summarize the findings.

RESULTS AND DISCUSSION

1. Pulmonary Delivery as a Coupled Transport System:

Pulmonary drug delivery works through a series of connected processes. First, drug particles are deposited in different regions of the lungs. After deposition, the drug dissolves and is released, then it diffuses across the epithelial barriers of the lungs, and finally enters the systemic circulation. These processes are linked with each other and together determine how much of the drug becomes available in the body. Thus: Pulmonary bioavailability is governed by transport coupling, not a single step.

2. Particle Deposition as the Initial Determinant:

Particle size is the main factor that determines where drug particles deposit in the lungs. Particles larger than 5 μm usually deposit in the upper airways by impaction, while particles between 1–5 μm reach the deep lungs and alveolar region mainly by sedimentation. Very small particles smaller than 0.5 μm deposit by diffusion. These deposition mechanisms decide whether the particles can reach the areas suitable for systemic absorption.[2]. However:

Deposition location defines potential absorption, not actual bioavailability.

3. Absorption Across the Alveolar Barrier: Once deposited, drugs must cross the pulmonary epithelium.



Several factors influence drug absorption in the lungs, including the thin alveolar membrane, high blood flow in the lungs, and the molecular diffusion properties of the drug. Because the alveolar region has a very thin barrier and rich blood supply, pulmonary delivery allows rapid absorption of the drug directly into the systemic circulation. [1]. However, the efficiency of drug absorption in the lungs depends on several factors such as drug solubility, membrane permeability, and the interaction of the drug with epithelial cells. These factors determine how easily the drug can dissolve, pass through the lung barrier, and enter the bloodstream.

4. **Competing Clearance Mechanisms:** Clearance processes greatly reduce the amount of drug available for absorption in the lungs. Mucociliary clearance removes drug particles from the conducting airways by moving them out of the respiratory tract, while alveolar macrophages engulf particles that reach the deep lung regions. These natural defense mechanisms compete with drug absorption and reduce the time the drug remains in the lungs for effective uptake. [3]. Thus: Pulmonary delivery involves a balance between absorption and clearance.
5. **Deposition–Absorption–Clearance Coupling:** A key insight is that systemic bioavailability depends on the interaction of three connected processes: deposition, absorption, and clearance. Deposition determines where the drug particles settle in the lungs, absorption determines how much drug enters the bloodstream, and clearance determines how much drug is removed before absorption. For example, deep lung deposition offers high absorption potential but also exposes particles to macrophage clearance, while upper airway deposition may allow longer retention but provides limited systemic absorption. Therefore, improving only one factor does not guarantee effective drug delivery.
6. **Trade-Off Between Retention and Absorption:** Pulmonary delivery involves a basic trade-off between absorption and clearance. Faster drug absorption can increase exposure to clearance mechanisms, while longer retention in the lungs may reduce access to systemic circulation. This creates a dynamic balance where effective drug delivery depends on optimizing how long the drug stays in the lungs in relation to how quickly it can be absorbed into the bloodstream.
7. **Critical Gap: Lack of Integrated Predictive Models:** Current research has several limitations because deposition, absorption, and clearance are often studied separately instead of as connected processes. There is a lack of integrated transport models and limited predictive frameworks for designing effective formulations. Important factors such as particle size, aerodynamic behavior, lung physiology, and clearance kinetics are rarely combined into a single unified model, which makes it difficult to accurately predict pulmonary drug delivery performance.

Table 1. Coupled Processes Governing Pulmonary Drug Delivery

Process	Functional	Role Limitation
Deposition	Determines lung region	Does not ensure absorption
Absorption	Enables systemic uptake	Depends on drug properties
Mucociliary clearance	Removes particles	Reduces bioavailability
Process	Functional	Role Limitation
Macrophage uptake	Eliminates particles	Limits deep lung delivery
Particle engineering	Controls deposition	Trade-off with clearance

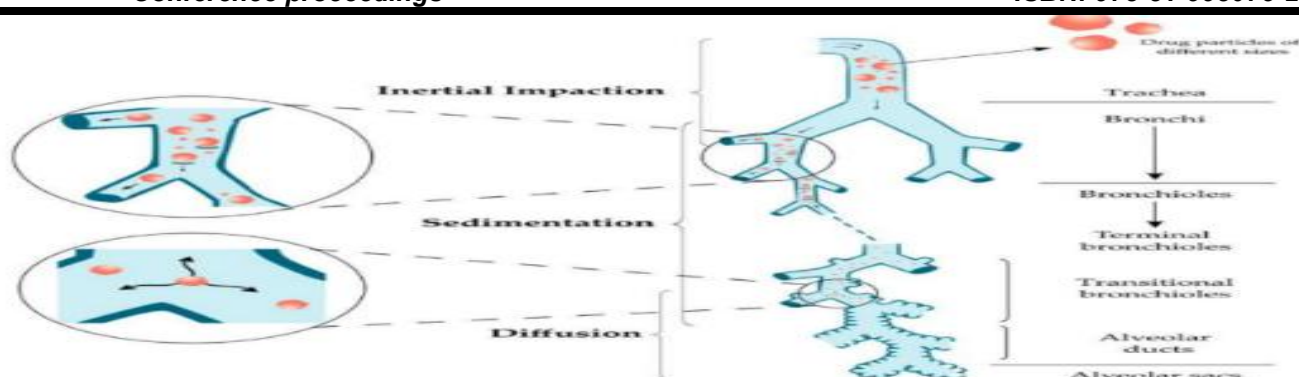


Figure 1 : Particle deposition mechanisms according to particle size. (4)

CONCLUSION: This review shows that inhalable drug delivery systems should be understood as transport-controlled systems based on the coupling of deposition, absorption, and clearance, rather than simply as an alternative to conventional drug delivery routes. Pulmonary delivery efficiency depends on several connected processes where particle deposition provides access to the lungs, but does not guarantee absorption. Clearance mechanisms such as mucociliary and macrophage clearance compete with drug absorption, and systemic bioavailability depends on the balance between these processes. Inhalable drug delivery is therefore determined not only by where particles deposit, but also by whether they remain in the lungs long enough to be absorbed before being cleared.

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Thiolated Polymer–Mucosa Interactions as Multi-Barrier Modulators in Buccal Peptide Delivery: A Mechanistic Analysis of Mucoadhesion, Permeation, And Enzyme Inhibition

Arpita Nandi, And Debabrata Ghosh Dastidar*

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Peptide therapeutics face significant delivery challenges due to enzymatic degradation, poor epithelial permeability, and rapid clearance, resulting in low systemic bioavailability following conventional administration. Buccal drug delivery offers a promising alternative by bypassing first-pass metabolism; however, its effectiveness is constrained by limited residence time, restricted permeation, and enzymatic degradation within the mucosal environment. Traditional mucoadhesive polymers rely on weak non-covalent interactions, which are insufficient to ensure prolonged retention and effective absorption. This highlights a fundamental limitation in buccal delivery systems, where multiple biological barriers act simultaneously. Recent literature identifies thiolate polymers (thiomers) as multifunctional excipients capable of overcoming these barriers through chemical modification of polymer backbones. This leads to a central mechanistic question: Do thiolate polymers function only as mucoadhesive agents, or as integrated modulators of multiple biological barriers?

MATERIALS AND METHODS

This review was conducted using a PRISMA-based systematic approach. Literature was searched in PubMed, Scopus, Web of Science, and ScienceDirect using keywords related to thiolate polymers, mucoadhesion, and buccal peptide delivery. Only peer-reviewed articles published between 2020 and 2025 were included. Studies were included if they investigated thiolate polymer (theorem)- based systems for buccal or mucosal drug delivery with mechanistic evaluation. Non-thiolate systems and descriptive studies without mechanistic insight were excluded. A critical synthesis approach was applied to analyze and integrate the findings.

RESULTS AND DISCUSSION

3.1 Buccal Delivery as a Multi-Barrier System Buccal: Drug delivery faces multiple simultaneous barriers, including short residence time due to saliva washout, low epithelial permeability that restricts drug absorption, and enzymatic degradation of sensitive molecules such as peptides. Since these challenges occur together, improving only one parameter is often insufficient, making buccal delivery fundamentally a multi-barrier transport problem requiring integrated delivery strategies.

3.2 Mucoadhesion via Disulfide Bond Formation [1,2]: Thiolate polymers enhance mucoadhesion by forming covalent disulfide bonds with cysteine-rich mucin through thiol–disulfide exchange reactions, creating strong and stable polymer–mucus interactions that prolong residence time, reduce drug washout, and improve drug localization at the buccal mucosal surface compared with conventional polymers.

3.3 Permeation Enhancement Mechanisms [2]: Thiolate polymers improve buccal drug absorption by enhancing epithelial permeation through tight junction modulation, increased paracellular transport, membrane interaction, and possible efflux pump inhibition, making permeation enhancement essential alongside mucoadhesion.

3.4 Enzyme Inhibition and Drug Protection [1,2]: Thiolate polymers protect peptide drugs from rapid



mucosal enzymatic degradation by interacting with proteolytic enzymes, chelating essential metal ions needed for enzyme activity, and providing steric shielding around drug molecules, thereby reducing degradation and improving peptide stability during buccal delivery. **3.5 Integrated Mechanistic Triad:** Thiolate polymers function through an integrated mechanistic triad by enhancing mucoadhesion for increased retention, improving permeation for better epithelial transport, and inhibiting enzymes to increase peptide stability, demonstrating that thiomers act as multi-barrier modulators rather than single-function excipients in buccal drug delivery. **3.6 Trade-Off: Adhesion vs Drug Release:** Although thiolated polymers offer multiple advantages, excessive mucoadhesion and strong cross-linking can reduce drug diffusion and slow release, making the degree of thiolation a critical factor in balancing retention, permeation, and controlled drug release for optimal buccal delivery. **3.7 Critical Gap: Lack of Predictive Design Frame:** A major limitation in current thiolated polymer research is the lack of predictive design frameworks, as most studies report improved performance without quantitatively correlating thiolation degree with drug delivery outcomes, separating the individual effects of adhesion, permeation, and enzyme inhibition, or establishing clear structure–function relationships.

Table 1. Mechanistic Contributions of Thiolated Polymers

Mechanism	Functional Role	Outcome
Disulfide bonding	Strong mucoadhesion	Increased residence time
Tight junction modulation	Permeation enhancement	Increased drug flux
Enzyme interaction	Protease inhibition	Improved stability
Polymer structure	Controls interaction	Affects release
Thiolation degree	Functional tuning	Determines performance

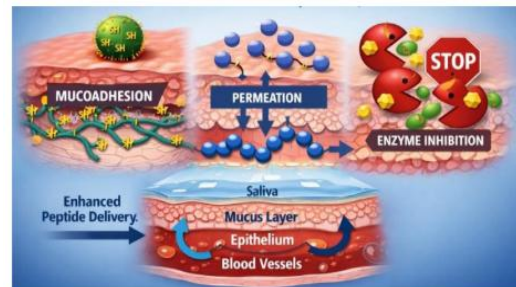


Figure 1: Multi-Barrier Buccal Delivery Model

CONCLUSION

Thiolate polymers are established as multifunctional barrier modulators in buccal peptide delivery, as they simultaneously improve mucoadhesion, permeation, and drug stability while addressing the multiple interacting barriers of the buccal mucosa. Their ability to form disulfide bonds provides a clear mechanistic advantage over conventional polymers, although optimal performance depends on carefully balancing adhesion, permeation, and drug release within the mucosal environment.

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Competing Transport Mechanisms Across the Nasal Mucus Barrier: Balancing Mucoadhesion And Mucopenetration In Intranasal Drug Delivery

Sanjhbati Roy, And Debabrata Ghosh Dastidar*

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Intranasal drug delivery has emerged as a promising non-invasive route for systemic and central nervous system targeting due to its rapid absorption and ability to bypass first-pass metabolism and, in some cases, the blood–brain barrier [1]. However, its efficiency is fundamentally constrained by the nasal mucus barrier, which restricts drug diffusion and promotes rapid mucociliary clearance, thereby limiting residence time and bioavailability [1]. The mucus layer is a viscoelastic, selectively permeable barrier composed primarily of mucin glycoproteins that trap foreign particles through physicochemical interactions and subsequently remove them via mucociliary transport [2]. This creates a fundamental delivery challenge: achieving sufficient retention while ensuring effective transport across the mucus layer. Recent literature identifies two dominant yet mechanistically opposing strategies—mucoadhesion and microgeneration—to overcome this barrier. This raises a central mechanistic question: Should drug delivery systems adhere to mucus to enhance retention, or avoid interaction to enable transport?

MATERIALS AND METHODS

This study was conducted using a PRISMA-based systematic review framework. Literature searches were carried out across PubMed, Scopus, Web of Science, and ScienceDirect using the keywords “intranasal drug delivery mucus barrier,” “mucoadhesion vs microgeneration,” and “polymer–mucus interaction nanocarriers.” The review was limited to peer-reviewed publications published between 2020 and 2025. Studies were included if they focused on intranasal drug delivery systems, mucoadhesive and mucus-penetrating formulations, and mechanistic or transport-based investigations. Studies were excluded if they involved non-nasal mucosal systems or were purely descriptive in nature. A critical synthesis approach was used to analyze and summarize the selected literature.

RESULTS AND DISCUSSION

1. **Mucus Barrier as a Dynamic Transport:** Constraint The nasal mucus barrier is not a static structure but a dynamic system that regulates particle transport through steric hindrance caused by its mesh-like network, adhesive interactions with mucins, and continuous mucociliary clearance. Nanoparticles are often trapped within the mucus due to hydrogen bonding, van der Waals forces, and electrostatic interactions, which can result in their rapid elimination before they reach the epithelial surface.[2] Therefore, failure of drug delivery commonly occurs because of restricted diffusion along with rapid clearance from the nasal cavity.
2. **Mucoadhesion: Enhancing Retention via Interaction:** Mucoadhesive systems are designed to enhance interaction with nasal mucus by using polymers such as chitosan. These systems work through mechanisms like hydrogen bonding, electrostatic interactions, and in advanced formulations, covalent interactions. As a result, they can increase the residence time of the drug in the nasal cavity and maintain a higher local drug concentration. However, excessively strong adhesive interactions may immobilize the carriers within the mucus layer, thereby reducing their ability to penetrate through the mucus and reach the epithelial surface. [3].
3. **Enhancing Transport via Reduced Interaction:** Compensating systems are engineered to minimize interactions with nasal mucus in order to improve particle movement through the mucus layer. Common strategies include the use of hydrophilic coatings such as PEGylation, neutral surface charge, and reduced hydrophobic interactions. These modifications allow rapid diffusion through the mucus mesh and better access to the epithelial surface. However, because these systems interact less with mucus, they often have shorter residence time in the nasal cavity and are more easily cleared. Thus, microgeneration enhances mobility, but at the cost of reduced retention.
4. **Fundamental Trade-Off: Adhesion vs Diffusion:** Mucoadhesion and microgeneration represent competing transport mechanisms



in intranasal drug delivery. Increased adhesion can improve residence time within the nasal cavity, but it may also reduce diffusion through the mucus layer. On the other hand, increased penetration enhances diffusion across mucus, but often decreases residence time. Recent studies emphasize that effective drug delivery depends on balancing these opposing effects rather than optimizing only one mechanism.[4]

5. **Hybrid Systems: Resolving the Trade-Off:** Emerging strategies aim to combine both mucoadhesion and microgeneration within a single delivery system. These include mucoadhesive-to-compenetrating nanoparticles, surface-switching systems, and layered polymer architectures. Such systems are designed to initially adhere to the mucus layer, allowing sufficient residence time, and then subsequently penetrate through the mucus toward the epithelial surface. As a result, these dual-functional systems demonstrate improved transport efficiency compared with single-mechanism approaches [2].
6. **Critical Gap: Lack of Predictive Transport Models:** Despite extensive research, several key limitations still remain in the field of intranasal drug delivery. These include the lack of quantitative models that clearly link particle properties with transport behavior, limited integration of mucus rheology and turnover dynamics, and the absence of standardized evaluation frameworks. Important parameters such as particle size, surface charge, hydrophilicity, and mucus composition are often studied separately and are rarely combined into unified predictive systems.

Table 1. Competing Mechanisms in Nasal Drug Transport

Mechanism	Functional Role	Limitation
Mucoadhesion	Increased retention	Reduced diffusion
Mucopenetration	Enhanced diffusion	Reduced residence time
Mucociliary clearance	Barrier defense	Rapid drug removal
Polymer interaction	Controls adhesion/penetration	Difficult to optimize
Surface modification	Modulates transport	Trade-off effects

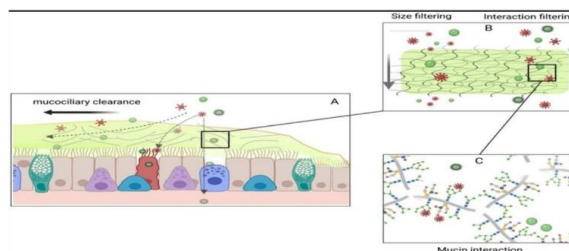


FIG 1 : Competing Transport Mechanism Model [5]

CONCLUSION

This review demonstrates that intranasal drug delivery should be understood as a transport problem governed by competing mechanisms across the mucus barrier. The analysis reveals that mucus functions as a dynamic barrier that limits diffusion while promoting rapid clearance. Mucoadhesive systems can enhance retention within the nasal cavity, but they may also restrict particle transport through the mucus layer. In contrast, compenetrating systems improve diffusion across mucus but often reduce residence time. Therefore, optimal intranasal drug delivery requires a balance between these opposing mechanisms. Effective delivery is not achieved by maximizing adhesion or penetration alone, but by carefully controlling polymer–mucus interactions to maintain both retention and transport efficiency.

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Polymeric Micelles in Targeted Cancer Therapy: A Critical Analysis of Tumor Targeting Mechanisms and Microenvironmental Constraints

Saptak Chakraborty, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Conventional chemotherapy remains fundamentally limited by poor selectivity, systemic toxicity, and inefficient accumulation of therapeutic agents at tumor sites. Polymeric micelles have been developed to address these limitations by improving solubility, prolonging circulation time, and enhancing tumor localization of hydrophobic drugs through nanoscale carrier design [1]. Structurally, these systems are formed via the self-assembly of amphiphilic block copolymers into core-shell architectures, where the hydrophobic core enables drug encapsulation and the hydrophilic corona stabilizes the carrier in biological environments. Their small size and prolonged circulation facilitate accumulation in tumors via the enhanced permeability and retention (EPR) effect, which is often considered the primary basis for passive targeting [1][2]. However, increasing evidence suggests that tumor targeting is not an intrinsic property of polymeric micelles but an emergent outcome governed by interactions with tumor biology. This challenges the conventional assumption that nanocarrier design alone determines targeting efficiency and instead raises a deeper mechanistic question: Is targeting a property of the carrier, or a consequence of its interaction with a highly variable tumor microenvironment?

MATERIALS AND METHODS:

This study was conducted using a PRISMA-based systematic review framework. Literature was collected from PubMed, Scopus, Web of Science, and ScienceDirect using keywords including “polymeric micelles tumor targeting,” “EPR variability nanocarriers,” and “tumor microenvironment drug delivery.” The review was restricted to peer-reviewed studies published between 2020 and 2025, with inclusion criteria focused on mechanistic analyses of micelle-based delivery and tumor interaction, while purely descriptive studies were excluded. A critical synthesis approach was applied to identify mechanistic dependencies, transport limitations, and translational gaps.

RESULTS AND DISCUSSION:

Polymeric micelles function as nanoscale carriers that improve pharmacokinetics and enable passive tumor accumulation; however, their performance is fundamentally constrained by the variability of the EPR effect itself. Although tumor vasculature is often described as leaky, facilitating nanoparticle extravasation, studies show that vascular permeability, interstitial pressure, and perfusion vary significantly across tumor types and even within different regions of the same tumor, leading to highly heterogeneous accumulation patterns [1][2]. As a result, EPR-mediated targeting is neither uniform nor predictable, and passive accumulation alone cannot ensure effective delivery to tumor cells. To overcome these limitations, active targeting strategies have been introduced through ligand-functionalized micelles designed to bind specific receptors on cancer cells. While this improves recognition and cellular interaction, it does not resolve the fundamental transport limitations within tumors. Receptor expression is heterogeneous, and many target sites remain inaccessible due to physical barriers within the tumor microenvironment. Consequently, ligand-based targeting enhances binding specificity but does not guarantee deeper tissue penetration or uniform drug distribution, indicating that targeting efficiency is constrained more by biological accessibility than by molecular recognition alone [2]. Beyond targeting mechanisms, the stability of polymeric micelles in systemic circulation represents another critical limitation. These systems are inherently dynamic and may undergo premature disassembly or drug leakage due to dilution below the critical micelle concentration or interactions with plasma proteins. Such instability reduces the fraction of drug that remains encapsulated during circulation, thereby limiting the amount that ultimately reaches the tumor site. This highlights a key disconnect between in vitro stability and in vivo performance, where biological conditions significantly alter carrier behavior [2]. Even when micelles successfully accumulate in tumors, their ability to penetrate and distribute within tumor tissue is severely restricted by the tumor microenvironment. Dense extracellular matrix networks, elevated interstitial fluid pressure, heterogeneous perfusion, and hypoxic conditions collectively create a



complex barrier that limits nanoparticle transport beyond the perivascular region. These factors prevent uniform drug distribution and result in localized delivery rather than effective whole-tumor exposure [1]. Consequently, drug delivery efficiency is governed not only by nanocarrier design but by the interplay between carrier properties and tumor-specific physiological constraints. Taken together, effective delivery via polymeric micelles requires successful progression through multiple interdependent steps, including systemic stability, tumor accumulation, tissue penetration, controlled drug release, and cellular uptake. Failure at any one of these stages compromises overall therapeutic efficacy. This multi-step dependency reveals that targeting is not a singular event but a sequential transport process influenced by both material design and biological environment.

Parameter	Functional Role	Limitation
EPR effect	Passive accumulation	Highly heterogeneous
Ligand targeting	Cellular recognition	Limited accessibility
Micelle stability	Drug retention	Premature release
Tumor microenvironment	Transport regulation	Physical barriers
Drug release kinetics	Therapeutic action	Difficult to control

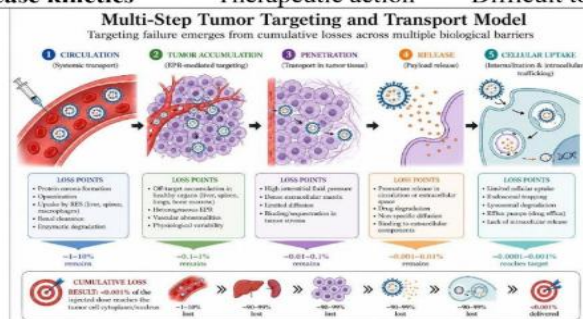


Figure 1: Multi-Step Tumor Targeting and Transport Model [3]

CONCLUSION

This review demonstrates that polymeric micelles should not be regarded as inherently targeted drug delivery systems but as transport modulators whose performance is determined by tumor microenvironmental interactions. While micelle design improves solubility and circulation behavior, targeting efficiency is constrained by variability in tumor vasculature, biological barriers to transport, and instability in systemic conditions. Polymeric micelles do not inherently target tumors; rather, targeting emerges from the balance between nanocarrier properties and tumor microenvironmental constraints, making effective delivery a system-level problem rather than a material-level solution.

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3. Multi Step Tumour Targeting Model. Generated using artificial intelligence tools developed by OpenAI, based on author-defined prompts. [Figure 1]



Protein–Protein Interaction Network Dysregulation in Autoimmune Diseases: A Systems-Level Analysis of Immune Signaling And Therapeutic Constraints

Kripa Agarwal, and Debabrata Ghosh Dastidar*
Guru Nanak Institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Autoimmune diseases result from disrupted immune signaling networks that disturb activation–tolerance balance. This review examines whether pathology arises from isolated molecular defects or broader protein interaction failures, highlighting evidence that disease progression is driven by dysregulated interconnected systems causing persistent activation and chronic inflammation.[3]. Autoimmune diseases arise when disrupted immune signaling networks upset the balance between activation and tolerance. This review evaluates whether pathology stems from isolated molecular defects or broader protein interaction failures, emphasizing evidence that disease progression reflects dysregulated interconnected systems driving activation, regulation, and chronic inflammation.

MATERIALS AND METHODS

This PRISMA-based systematic review synthesized literature from PubMed, Scopus, Web of Science, and ScienceDirect. Studies on protein–protein interaction networks, immune regulation, and autoimmune mechanisms were included, excluding single-target and non-immune studies. Critical synthesis identified mechanistic patterns, network disruptions, and translational gaps to support understanding of autoimmune pathogenesis and future network-based therapeutic strategies.

RESULTS AND DISCUSSION

1. **PPI Networks as the Structural Basis of Immune:** Signaling Protein–protein interaction networks connect proteins into complex signaling systems. In immunity, they integrate antigen signaling, cytokine communication, and transcriptional control, enabling coordinated immune responses. This interconnected structure ensures cellular processes work collectively, maintaining dynamic regulation and effective immune function.[1]
2. **Network Dysregulation in Autoimmune Diseases:** Autoimmune diseases result from dysregulated protein–protein interaction networks that shift immune signaling toward persistent activation. Abnormal receptor interactions, excessive cytokine signaling, and defective inhibitory pathways cause loss of self-tolerance and chronic inflammation. Evidence shows these diseases arise from interconnected immune networks rather than isolated gene defects, supporting systems-level understanding.[6].
3. **Hub Proteins and Network Centrality:** Within protein–protein interaction networks, highly connected hub proteins coordinate multiple signaling pathways, including cytokines such as TNF and interleukin pathways, and transcription regulators like STAT proteins. Disturbance of one hub can spread across the network, amplifying dysfunction. Proteome-wide studies show autoimmune diseases involve clusters of interacting proteins rather than isolated molecular targets.[1].
4. **Feedback Loops and Network Amplification:** Protein–protein interaction networks regulate immune signaling through feedback control. In autoimmune diseases, disrupted positive and inhibitory feedback loops amplify inflammation and prevent immune resolution, causing chronic self-sustaining activation. These complex dynamics cannot be explained by single-pathway models, highlighting the need for a systems-level network perspective to understand immune dysfunction.
5. **Multi-Factor Interaction: Genetics, Environment, Epigenetics:** Within protein–protein interaction networks, hub proteins coordinate multiple signaling pathways, including cytokines like TNF and interleukins and transcription regulators such as STAT proteins. Disruption of a single hub can spread dysfunction throughout the network, amplifying immune imbalance. Proteome-wide analyses confirm that autoimmune diseases arise from interconnected clusters of interacting proteins rather than isolated molecular targets alone.[1].
6. **Therapeutic Limitation: Failure of Reductionist Approaches :** Current autoimmune therapies mainly target individual molecules, but often fail due to redundancy in protein–protein interaction networks, where alternate pathways compensate for blocked components. This reduces effectiveness and often requires broad immunosuppression, causing side effects. These limitations show that single-target approaches are insufficient to address the complexity of interconnected immune signaling



networks.

7. **Emerging Direction: Network-Based Therapeutics** Recent therapeutic advances focus on network-level interventions for autoimmune diseases, including targeted protein degradation, multi-target modulation, and interaction-specific inhibitors. These approaches influence multiple network components or specific protein interactions rather than single molecules. By restoring overall signaling balance, they offer a more precise and potentially effective strategy than traditional single-target therapies [7].

Table 1. Network-Level Features of Autoimmune Disease Pathogenesis

Network Component	Functional Role	Dysregulation Outcome
Cytokine interactions	Signal amplification	Chronic inflammation
Receptor–ligand binding	Immune activation	Persistent signaling
Regulatory proteins	Immune suppression	Loss of tolerance
Hub proteins	Network coordination	System-wide propagation
Feedback loops	Signal control	Self-sustained activation

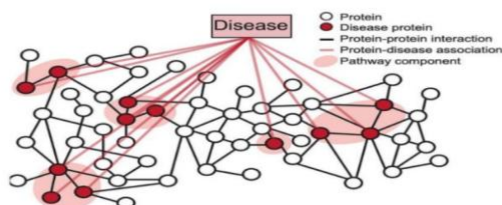


Figure 1: PPI Network Dysregulation Model [8]

CONCLUSION:

This review shows that autoimmune diseases are systems-level disorders caused by dysregulated protein–protein interaction networks rather than isolated molecular defects. Immune dysfunction arises from disrupted network balance, altered feedback regulation, and hub proteins amplifying pathological signals. These findings expose the limitations of single-target therapies and support redefining autoimmune diseases as network-driven disorders. Effective treatment should focus on modulating interconnected interaction systems to restore immune balance and address the complexity of disease mechanisms.

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Biosurfactant–Antibiotic Synergy as a Dual-Target Strategy Against Biofilms: A Critical Analysis Of Structure–Penetration Mechanisms

Arpan Sen, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Biofilm-associated infections represent a major therapeutic challenge due to their intrinsic resistance to conventional antibiotic treatment. Within biofilms, microorganisms are embedded in an extracellular polymeric substance (EPS) matrix that acts as a physical barrier, limiting drug penetration and altering bacterial physiology, thereby reducing antibiotic efficacy. In addition to structural protection, biofilm-associated bacteria exhibit altered metabolic states and enhanced gene exchange, further contributing to antimicrobial resistance. Conventional antibiotic therapies primarily target planktonic bacteria and often fail to effectively eradicate biofilm-associated infections. This limitation reflects a fundamental mismatch between drug action and the dual nature of biofilm resistance—physical (EPS barrier) and biological (cellular adaptation). Recent literature highlights biosurfactants as promising adjunct agents due to their amphiphilic nature and ability to interact with both microbial membranes and biofilm matrices. This leads to a central mechanistic question: Can biosurfactants enhance antibiotic efficacy by overcoming structural barriers, or do they act as independent antimicrobial agents?

This review critically evaluates recent literature (2020–2025) to position biosurfactant–antibiotic combinations as dual-target systems addressing both biofilm structure and microbial viability.

MATERIALS AND METHODS

This study was carried out using a PRISMA-based systematic review method. Relevant articles were collected from databases such as PubMed, Scopus, Web of Science, and ScienceDirect using keywords like “biosurfactant antibiotic synergy biofilm,” “EPS disruption antimicrobial penetration,” and “biosurfactant antibiofilm mechanism.” Only peer-reviewed studies published between 2020 and 2025 were included. The selection focused on studies related to biosurfactant-mediated antibiofilm activity, antibiotic combination or synergy, and mechanisms of biofilm disruption, while non-biofilm studies and single-agent studies without mechanistic details were excluded. Finally, a critical analysis was performed to understand key mechanisms, interaction patterns, and existing research gaps.

RESULTS AND DISCUSSION

Biofilm Resistance as a Dual-Barrier System Biofilm Resistance as a Dual-Barrier System involving both physical and biological factors. The physical barrier is formed by the extracellular polymeric substance (EPS) matrix, which limits the penetration of antibiotics into the biofilm. At the same time, bacteria within the biofilm undergo biological adaptations such as reduced metabolic activity, formation of persisted cells, and exchange of resistance genes. Together, these mechanisms greatly decrease the effectiveness of antibiotics. Therefore, biofilm resistance is not only due to bacteria themselves, but also the combined effect of biofilm structure and bacterial behavior. **Biosurfactants: Structure-Disruptive Agents** Biosurfactants are molecules that have both water-loving (hydrophilic) and fat-loving (hydrophobic) parts, which allows them to interact easily with different components of biofilms. Studies show that biosurfactants can both break down existing biofilms and stop new ones from forming. In addition, they interfere with quorum sensing (bacterial communication), which reduces the production of virulence factors and weakens the bacteria. **Mechanistic Basis of Biosurfactant–Antibiotic Synergy** Recent studies show that biosurfactants can improve the effectiveness of antibiotics by working through multiple supportive mechanisms. They break down the EPS matrix, which helps antibiotics penetrate deeper into the biofilm. They also increase the permeability of bacterial cell membranes, allowing more drug to enter the cells. In addition, biosurfactants disrupt quorum sensing, reducing resistance and bacterial



communication. Because of these combined effects, antibiotics can reach and act on bacteria that were previously protected inside the biofilm. Studies also show that using biosurfactants with antibiotics can significantly lower the required antibiotic dose, indicating a true synergistic effect rather than just an additive one. Translational Gap: From Laboratory to Clinical Application There are several key challenges in this area. Biosurfactants often have issues with stability and large-scale production, and there are no standard methods for formulating them with antibiotics. Also, most studies are limited to laboratory experiments, with very few in vivo or clinical validations. In real infections, biofilms are much more complex than in controlled lab conditions. Therefore, even though current research shows good effectiveness, it still lacks strong potential for practical clinical use.

Component	Functional Role	Outcome
EPS matrix	Physical barrier	Limits antibiotic penetration
Biosurfactant	Matrix disruption	Enhances drug diffusion
Membrane interaction	Increased permeability	Improved drug uptake
Antibiotic	Antimicrobial action	Bacterial killing
Quorum sensing inhibition	Reduced virulence	Biofilm destabilization

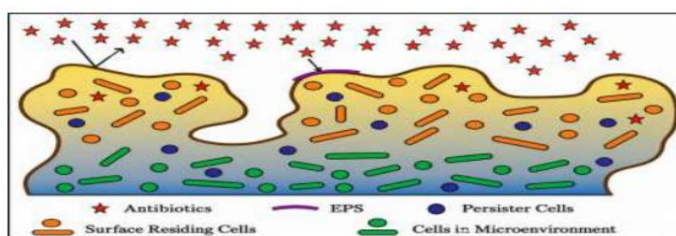


Fig 1 :Dual-Target Biofilm Disruption Model

CONCLUSION

This review shows that biosurfactant–antibiotic combinations work as dual-target systems, attacking both the structure of the biofilm and the bacteria inside it. Biofilm resistance comes from both the protective EPS structure and bacterial adaptations. Biosurfactants help by breaking down the EPS and allowing antibiotics to penetrate more easily, so antibiotics can work better. The overall effect depends on how these two components interact, not just their individual actions. Therefore, biosurfactants can be seen as supporting agents that improve antibiotic access, highlighting the importance of combined strategies that target both biofilm structure and bacterial survival.

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Molecular Docking Analysis Of Tesetaxel Across β -Tubulin Mutants And Biii Isotype: A Multi-Target Approach

Titas Das, And Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Microtubules are essential cytoskeletal components composed of α/β -tubulin heterodimers and are involved in key cellular processes such as mitosis, intracellular transport, and structural maintenance. Their dynamic behaviour is regulated by conformational changes in β -tubulin, particularly in the M-loop region, which governs lateral protofilament interactions [1]. Tesetaxel is a next-generation taxane derivative designed to improve pharmacokinetic and structural adaptability while maintaining microtubule stabilization capability. Like other taxanes, it binds to the taxoid pocket of β -tubulin and promotes microtubule polymerization by stabilizing the M-loop in an extended conformation [1][2]. Resistance to taxane-based agents arises due to β -tubulin isotype variation, particularly the β III-tubulin (TUBB3) isotype, and point mutations within the binding region. These mutations, including A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I, affect ligand binding through steric hindrance, electrostatic disruption, and conformational instability [2]. The present study investigates the binding behaviour of tesetaxel across wild-type β -tubulin, TUBB3 isotype, and multiple resistance-associated mutants using a multi-target docking approach.

MATERIALS AND METHODS

Tesetaxel was subjected to molecular docking against eleven β -tubulin targets, including wild-type, β III-tubulin (TUBB3), and nine mutant variants (A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I), using the GIRL server multi-target docking platform. Ligand conformations were generated using ETKDGV3 and optimized using the UFF force field. Docking was performed using the SMINA engine with an exhaustiveness parameter of 8 and an energy window of 3 kcal/mol, generating multiple binding modes. An ensemble docking approach was applied, and the best binding affinity for each target was selected. Docking scores (kcal/mol) were used to evaluate ligand–protein interaction strength.

RESULTS AND DISCUSSION

Table 1. Docking Score Distribution Across β -Tubulin Variants

Target	Docking Score (kcal/mol)
Wild-type β -tubulin	–9.04
TUBB3 (β III)	–6.87
Mutants (range)	–6.03 to –8.00

The results indicate strong binding to wild-type β -tubulin, followed by a noticeable reduction in binding affinity across mutant variants and the TUBB3 isotype. The docking analysis demonstrated that tesetaxel exhibits reduced binding affinity toward



structurally altered β -tubulin variants compared to the wild-type protein[2]. A decrease in docking score was observed from -9.04 kcal/mol in wild-type β -tubulin to -6.87 kcal/mol in the β III-tubulin (TUBB3) isotype, reflecting the inherent structural differences associated with the β III isotype, including increased conformational flexibility and altered hydrophobic characteristics of the taxoid binding pocket. The enhanced flexibility of the binding site likely increases the energetic requirement for ligand stabilization, resulting in reduced binding affinity[3]. However, the interaction remained within an acceptable binding range, indicating partial retention of binding capability despite isotype-associated structural variation. Mutation-specific analysis further revealed that tesetaxel is sensitive to alterations affecting the binding pocket, M-loop region, structural core, and protein interface residues. Binding pocket mutations such as A250V and F272V introduced steric hindrance and loss of aromatic interactions, leading to displacement of the ligand from its optimal orientation and decreased hydrophobic stabilization[4]. Similarly, M-loop mutations T276I and R284N altered local flexibility, hydrogen bonding potential, and electrostatic interactions, producing moderate reductions in binding affinity and indicating sensitivity toward M-loop structural perturbations[3][4]. Core structural mutations including A233T and D199N also demonstrated reduced docking scores, suggesting that polarity introduction and electrostatic alterations destabilize the taxoid binding pocket and affect ligand interaction. In addition, allosteric and interface mutations such as A187T, S174A, and R308C produced variable effects on docking affinity, with A187T maintaining relatively stronger binding while S174A and R308C resulted in significant and moderate reductions in ligand stabilization, respectively[5]ss. Overall, the observed variation in docking scores suggests that tesetaxel binding is influenced by both direct and indirect structural perturbations within β -tubulin. The wider docking score distribution compared to more mutation-tolerant taxanes indicates that tesetaxel exhibits partial dependence on specific residue interactions and remains moderately sensitive to conformational changes within the taxoid binding pocket.

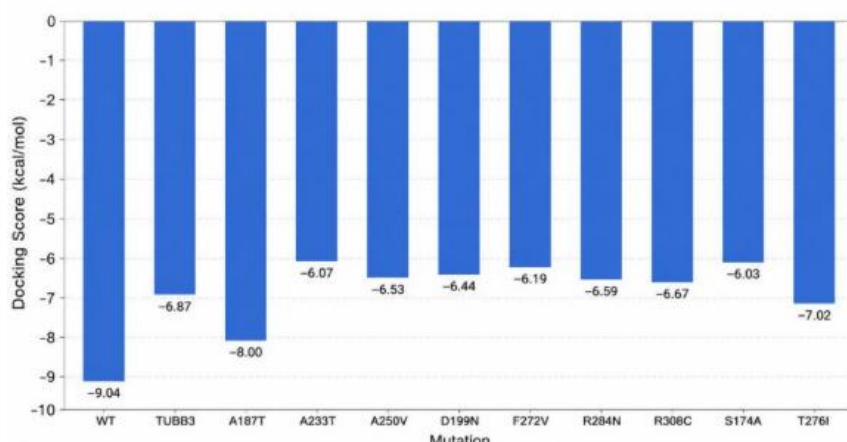
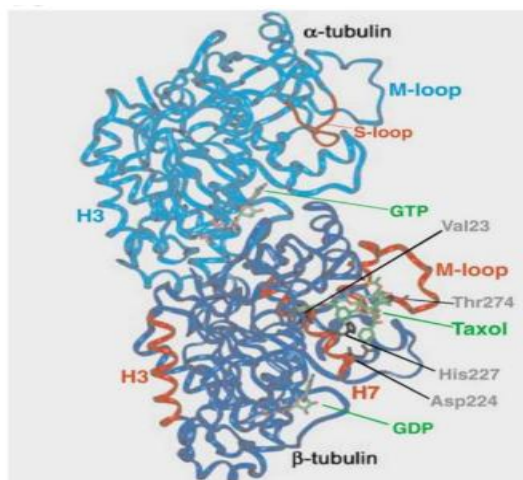


Figure 1. Structural representation of β -tubulin highlighting taxoid binding pocket and mutation sites.

Figure 2. Docking score distribution of tesetaxel across wild-type,

[Adapted From: doi: 10.1038/sj.onc.1206934]

CONCLUSION



The present study demonstrates that tesetaxel exhibits strong binding affinity toward wild-type β -tubulin but shows a noticeable reduction in binding across β III-tubulin and mutation-bearing variants. Mutations affecting the binding pocket and M-loop region significantly influence ligand binding, while allosteric mutations contribute indirectly to reduced interaction stability. The observed variation in docking scores suggests that tesetaxel exhibits moderate adaptability to structural perturbations but remains sensitive to mutations that disrupt key interactions within the taxoid binding pocket. These findings provide insight into the structural determinants governing ligand–tubulin interactions and may inform the design of improved taxane derivatives with enhanced mutation tolerance.

ACKNOWLEDGMENT

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Transformation Of Drug Release Mechanisms from Chitosan Microparticles to Tablets: A Multi-Scale Analysis Of Structural Reorganization And Diffusion Control

Aritra De and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Chitosan-based microparticles have been widely studied for controlled drug delivery due to their tunable porosity, swelling behavior, and diffusion-controlled release properties. However, for practical pharmaceutical applications, these microparticles are often further processed into tablet dosage forms, introducing an additional level of structural complexity. While the release behavior of microparticles is relatively well characterized, the transformation of these systems into tablets results in significant alteration of drug release mechanisms, which remains insufficiently understood. Compression of microparticles into tablets, induces mechanical deformation, structural rearrangement, and inter-particle bonding, leading to the formation of a consolidated matrix. Studies demonstrate that chitosan microparticles undergo plastic deformation under compression, forming dense structures with altered porosity and diffusion characteristics [1]. This structural transformation fundamentally changes how drug molecules diffuse through the system. Importantly, drug release from microparticles is primarily governed by diffusion through individual particles, whereas in tablet systems, release becomes dependent on interconnected diffusion pathways across a compressed matrix. Experimental evidence shows that compression can either accelerate release (due to particle rupture) or retard it (due to matrix densification), depending on formulation and process conditions [2]. This leads to a critical research question: Does tableting preserve microparticle release behavior, or does it create a fundamentally new diffusion-controlled system? This review critically evaluates recent literature (2020–2025) to establish that tableting represents a multi-scale structural transformation, redefining drug release mechanisms from particle-level to matrix-level diffusion.

MATERIALS AND METHODS:

This study was conducted as a systematic review using a PRISMA-based analytical framework to ensure structured literature selection and reproducibility. Literature searches were performed across PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar. Search terms included: “chitosan microparticles tablet drug release”, “compression effect microparticles release kinetics”, “matrix tablets chitosan diffusion mechanisms”. The search was restricted to peer-reviewed articles published between 2020 and 2025 in English. Inclusion criteria comprised studies addressing compression of microparticles, tablet formation, and drug release behavior. Exclusion criteria included unrelated dosage forms, incomplete datasets, and duplicate studies. Articles were screened via title, abstract, and full-text analysis. Extracted data included compression parameters, structural changes, and release kinetics.

RESULTS AND DISCUSSION:

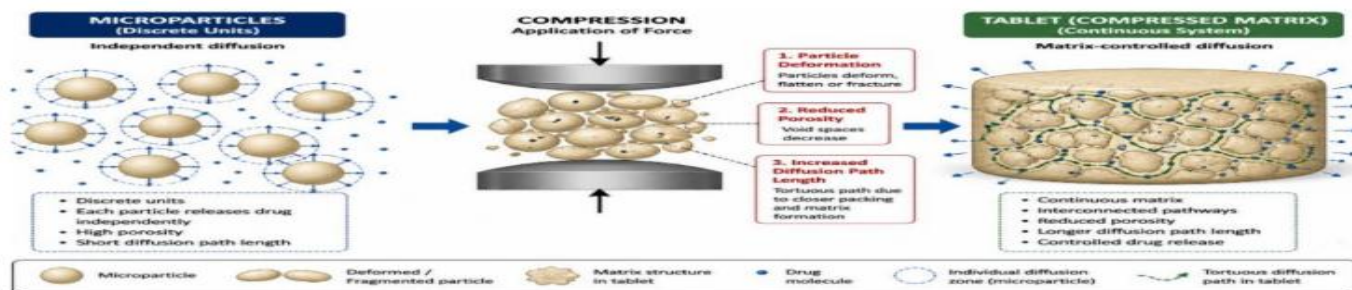


- 1. Structural Transformation During Compression:** of microparticles into tablets results in significant structural changes, including: Particle deformation (plastic or elastic), reduction in inter-particulate void spaces, formation of a continuous matrix. Studies show that chitosan microparticles exhibit plastic deformation under compression pressure, enabling the formation of coherent tablets [1]. This process reduces porosity and alters internal architecture, which directly impacts drug transport.
- 2. Transition from Particle-Level to Matrix-Level Diffusion:** In microparticles, drug release is governed by diffusion through individual particles. However, in tablets, release occurs through a continuous matrix formed by compressed particles, where diffusion pathways span multiple particles. This transformation results in: increased diffusion path length, reduced permeability, formation of tortuous pathways as a result, drug release becomes slower and more controlled, transitioning from particle-level diffusion to matrix-controlled transport.
- 3. Compaction-Induced Damage and Its Consequences:** A critical issue in tableting is the potential damage to microparticle structure during compression. Studies show that compression can: rupture polymer coatings, collapse internal pores, disrupt encapsulation. This can lead to increased burst release, particularly when protective structures are not maintained [2]. However, the inclusion of cushioning excipients (e.g., microcrystalline cellulose) has been shown to protect particle integrity, reducing structural damage and preserving controlled release behavior [2].
- 4. Role of Excipients and Matrix Formation:** Tablet formulation introduces additional variables, including binders, fillers, and lubricants, which influence structural organization. Excipients can: enhance compressibility, modify matrix density, influence diffusion pathways for example, increasing filler content can reduce drug release rate by providing a cushioning effect and preserving microparticle structure during compression [2]. Thus, drug release in tablets is governed not only by microparticle properties but also by secondary matrix formation mechanisms.
- 5. Multi-Scale Diffusion Control:** A key insight is that drug release in tablet systems operates across multiple scales: Micro-scale: diffusion within individual particles, Meso-scale: diffusion between particles, Macro-scale: diffusion across the tablet matrix, this multi-scale behavior results in complex release kinetics that cannot be explained by single-mechanism models.
- 6. Critical Gap:** Lack of Multi-Scale Predictive Models. Despite extensive studies, there is no predictive framework linking: microparticle properties, compression parameters, tablet structure → Drug release behavior. Current models fail to integrate multi-scale diffusion processes, limiting rational design of tablet-based delivery systems.



Table 1. Comparison of Drug Release Mechanisms: Microparticles vs Tablets

Feature	Microparticles	Tablets (Compressed System)
Structural level	Individual particles	Continuous matrix
Porosity	High, particle-specific	Reduced, matrix-controlled
Diffusion pathway	Short, localized	Long, tortuous
Release mechanism	Particle diffusion	Matrix diffusion
Effect of compression	Not applicable	Alters structure and release
Release rate	Faster	Slower, sustained



CONCLUSION

This review demonstrates that compression of chitosan microparticles into tablets results in a fundamental transformation of drug release mechanisms, shifting from particle-level to matrix-level diffusion control. The analysis reveals that: Compression induces structural reorganization and reduces porosity, drug release transitions from localized to multi-scale diffusion, particle integrity and excipient selection critically influence release behavior, tableting introduces new variables beyond formulation. A major limitation in current research is the absence of predictive multi-scale models linking microparticle properties to tablet performance. Tableting should be viewed as a structural transformation process that redefines drug release mechanisms, requiring integrated multi-scale design approaches rather than simple extrapolation from microparticle systems.

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Determinants Of Initial Burst Release in Chitosan Microparticles: Crosslinking-Driven Network Architecture and Diffusion-Controlled Release Mechanisms

Sourav Neogi, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Chitosan–tripolyphosphate (TPP) microparticles have been extensively explored as drug delivery systems due to their biocompatibility, mild fabrication conditions, and tenable release behaviour; however, a persistent and unresolved limitation across the literature is the occurrence of initial burst release, which leads to uncontrolled drug discharge and reduced therapeutic efficiency. Despite decades of research, reported release profiles remain highly inconsistent, indicating a lack of mechanistic clarity in understanding early-stage release kinetics. Traditionally, burst release has been attributed to surface-associated drug molecules loosely bound to the particle exterior, but while this explanation is widely accepted, it fails to account for observations where burst release persists even in systems with high encapsulation efficiency and minimal surface drug. Experimental evidence suggests that release behaviours is strongly influenced by formulation parameters such as crosslinking conditions, polymer concentration, and particle morphology, indicating that deeper structural factors are involved [1]. Recent studies increasingly point toward the role of internal network architecture, governed by ionic crosslinking between chitosan and TPP, as a primary determinant of release behaviour, with crosslinking density directly influencing matrix compactness, porosity, and water penetration, which collectively control diffusion pathways within the polymer system [2]. This leads to a critical research question: is initial burst release a surface phenomenon, or a manifestation of diffusion through a structurally heterogeneous polymer network? This review critically evaluates recent literature (2020–2025) to reframe burst release as a network-controlled diffusion phenomenon rather than a formulation artifact.

MATERIALS AND METHODS

This study was conducted as a systematic review using a PRISMA-based approach for structured and reproducible literature selection. Articles were collected from PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using relevant keywords and Boolean operators. Only English-language studies published between 2020 and 2025 were included. Studies focusing on chitosan–TPP microparticles with reported drug release behaviour were selected, while irrelevant and duplicate studies were excluded. Screening was done through title, abstract, and full-text review. Data on formulation, crosslinking, release kinetics, and structure were extracted, and a critical analysis was performed to identify trends and research gaps.

RESULTS AND DISCUSSION: 1. Variability in Burst Release Behaviour Burst release shows high variability across studies. Some formulations release drugs rapidly within minutes, while others show slower, controlled release. This indicates that no single factor governs the process. Experimental issues such as particle aggregation and non-standardized testing conditions can also affect results, contributing to this variability [1]. **2. Limitations of the Surface Drug Hypothesis:** The common explanation of burst release as surface drug diffusion is incomplete. Burst release often occurs even with high encapsulation efficiency and varies with crosslinking conditions and internal structure. This suggests that internal drug distribution and matrix properties play a major role. **3. Role of Crosslinking Density:** Crosslinking between chitosan and TPP determines the internal network structure. Higher crosslinking produces a dense matrix with smaller pores and slower drug diffusion, while lower crosslinking leads to a looser, more porous structure and faster release. Studies confirm that increased crosslinking reduces drug release rates [2][3]. **4. Diffusion-Controlled Release:** The initial burst phase is mainly governed by diffusion. Rapid water penetration into the polymer network allows drug molecules to move quickly through pores and channels, creating fast release pathways. **5. Structural Heterogeneity:** Chitosan–TPP microparticles are structurally heterogeneous. Variations in crosslinking and density



create regions with different diffusion rates, leading to non-uniform and unpredictable burst release. Thus, burst release is better explained by internal structural heterogeneity rather than only surface effects.

Table 1. Influence of Crosslinking Parameters on Drug Release Behavior

Parameter	Effect on Network Structure	Impact on Burst Release
Chitosan:TPP ratio	Determines crosslinking density	Lower ratio → higher burst
TPP concentration	Increases ionic crosslinking	Higher concentration → reduced burst
Crosslinking time	Enhances network stability	Longer time → slower release
Polymer MW	Affects chain entanglement	Higher MW → reduced diffusion
pH of system	Influences ionization	Lower pH → tighter structure

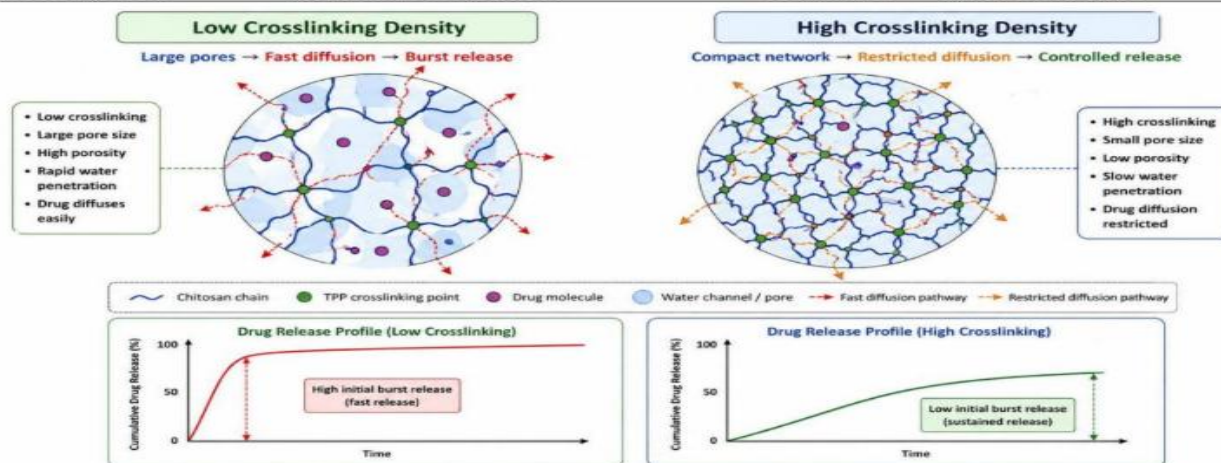


Figure 1 :Crosslinking Density vs Diffusion Pathway Model (generated by AI)

CONCLUSION

Initial burst release in chitosan–TPP microparticles is (1) a diffusion-controlled process governed by internal network architecture, with crosslinking density as the primary determinant; however, (2) surface-associated drug, structural heterogeneity, and experimental inconsistencies influence early release and limit interpretation; (3) this highlights the need for network-based design strategies; (4) a key limitation is the lack of predictive models linking formulation to release kinetics; therefore, (5) burst release should be redefined as a network-controlled diffusion phenomenon requiring precise crosslinking control for predictable performance.

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Influence Of Binder-Induced Matrix Formation on Drug Release from Microparticle-Based Tablets: A Multi-Scale Diffusion Control Perspective

Aritra Das, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Microparticle-based drug delivery systems are frequently compressed into tablets to achieve practical dosage forms with improved handling and patient compliance. While microparticles inherently exhibit diffusion-controlled release, the incorporation of binders and excipients during tableting introduces an additional level of structural complexity. This leads to the formation of a secondary matrix, fundamentally altering the drug release mechanism. Binders are traditionally considered formulation aids that improve tablet mechanical strength and cohesion. However, emerging evidence suggests that binders actively influence drug release by modifying matrix density, porosity, and diffusion pathways [1]. In particular, hydrophilic binders such as chitosan, polyvinylpyrrolidone (PVP), and cellulose derivatives contribute to the formation of gel-like structures upon hydration, which act as diffusion barriers. Studies demonstrate that binder concentration significantly affects drug release kinetics. For instance, reduction in binder content can increase drug release rates, while higher binder levels enhance matrix integrity and retard drug diffusion [2]. Furthermore, binders can interact with microparticles during compression, influencing particle integrity and inter-particulate bonding. This raises a critical mechanistic question: does drug release in microparticle-based tablets depend on microparticle properties, or is it dominated by binder-induced matrix formation? This review critically evaluates recent literature (2020–2025) to establish that binders act as active structural regulators, transforming release mechanisms from particle-controlled to matrix-controlled diffusion systems.

MATERIALS AND METHODS

This study was carried out as a systematic review using a PRISMA-based approach to ensure a clear and reproducible selection of literature. Relevant studies were searched from databases such as PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using keywords like “chitosan binder tablet drug release,” “microparticle compression binder effect release kinetics,” and “matrix tablet excipient diffusion control.” Only peer-reviewed articles published in English between 2020 and 2025 were included. Studies were selected based on their focus on binder effects, matrix tablet formation, microparticle compression, and drug release mechanisms, while unrelated dosage forms, incomplete studies, and duplicate papers were excluded. The screening process involved reviewing titles, abstracts, and full texts, and important data such as binder type, concentration, matrix structure, and drug release patterns were extracted. Finally, the collected information was analysed using a critical synthesis method to understand relationships between formulation process, structure, and drug release behaviour, and to identify gaps in existing research.

RESULTS AND DISCUSSION

1. Binder-Induced Matrix Formation: Binders play a fundamental role in tablet formation by promoting particle adhesion and cohesion during compression. However, beyond mechanical function, binders actively contribute to the formation of a continuous matrix, which governs drug release behaviour. During hydration, hydrophilic binders absorb water, swell, and form



a gel layer around the microparticles, which acts as a barrier to drug diffusion. This gel layer controls how water enters the system, how the drug dissolves, and how quickly it diffuses out. As a result, drug release is influenced not only by the properties of the microparticles but also by the behaviour of the binder-formed matrix. [1]. **2. Effect of Binder Concentration on Drug Release:** Binder concentration plays an important role in determining matrix density and drug release rate. At low binder levels, the matrix is weaker, allowing faster drug release, while at high binder levels, a denser matrix forms, slowing down the release. Studies show that decreasing binder concentration increases drug release, whereas increasing it slows release by strengthening the matrix and restricting diffusion. Therefore, binder concentration acts as a key regulator, balancing tablet strength and drug permeability. **3. Interaction Between Binder and Microparticles** A key mechanistic aspect is the interaction between binders and microparticles during compression. Binders help improve tablet structure by filling spaces between particles, protecting microparticles from breaking, and influencing how particles deform during compression. Excipients like microcrystalline cellulose can act as cushioning agents, reducing damage to microparticles and helping maintain controlled drug release. However, if too much binder is used, it can form a dense matrix around the microparticles, which limits their individual diffusion and may slow down drug release excessively. **4. Transition to Matrix-Controlled Drug Release** In microparticle-based tablets without binders, drug release mainly depends on diffusion from individual particles. When a binder is added, the release mechanism shifts to matrix-controlled diffusion, where the drug must pass through the microparticle structure, the surrounding binder matrix, and the interconnected pathways within it. This increases the distance the drug has to travel, reduces permeability, and leads to a slower, more sustained release. As a result, the system changes from a collection of separate particles to a continuous matrix system.

5. Multi-Scale Diffusion Control

Binder-based systems exhibit multi-scale diffusion: • Micro-scale → within microparticles • Meso-scale → particle–binder interface • Macro-scale → tablet matrix This multi-level control creates complex release kinetics that cannot be described by simple diffusion models. **6. Critical Gap: Lack of Integrated Binder–Structure–Release Models**

Despite extensive research, there is still no clear predictive model that directly links binder type and concentration with matrix structure and drug release behaviour. Most studies consider binders simply as formulation components rather than key factors that actively influence the structure of the system. This limits a deeper mechanistic understanding of how binders control drug release kinetics.

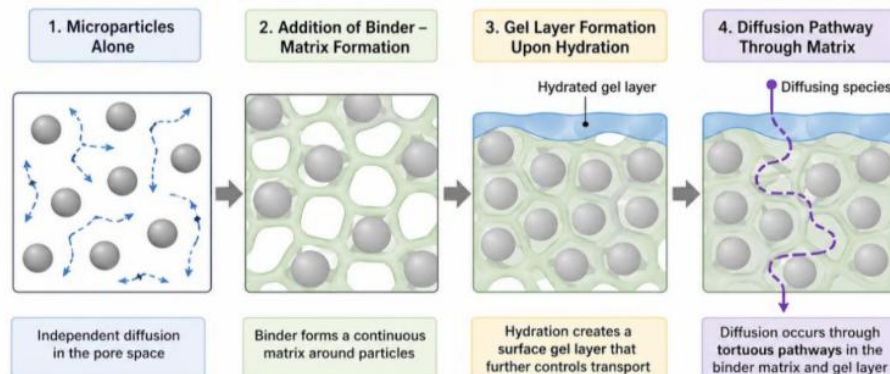


Figure 1: Binder-Induced Matrix Transformation Model [This figure is an original work and is distributed under the Creative Commons Attribution 4.0 International License (CC BY 4.0)]

CONCLUSION: This review demonstrates that binders are not passive excipients but active regulators of drug release behaviour in microparticle-based tablet systems. The analysis reveals that:

- Binder incorporation leads to formation of a secondary matrix
- Drug release transitions from particle-controlled to matrix-controlled diffusion
- Binder concentration and type significantly influence release kinetics
- Multi-scale diffusion mechanisms govern overall release behavior

A major limitation in current research is the absence of predictive models integrating binder properties with structural and functional outcomes. Binders should be redefined as structural modulators that govern multi-scale diffusion processes, requiring their integration into rational design strategies for controlled drug delivery systems.

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Preparation and optimization of Amoxicillin-Loaded HPMC core coated with Zinc Stearate nanoparticles using a QbD approach for enhanced antibacterial activity

Rini Das, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Amoxicillin is a widely used broad-spectrum antibiotic; however, its clinical effectiveness is often limited by rapid systemic clearance, short half-life, and increasing antimicrobial resistance, leading to reduced bioavailability and frequent dosing. Polymeric carriers such as Hydroxypropyl methylcellulose (HPMC) have been extensively studied for controlled drug delivery due to their biocompatibility and sustained release properties [3]. Despite this, conventional HPMC-based systems may suffer from premature drug release and lack additional antimicrobial functionality [1]. This study addresses whether a core-shell nanoparticle system can enhance stability and antibacterial efficacy of amoxicillin [2] [4]. To overcome these limitations, a hydrophobic coating using Zinc stearate was employed. Unlike stearic acid, zinc stearate not only provides a diffusion barrier for controlled release but also offers potential antimicrobial synergy due to zinc ions. Thus, incorporating zinc stearate enables a multifunctional system combining controlled delivery with enhanced antibacterial performance.

MATERIALS AND METHODS: Amoxicillin, Hydroxypropyl methylcellulose (HPMC), Zinc stearate, hexane, Tween 20 and propylene glycol were used for nanoparticle preparation. Zinc stearate nanoparticles were initially prepared using a modified emulsification-solvent evaporation method. Subsequently, HPMC was incorporated to form the core, followed by zinc stearate coating and loading of amoxicillin in the core to obtain core-shell nanoparticles. A Quality by Design (QbD)-based Design of Experiments (DoE) approach with 11 experimental runs was employed for optimization. The independent variables included HPMC concentration and zinc stearate concentration, while drug amount remained constant. Particle size and polydispersity index (PDI) were selected as critical response parameters due to their influence on nanoparticle stability and performance. Particle size and polydispersity index (PDI) were measured using dynamic light scattering (DLS). Fourier-transform infrared (FTIR) spectroscopy was performed to confirm drug incorporation, assess compatibility between drug and excipients, and verify the structural arrangement of the formulation. The FTIR analysis also confirmed the presence of Hydroxypropyl methylcellulose in the core and Zinc stearate on the surface, supporting the formation of a core-shell nanoparticle system. Antibacterial activity of the optimized formulation was evaluated using a minimum inhibitory concentration (MIC) assay against the selected bacterial strain. Statistical analysis was carried out using ANOVA to determine the significance of formulation variables on the response parameters.

RESULTS AND DISCUSSION: The nanoparticles were successfully formed through a stepwise process, confirming the development of a core-shell system. Zinc stearate nanoparticles exhibited an average particle size of 38.66 nm. Upon incorporation of Hydroxypropyl methylcellulose (HPMC), the particle size increased to 107.8 nm, indicating successful formation of the polymeric core. Further coating and drug loading resulted in final amoxicillin-loaded core-shell nanoparticles with an average size of 390.3 nm and a PDI of 0.5, suggesting moderate size distribution. The Design of Experiments (DoE) analysis revealed that formulation variables significantly influenced nanoparticle characteristics. ANOVA results showed p-



values <0.05, confirming statistical significance. The optimized formulation exhibited desirable properties, including nanoscale size and acceptable PDI, indicating its suitability for effective drug delivery.

Table 1. Particle size and PDI at different formulation stages

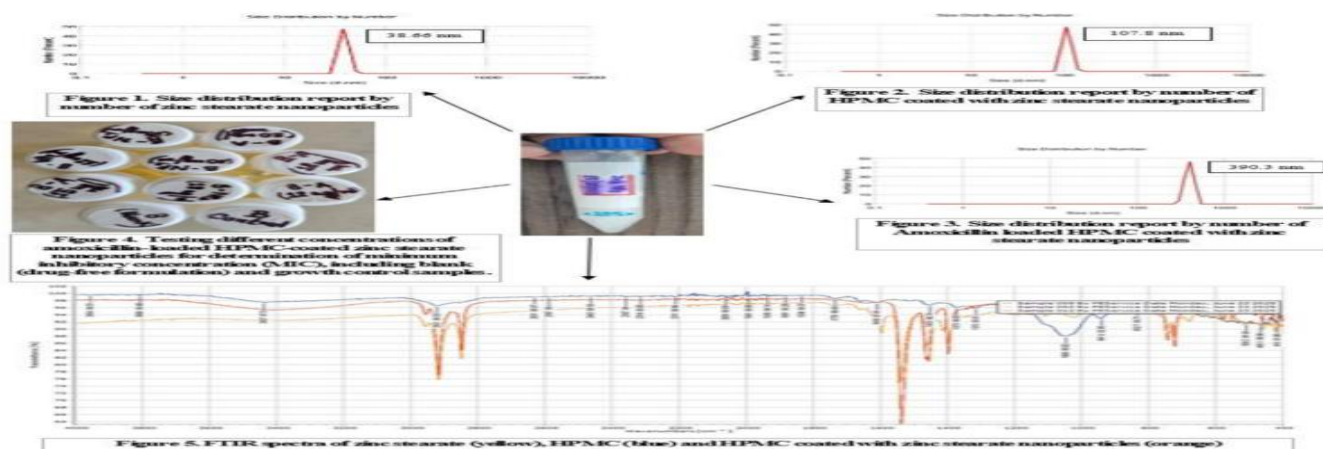
Formulation Stage	Particle Size (nm)	PDI
Zinc stearate nanoparticles	38.66	0.3
HPMC coated with zinc stearate nanoparticles	107.8	0.6
Amoxicillin loaded HPMC coated with zinc stearate nanoparticles	390.3	0.5

Comparative FTIR analysis of the pure components and the final nanoparticle formulation confirmed successful core-shell formation and drug encapsulation. Hydroxypropyl methylcellulose exhibited a characteristic broad O-H stretching peak in the range of 3400–3450 cm⁻¹, which appeared at 3437 cm⁻¹ in the final formulation with reduced intensity and slight broadening, indicating that HPMC is present but embedded within the core rather than exposed on the surface. The C-H stretching peak of HPMC (2900–2950 cm⁻¹) was retained at 2918 cm⁻¹, confirming the presence of the polymer backbone. Amoxicillin showed a characteristic β -lactam carbonyl peak at 1740–1770 cm⁻¹ in its pure form; however, this peak was not observed in the final formulation, suggesting that the drug is encapsulated within the core and not present on the surface. Additionally, the amide carbonyl peak (~1650–1680 cm⁻¹) appeared reduced or overlapped, further supporting physical entrapment within the polymer matrix. Zinc stearate exhibited a distinct carboxylate (COO⁻) peak at 1530–1550 cm⁻¹, which was retained at ~1540 cm⁻¹ in the formulation, confirming its presence on the nanoparticle surface. The alkyl C-H stretching of zinc stearate overlapped with HPMC peaks, indicating formation of a lipid layer. The absence of new peaks confirmed that no chemical interaction occurred, indicating successful physical encapsulation of the drug.

Table 2. Comparative FTIR analysis of pure components and final nanoparticles

Component	Pure peak (cm ⁻¹)	Functional group	Observation in final formulation	Interpretation
Hydroxypropyl methylcellulose	3400–3450	O–H stretching	Broad peak at 3437 cm ⁻¹ (reduced intensity)	HPMC present but embedded in core (not surface exposed)
HPMC	2900–2950	C–H stretching	Peak at 2918 cm ⁻¹ retained	Confirms polymer backbone in system
Amoxicillin	1740–1770	β -lactam C=O	Not observed (masked)	Drug encapsulated within core, not surface present
Amoxicillin	1650–1680	Amide C=O	Overlapped / reduced	Interaction with polymer matrix (physical entrapment)
Zinc stearate	1530–1550	COO ⁻ asymmetric stretching	Peak at ~1540 cm ⁻¹ retained	Confirms zinc stearate coating on surface
Zinc stearate	2850–2920	C–H stretching (alkyl chain)	Overlaps with HPMC peak	Confirms lipid layer presence

The antibacterial activity study demonstrated that the amoxicillin-loaded nanoparticles exhibited significant inhibitory effects with a minimum inhibitory concentration (MIC) of 18 μ g/mL, indicating enhanced antibacterial efficacy. This improvement may be attributed to sustained drug release and the potential synergistic effect of zinc.



CONCLUSION

The study successfully developed a core-shell nanoparticulate system comprising amoxicillin-loaded Hydroxypropyl methylcellulose coated with Zinc stearate using a QbD approach. The formulation exhibited nanoscale size with moderate polydispersity, confirming successful formation of a polymer-lipid hybrid system. FTIR analysis verified the presence of HPMC in the core and zinc stearate on the surface without chemical interaction, indicating physical encapsulation of the drug. The optimized nanoparticles showed effective antibacterial activity (MIC 18 µg/mL), likely due to controlled drug release and the synergistic effect of zinc. DoE and ANOVA ($p < 0.05$) confirmed the significant influence of formulation variables, ensuring robustness and reproducibility. Overall, this system represents a promising platform for improved amoxicillin delivery with enhanced stability and antibacterial efficacy.

ACKNOWLEDGMENT

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Preparation And Optimization of Ketoconazole Loaded Calcium Stearate Nanoparticles for Enhanced Antifungal Activity

Atanu Kundu, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Fungal infections remain a major therapeutic challenge, particularly in topical and ocular delivery where achieving adequate drug concentration at the site of infection is difficult. Ketoconazole (KTZ), a broad-spectrum imidazole antifungal, inhibits ergosterol biosynthesis but suffers from poor aqueous solubility and limited bioavailability, restricting its therapeutic effectiveness [1]. Several studies have demonstrated that nanocarrier-based systems can improve the solubility, retention, and antifungal efficacy of poorly soluble drugs such as ketoconazole [2]. However, many conventional lipid carriers face issues such as polymorphic instability, burst release, and drug expulsion during storage [2,3]. Calcium stearate was selected as a novel lipidic carrier owing to its biocompatibility, hydrophobicity, structural rigidity, and potential to provide better drug entrapment and sustained release compared with stearic acid-based systems [4]. Unlike stearic acid, calcium stearate forms a metal soap matrix that may improve nanoparticle stability and encapsulation efficiency. Therefore, this study aimed to develop and optimize ketoconazole-loaded calcium stearate nanoparticles using a Design of Experiments approach to overcome solubility limitations and enhance antifungal performance.

MATERIALS AND METHODS

Ketoconazole, calcium stearate, hexane, tween 20 and propylene glycol were used for nanoparticle preparation. Calcium stearate nanoparticles were prepared using a modified emulsification-solvent evaporation method. Blank nanoparticles and drug-loaded nanoparticles were formulated by varying key formulation parameters. Ketoconazole-loaded calcium stearate nanoparticles were optimized using a Quality by Design (QbD)-based Design of Experiments (DoE) approach comprising 11 experimental runs. Two independent formulation variables were selected: calcium stearate amount (Factor A) and dispersion volume (Factor B), while the drug amount (5 mg ketoconazole) was kept constant throughout all experiments. Calcium stearate was studied at a low level of 50 mg and a high level of 100 mg, whereas dispersion volume was varied between 10 mL (low level) and 30 mL (high level). For optimization, particle size and polydispersity index (PDI) were chosen as critical response parameters due to their significant influence on nanoparticle stability, uniformity, and overall performance of the final formulation. Statistical analysis of the experimental design was carried out using ANOVA to evaluate the significance of formulation variables and identify the optimized formulation. The prepared formulations were further characterized using Dynamic Light Scattering (DLS) to determine particle size distribution and PDI, while Fourier Transform Infrared (FTIR) spectroscopy was employed to assess drug-excipient compatibility and confirm successful drug encapsulation within the calcium stearate matrix.

RESULTS AND DISCUSSION: The prepared calcium stearate nanoparticles exhibited nanoscale size distribution. Blank nanoparticles showed an average size of approximately 38.53 nm, whereas ketoconazole-loaded nanoparticles exhibited a size of around 190 nm with a PDI of ~0.2, indicating uniform dispersion.



Table 1. Particle size and PDI at different formulation stages

Formulation Stage	Particle Size (nm)	PDI
Calcium stearate nanoparticles	38.53	0.4
Final core-shell nanoparticles (drug-loaded)	191.2	0.71

Table 2. FTIR spectral interpretation of formulation

Functional Group / Peak	Pure Ketoconazole (cm ⁻¹)	Pure Calcium Stearate (cm ⁻¹)	KTZ-Loaded CaSt NPs (cm ⁻¹)	Interpretation
C=O stretching	~1645	—	Reduced intensity	Drug present but embedded in core
Aromatic C=C / C=N	~1510–1515	—	Weak/partially masked	Suggests drug encapsulation
COO ⁻ asymmetric stretch	—	~1575	Retained (~1575)	Confirms CaSt matrix maintained
CH ₂ bending	—	~1465	Retained	Lipid structure preserved
CH ₂ stretching	—	~2918, 2850	Dominant peaks retained	Surface dominated by CaSt coating
New interaction peaks	—	—	Absent	No chemical interaction, physical encapsulation

FTIR analysis confirmed the presence of characteristic functional groups of calcium stearate and ketoconazole. The carboxylate (COO⁻) stretching vibration was observed at ~1575 cm⁻¹. The absence of new peaks in drug-loaded nanoparticles indicated no chemical interaction, confirming physical encapsulation of the drug. The antifungal activity study demonstrated that the KTZ-loaded nanoparticles exhibited significant inhibitory effects, with a minimum inhibitory concentration (MIC) of approximately 20 µg/mL. This result indicates enhanced antifungal activity compared to conventional formulations. The DoE analysis revealed that formulation variables significantly influenced nanoparticle characteristics. ANOVA results showed p-values <0.05, confirming statistical significance. The optimized formulation exhibited desirable properties, including sub-200 nm particle size and narrow PDI, making it suitable for effective drug delivery.

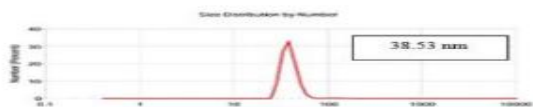


Figure 1. Size distribution report by number of calcium stearate nanoparticles

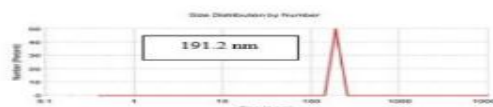


Figure 2. Size distribution report by number of Ketoconazole loaded calcium stearate nanoparticles

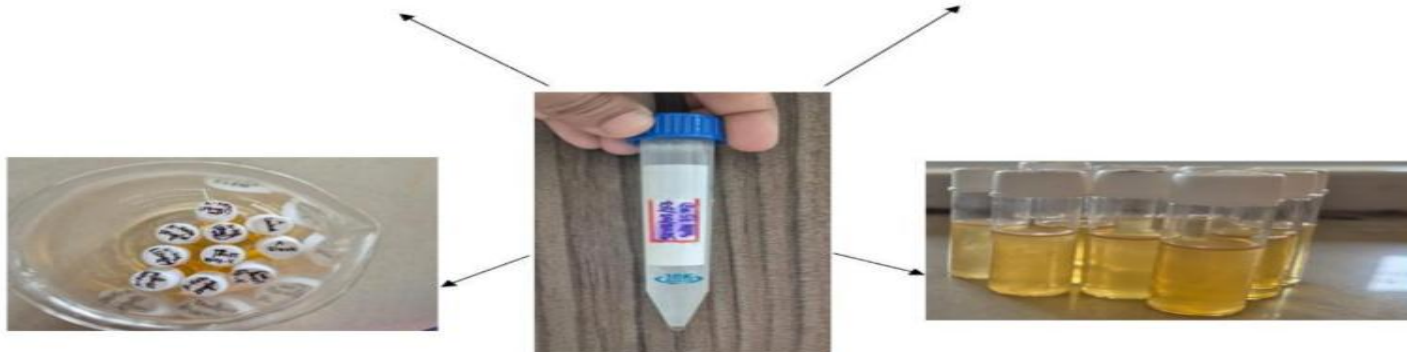


Figure 3. Testing different concentrations of ketoconazole loaded calcium stearate nanoparticles for determination of minimum inhibitory concentration (MIC), including blank (drug-free formulation) and growth control samples



CONCLUSION

The present study successfully developed and optimized ketoconazole-loaded calcium stearate nanoparticles using a systematic Design of Experiments approach. The nanoparticles demonstrated nanoscale size, uniform distribution, and effective drug encapsulation without chemical interaction. Enhanced antifungal activity was observed in vitro, indicating improved therapeutic potential. These findings suggest that calcium stearate nanoparticles are a promising carrier system for improving the delivery of poorly soluble antifungal drugs like ketoconazole, particularly for topical and ocular applications. Further studies may focus on in vivo evaluation and long-term stability.

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Synthesis And Structural Characterization of Hydrophobically Modified Carboxymethyl Chitosan for Haemostatic Applications

Soumyadeep Saha, and Dr. Debabrata Ghosh Dastidar*
Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Uncontrolled bleeding is a critical concern in trauma management, surgical procedures, and emergency care, often leading to severe complications and mortality if not rapidly controlled. The development of efficient haemostatic materials that can promote rapid clot formation and ensure biocompatibility has therefore gained significant attention in biomedical research. Among natural polymers, chitosan, a cationic polysaccharide derived from chitin, is widely recognized for its inherent haemostatic properties, biodegradability, and non-toxicity[1]. Its positive charge enables electrostatic interaction with negatively charged red blood cells (RBCs) and platelets, promoting aggregation and accelerating clot formation[1]. Despite these advantages, chitosan exhibits poor solubility at physiological pH (~7.4), limiting its effectiveness in blood-contact applications [4]. It remains soluble only in acidic conditions due to protonation of amino groups, which restricts its practical utility. To overcome this limitation, chemical modification such as carboxymethylation has been employed to produce carboxymethyl chitosan (CMC), a water-soluble derivative with improved functionality at neutral pH[2]. Recent studies suggest that introducing hydrophobic groups into chitosan derivatives enhances haemostatic activity by facilitating stronger interaction with cell membranes through hydrophobic insertion, thereby promoting cellular aggregation. However, excessive hydrophobicity can compromise aqueous solubility, creating a need for a balanced modification strategy[4]. This study addresses the question of whether hydrophobically modified carboxymethyl chitosan (HM-CMC) can be synthesized to achieve both enhanced solubility and improved haemostatic performance under physiological conditions. The proposed approach involves combining hydrophilic carboxymethyl groups with controlled hydrophobic modification to optimize polymer functionality[1]. Current research indicates promising outcomes with individual modifications, yet limited work has explored their combined effect. Therefore, this study focuses on the synthesis and structural characterization of HM-CMC as a potential advanced haemostatic biomaterial[3]

METHODS: In the present study, chitosan was modified via a two-step chemical approach. Initially, N-alkylation was carried out by using glacial acetic acid, DMSO (as solvent), dodecanal (C-12), NaBH₃CN (as reducing agent), to incorporate hydrophobic moieties. This was followed by carboxymethylation using iso-propanol, NaOH and monochloroacetic acid, to enhance aqueous solubility by introducing hydrophilic functional groups. Then, the prepared sample was dried maintaining the



temperature under 40°C. Structural confirmation of functional group modification was carried out using Fourier-Transform Infrared (FTIR) spectroscopy. Preliminary interaction studies with blood components were assessed using microscope.

RESULTS AND DISCUSSION The prepared chitosan derivative was found to be white in colour. The FTIR analysis shows characteristic spectral changes corresponding to successful incorporation of carboxymethyl and alkyl groups, confirming dual modification. This creates an amphiphilic polymer system—hydrophilic segments promote solubility, while hydrophobic domains enhance interfacial interactions. Under the microscope, observations indicated visible aggregation behaviour of blood cells in the presence of the modified polymer, suggesting improved polymer–cell interaction. It can be understood that this interaction is driven by electrostatic attraction along with hydrophobic association at the cellular interface, which is mechanistically relevant for haemostatic material design.

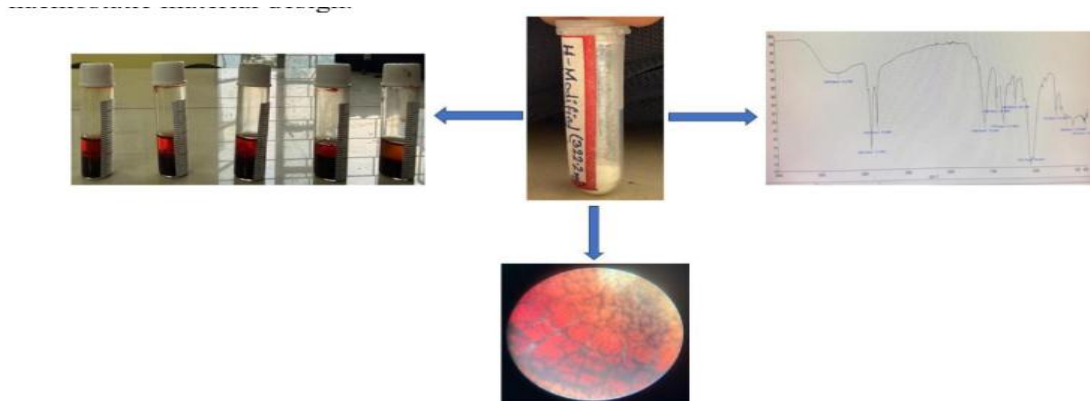


Figure 1. Showing the different characterization analysis of the synthesized N-alkylated carboxymethylated chitosan derivative

Table1. Comparative FTIR spectra of native chitosan and its chemically modified derivatives illustrating the introduction of hydrophobically modified derivative and hydrophobically modified carboxymethyl chitosan derivative

Wave number (cm ⁻¹)	Native Chitosan	Hydrophobically Modified Chitosan	Hydrophobically Modified Carboxymethyl Chitosan	Interpretation
3350–3400	Broad O–H and N–H stretching	Slight shift, reduced intensity	Further broadening/shift	Hydrogen bonding altered due to substitution; reduced free –NH ₂ groups
2920 & 2850	Weak/less intense C–H stretching	Strong peaks appear	Strong peaks retained	Introduction of alkyl chains (–CH ₂ –) confirms N-alkylation
1250–1260	Weak/absent	Slight increase	More prominent	Indicates introduction of substituted functional groups
1600–1550	Weak in native	Moderate	Strong COO ⁻ asymmetric stretch	Confirms carboxymethylation
1400–1450	Weak	Moderate	COO ⁻ symmetric stretch appears	Clear evidence of carboxylate groups



(~1510–1515 cm⁻¹) were weak or partially masked, further supporting drug encapsulation. In contrast, the characteristic carboxylate (COO⁻) asymmetric stretching peak of calcium stearate at ~1575 cm⁻¹ was retained without significant shift, confirming the integrity of the lipid matrix. The CH₂ bending (~1465 cm⁻¹) and CH₂ stretching (~2918 and 2850 cm⁻¹) peaks remained prominent, indicating that the nanoparticle surface is dominated by calcium stearate. Importantly, no new peaks were observed in the spectrum, confirming the absence of chemical interaction between ketoconazole and excipients. These spectral changes collectively indicate successful formation of a stable nanoparticle system with ketoconazole physically entrapped within the calcium stearate matrix.

CONCLUSION

The study successfully synthesized hydrophobically modified carboxymethyl chitosan through a two-step chemical modification involving N-alkylation followed by carboxymethylation. FTIR analysis confirmed the introduction of both hydrophobic alkyl chains and hydrophilic carboxymethyl groups, indicating successful structural modification. The resulting polymer exhibited amphiphilic characteristics, combining improved aqueous solubility with enhanced interfacial interaction capability. Microscopic observations demonstrated aggregation of blood cells, suggesting improved polymer–cell interaction driven by electrostatic and hydrophobic forces, which is critical for haemostatic activity. Overall, the developed material shows promising potential as an advanced haemostatic agent.

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Formulation and Optimization of Ketoconazole-Loaded Stearic Acid Solid Lipid Nanoparticles for Enhanced Antifungal Activity

Muntazima Khatun, and Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Fungal infections remain a significant global health concern, particularly due to the increasing prevalence of resistant strains and the limitations associated with conventional antifungal therapies. Ketoconazole, a broad-spectrum imidazole antifungal agent, is widely used for the treatment of various superficial and systemic fungal infections. However, its clinical effectiveness is often limited by poor aqueous solubility, low bioavailability, and potential systemic side effects, which necessitate the development of advanced drug delivery systems.[1]. Solid lipid nanoparticles (SLNs) have emerged as promising carriers for lipophilic drugs like ketoconazole due to their biocompatibility, controlled drug release, and ability to enhance drug stability. Stearic acid, a physiologically acceptable lipid, is commonly employed as a matrix material in SLN formulation owing to its favourable safety profile and ability to encapsulate hydrophobic drugs efficiently. Incorporation of ketoconazole into stearic acid-based SLNs can potentially improve its solubility, enhance therapeutic efficacy, and reduce adverse effects [1,3]. Despite these advantages, the formulation of SLNs requires careful optimization of critical parameters such as lipid concentration, surfactant concentration, and processing conditions to achieve desirable particle size and uniformity. In this context, the application of Design of Experiments (DoE) provides a systematic and efficient approach to optimize formulation variables and understand their influence on key characteristics such as particle size and polydispersity index (PDI).[2]

MATERIALS AND METHODS:

Stearic acid-based solid lipid nanoparticles (SLNs) were prepared using a lipid-based nanoparticle preparation method under controlled experimental conditions. Stearic acid was used as the lipid matrix, while ethanol served as the organic solvent for dissolving both the lipid and the drug. Tween 20 was employed as a surfactant to stabilize the formulation and facilitate the formation of nanoparticles. Initially, blank SLNs were prepared to establish baseline formulation characteristics. Subsequently, drug-loaded SLNs were developed by incorporating ketoconazole into the lipid phase. The preparation process involved dissolving stearic acid and drug in ethanol, followed by controlled mixing with an aqueous phase containing Tween 20 under continuous stirring. The system was further subjected to homogenization to achieve uniform particle size distribution and enhance formulation stability. Different formulations were designed by varying key parameters such as lipid concentration, surfactant concentration, and processing conditions to evaluate their influence on nanoparticle characteristics. The prepared SLNs were characterized using Dynamic Light Scattering (DLS) to determine particle size and polydispersity index (PDI), which are critical indicators of formulation uniformity and stability. The antifungal activity of the ketoconazole-loaded SLNs was evaluated using minimum inhibitory concentration (MIC) studies to assess their biological efficacy. A Design of Experiments (DoE) approach was employed to systematically optimize the formulation variables and study their effect on dependent responses such as particle size and PDI. Statistical analysis was performed using analysis of variance (ANOVA) to determine the significance of formulation variables.



RESULTS AND DISCUSSION: Dynamic Light Scattering (DLS) analysis revealed that the stearic acid nanoparticles exhibited particle sizes of approximately 200 nm for blank formulations, while intermediate formulations showed particle sizes of around 255 nm. Upon drug loading, the particle size increased to 296 nm, indicating successful incorporation of the drug into the lipid matrix. The increase in particle size can be attributed to the presence of drug molecules within the lipid core and possible surface interactions. The polydispersity index values were found to be within an acceptable range, indicating uniform particle size distribution and good stability of the formulations. The antimicrobial evaluation using MIC studies demonstrated that the drug-loaded nanoparticles exhibited effective inhibitory activity, suggesting improved drug performance compared to conventional formulations. The Design of Experiments (DoE) approach enabled a systematic understanding of the formulation variables and their interactions. ANOVA results showed p-values less than 0.05, indicating that the formulation variables had a statistically significant effect on particle size and PDI. These findings emphasize the importance of optimization in achieving nanoparticles with desired physicochemical characteristics and enhanced performance.

Table 1. Particle size and PDI at different formulation stages

Formulation Stage	Particle Size (nm)	PDI
Stearic acid nanoparticles	200	1
Final core-shell nanoparticles (drug-loaded)	255	1

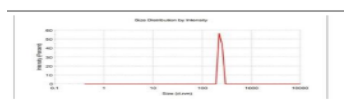


FIG1:Size distribution report of drug loaded SLN is 200 nm

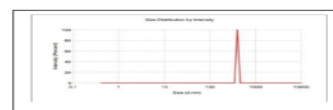


FIG 2:Size distribution report of drug loaded SLN is 390 nm

CONCLUSION

The present study successfully developed and optimized stearic acid-based solid lipid nanoparticles with desirable physicochemical properties and enhanced antimicrobial activity. The observed increase in particle size upon drug loading confirmed successful drug incorporation, while acceptable PDI values indicated good formulation stability. Statistical analysis confirmed the significant influence of formulation variables on nanoparticle characteristics. Overall, the optimized SLNs demonstrate strong potential as effective drug delivery systems for improved therapeutic outcomes.

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Nanoformulations For Phytochemicals: A Critical Analysis of Multi-Mechanistic Bioavailability Enhancement and Translational Limitations

Dhrubajyoti Dhara, and Dr. Debabrata Ghosh Dastidar*
Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Phytochemicals exhibit significant pharmacological potential, including antioxidant, anti-inflammatory, and anticancer activities. However, their clinical translation remains limited due to intrinsic physicochemical and biological constraints such as poor water solubility, low permeability, rapid metabolism, and instability in physiological environments [1][4]. These limitations result in extremely low oral bioavailability, often rendering otherwise potent bioactive compounds therapeutically ineffective. Nanotechnology-based drug delivery systems have emerged as a promising strategy to overcome these barriers. Nano formulations such as liposomes, nano emulsions, polymeric nanoparticles, and solid lipid nanoparticles are widely reported to enhance solubility, improve stability, and enable targeted delivery of phytochemicals [2][6]. However, despite extensive research and promising preclinical outcomes, translation into consistent clinical success remains limited.

MATERIALS AND METHODS

This study was conducted as a systematic review following a PRISMA-based analytical framework. Relevant literature was collected from PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using search terms related to nano formulations, phytochemical bioavailability, and nanocarrier absorption pathways. The review included peer-reviewed articles published between 2020 and 2025, focusing on studies involving nano formulations of phytochemicals, mechanistic insights into bioavailability enhancement, and in vitro–in vivo correlations, while excluding non-nano delivery systems and purely descriptive studies. A critical synthesis approach was applied to identify key mechanisms, inconsistencies, and translational gaps.

RESULTS AND DISCUSSION

1. **Multi-Mechanistic Basis of Bioavailability Enhancement** Nano formulations improve the bioavailability of phytochemicals through multiple interacting mechanisms rather than a single pathway. Reduction in particle size increases surface area and enhances dissolution, while encapsulation improves dispersion and protects compounds from degradation. Stabilization further prevents oxidation and enzymatic breakdown. As a result, phytochemicals like curcumin, resveratrol, and quercetin show significantly enhanced absorption and therapeutic efficacy when delivered via nanocarriers.
2. **Role of Biological Interactions in Absorption** Beyond physicochemical improvements, nano formulations also modulate biological processes that govern drug absorption by enhancing membrane permeability, protecting drugs from first-pass metabolism, increasing gastrointestinal residence time, and promoting lymphatic uptake. These combined effects demonstrate that improved bioavailability arises from complex interactions between the drug, carrier, and biological system, rather than from solubility enhancement alone.
3. **Discrepancy Between In Vitro and In Vivo Performance** Many nano formulation studies report significant improvements in solubility, dissolution rate, and stability; however, these enhancements do not always translate into better in vivo bioavailability



or therapeutic outcomes. This discrepancy is mainly due to the complex gastrointestinal environment, enzymatic degradation, and interactions with biological membranes and proteins. Consequently, the lack of reliable in vitro–in vivo correlation (IVIVC) remains a major limitation in nano formulation research. **4. Translational Barriers: Scale-Up and Reproducibility** Despite promising results, several challenges limit the clinical translation of nano formulations, including difficulties in large-scale manufacturing, batch-to-batch variability, stability during storage and administration, and regulatory as well as safety concerns. Scaling up from laboratory to industrial production often affects particle consistency and quality, while stability issues such as aggregation or degradation further complicate their use. Additionally, strict regulatory requirements demand thorough evaluation of safety and reproducibility, which slows approval processes. As highlighted in recent studies, a significant gap still exists between successful laboratory outcomes and reliable clinical application, making translation a major challenge in nano formulation research. **5. Critical Gap: Lack of Integrated Mechanistic Framework** A major limitation in current research is the lack of predictive models that can effectively link formulation parameters and biological interactions to overall bioavailability outcomes. Most studies tend to focus on individual mechanisms in isolation rather than integrating them into a unified framework. This fragmented approach restricts a comprehensive understanding and limits the rational design and optimization of nano formulations for improved therapeutic performance.

Table 1. Mechanisms and Limitations of Nanoformulations in Phytochemical Delivery

Mechanism	Functional Role	Limitation
Particle size reduction	Enhances dissolution	Does not ensure absorption
Encapsulation	Improves stability	May limit drug release
Permeability enhancement	Facilitates absorption	Variable across tissues
Lymphatic uptake	Bypasses metabolism	Not universally applicable
Controlled release	Sustains drug levels	Complex kinetics

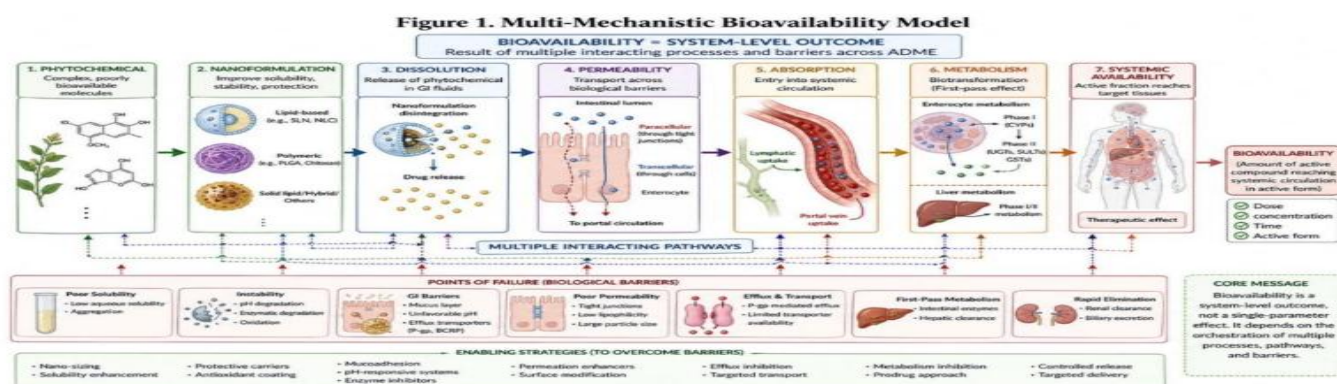


Figure 1. Multi-Mechanistic Bioavailability Model: From Phytochemical to Systemic Disposition

CONCLUSION



This review demonstrates that nano formulations enhance phytochemical bioavailability through a multi-mechanistic process involving both physicochemical and biological interactions, rather than simple solubility improvement. The analysis shows that improved bioavailability results from the combined effects of dissolution, permeability, and interactions with biological systems, while solubility enhancement alone is not sufficient to ensure therapeutic efficacy. It also highlights that in vitro success often does not translate into in vivo outcomes and that significant translational challenges persist due to issues of scalability and reproducibility. Therefore, nano formulations should be viewed as multifunctional delivery systems that modulate drug–biological interactions, requiring integrated design strategies that consider physicochemical properties, biological barriers, and manufacturing constraints for effective clinical application.

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Phytosomal Delivery Of Myricetin Enhances Its Solubility And Bioavailability

Ritam Roy¹, Anuj Kumar Borah², and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

2The Assam Royal Global University, NH-37, opp. Tirupati Balaji Temple, Setouchi, Guwahati, Assam
781035

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Myricetin is a naturally occurring flavonoid widely present in fruits, vegetables, and medicinal plants, known for its potent antioxidant, anti-inflammatory, and anti-diabetic activities. Due to its ability to modulate oxidative stress and glucose metabolism, it has attracted significant interest as a therapeutic agent for metabolic disorders. However, despite its promising pharmacological potential, the clinical application of myricetin remains limited due to its poor aqueous solubility, low permeability, and inadequate oral bioavailability. These limitations result in reduced dissolution, poor absorption, and consequently, suboptimal therapeutic efficacy [1]. Thus, the major problem addressed in this study is how to improve the solubility and bioavailability of myricetin to enhance its pharmaceutical performance. The key research question is whether a lipid-based drug delivery system can effectively overcome these limitations and improve the physicochemical and biopharmaceutical properties of myricetin.[2].

MATERIALS AND METHODS

Myricetin-loaded phytosomes were prepared using the thin film hydration method, where accurately weighed myricetin and soya lecithin were dissolved in ethanol, followed by magnetic stirring and controlled solvent evaporation to form a thin lipid film, which was further processed into a free-flowing complex; a pH 6.8 phosphate buffer was prepared for evaluation studies. A series of formulations (F1–F5) with varying drug–phospholipid ratios were developed and characterized for particle size and polydispersity index using DLS, drug–lipid interaction via FTIR, and solubility enhancement using RP-HPLC under optimized conditions, enabling identification of the formulation with improved physicochemical properties and drug availability.

RESULTS AND DISCUSSION

Dynamic Light Scattering (DLS) analysis was performed to evaluate the particle size distribution and homogeneity of the prepared myricetin–phospholipid phytosome formulations in both pH 6.8 phosphate buffer and distilled water. A clear difference in particle size behaviour was observed depending on the dispersion medium. In phosphate buffer, the formulations exhibited comparatively smaller Z-average particle sizes and better distribution profiles than in distilled water. Among the batches, formulation F3 (35:35) showed the smallest particle size (~190.2 nm), followed by F5 (27:43) with ~265.8 nm and F2 (20:50)



with ~439.0 nm, indicating relatively better dispersion and reduced aggregation. In contrast, formulations such as F1 (50:20) and F4 (43:27) showed significantly larger particle sizes (>1800 nm), suggesting poor dispersion and possible particle aggregation at higher drug concentrations. The polydispersity index (PDI) values in buffer ranged from 0.411 to 1.000, indicating moderate to high heterogeneity, with lower PDI values suggesting relatively more uniform particle distribution. In comparison, when the same formulations were dispersed in distilled water, a significant increase in particle size was observed across all batches, with Z-average values ranging from ~1420 nm to ~5827 nm, clearly indicating aggregation and instability in the aqueous medium. The PDI values were also higher (0.580–1.000), reflecting poor homogeneity and broad size distribution. This difference can be attributed to the absence of ionic strength and buffering capacity in distilled water, leading to reduced stabilization of phytosomal vesicles. Furthermore, size distribution data revealed multiple peaks and broader intensity patterns in water, whereas buffer systems showed comparatively narrower distributions. Among all formulations, F5 (27:43) demonstrated relatively improved performance in buffer with acceptable particle size and dispersion behaviour, suggesting an optimal balance between drug and phospholipid content. Overall, the DLS study indicates that pH 6.8 phosphate buffer provides a more suitable environment for Phyto some stability, and the optimized formulation exhibits improved physicochemical characteristics necessary for enhanced bioavailability. Fourier Transform Infrared Spectroscopy (FTIR) was employed to investigate the drug–phospholipid interaction and confirm the formation of the myricetin–phospholipid (Phyto some) complex.

Table 1. FTIR peak interpretation of myricetin and phytosomal formulations.

Wavenumber (cm ⁻¹)	Functional Group	Pure Myricetin	Phytosome (F1–F5)	Interpretation
3200–3400	–OH stretching (phenolic)	Broad peak present	Broadened and slightly shifted	Indicates hydrogen bonding between drug and phospholipid
2920–2850	C–H stretching (aliphatic)	Weak/less prominent	Strong peak observed	Confirms presence of phospholipid (soya lecithin)
~1730	C=O stretching (ester)	Less prominent	Strong peak appears	Confirms incorporation of phospholipid
1650–1700	C=O stretching (flavonoid)	Sharp peak present	Slight shift observed	Indicates interaction without chemical degradation
1500–1600	Aromatic C=C stretching	Present	Retained in all batches	Confirms structural integrity of myricetin
1000–1300	C–O and P=O stretching	Present (C–O)	Intensified peaks	Confirms formation of phytosomal complex
700–900	Aromatic bending vibrations	Present	Slight changes in intensity	Supports interaction and complex formation

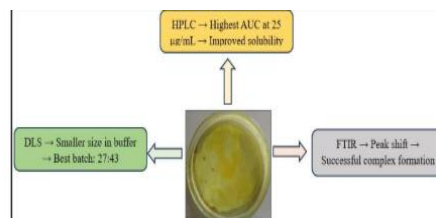


Figure 1. Graphical representation of the optimized myricetin phytosomal formulation highlighting key characterization outcomes, including particle size reduction (DLS), successful drug–phospholipid interaction (FTIR), and enhanced solubility (HPLC).

Reverse Phase High-Performance Liquid Chromatography (RP-HPLC) was employed to evaluate the solubility enhancement of myricetin in the phytosomal formulation. The solubility was assessed in terms of peak area (AUC), which is directly proportional to the concentration of dissolved drug. The results indicated that at 12 µg/mL, the AUC was 182,499, which increased significantly to 948,569 at 25 µg/mL, suggesting enhanced solubility and improved drug availability in the phytosomal system. However, at 50 µg/mL, a notable decrease in AUC (154,524) was observed. This reduction at higher concentration may be attributed to possible saturation of the system, aggregation of phytosomal particles, or reduced dispersion



efficiency, leading to lower effective solubility. The observed trend indicates that the phytosomal formulation exhibits an optimal solubility enhancement at intermediate concentration (25 µg/mL), beyond which the system may lose stability or exhibit limited solubilization capacity. Overall, the significant increase in AUC at optimized concentration confirms that phospholipid complexation effectively improves the solubility and dissolution behaviour of myricetin, thereby enhancing its potential bioavailability.

CONCLUSION

The present study successfully developed and optimized a myricetin-loaded phytosomal formulation using the thin film hydration method to overcome its poor solubility and bioavailability. Among the prepared formulations, the 27:43 (myricetin: phospholipid) ratio demonstrated optimal performance. DLS analysis confirmed improved particle size and stability in buffer, FTIR studies indicated successful drug–phospholipid interaction without chemical incompatibility, and HPLC results showed significant enhancement in solubility and drug availability. Overall, the findings suggest that the phytosomal approach is an effective strategy to improve the physicochemical properties and potential bioavailability of myricetin, with promising implications for anti-diabetic applications.

5. ACKNOWLEDGMENT

We acknowledge Guru Nanak Institute of Pharmaceutical Science and Technology for providing the necessary facilities, infrastructure, and academic environment to successfully carry out this study.

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Preparation And Characterization of Hydrophobic Carbon Quantum Dot Loaded Nanoparticle Of Heptadecanoic Acid

Vaskar Khan, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Nanotechnology has significantly transformed modern drug delivery systems by improving therapeutic efficiency, reducing side effects, and enabling targeted delivery. Among various nanomaterials, carbon dots have gained considerable attention due to their unique optical properties, high photostability, low toxicity, and excellent biocompatibility. These nanoscale carbon-based materials exhibit strong fluorescence, making them highly suitable for bioimaging and diagnostic applications. Carbon dots can be synthesized using simple, cost-effective methods such as pyrolysis of organic precursors. Oleyl alcohol serves as an efficient carbon source due to its hydrocarbon structure and ability to undergo thermal decomposition. However, standalone carbon dots may have limitations in stability and controlled delivery when applied in biological systems. To overcome these limitations, incorporation of carbon dots into lipid-based nanoparticles has emerged as a promising approach. Lipid nanoparticles provide a protective matrix, enhance bioavailability, and allow controlled release of encapsulated materials. Additionally, the combination of CDs with lipid carriers integrates both imaging and therapeutic functionalities, making it a potential theragnostic system. The present study focuses on the synthesis of carbon dots using a controlled pyrolysis method and their subsequent incorporation into lipid-based nanoparticles to develop a stable and efficient drug delivery platform.

MATERIALS AND METHODS

Preparation of Carbon Dots: Carbon dots were synthesized using oleyl alcohol as the precursor through a pyrolysis method. Initially, all glassware was thoroughly cleaned and dried to avoid contamination. A measured volume (5.00 mL) of oleyl alcohol was transferred into a sealed reagent bottle. The reaction environment was stabilized using a nitrogen flush to minimize oxidation and enhance fluorescence stability. The sealed bottle was immersed in a pre-heated oil bath maintained at 200°C ($\pm 2^\circ\text{C}$). The reaction was carried out for 45 minutes under controlled conditions. During the process, a gradual colour transition from clear to yellow, orange, and finally brown was observed, indicating the formation of carbon dots. After completion, the reaction mixture was allowed to cool naturally to prevent aggregation. The resulting carbon dot solution was collected and stored in amber-coloured vials to protect it from light exposure and maintain stability.

Preparation of Carbon Dot Loaded Nanoparticles: Lipid Phase Preparation: The lipid phase was prepared by dissolving 50 mg of heptadecanoic acid in ethanol, followed by the addition of 250 μL Span 20 and 1.2 mL of carbon dot solution. The mixture was heated at 70°C in a water bath until a clear homogeneous solution was obtained.



Aqueous Phase Preparation The aqueous phase consisted of 15 mL double distilled water containing 300 μ L Tween 20 and 1 mL propylene glycol. This mixture was stirred continuously using a magnetic stirrer to ensure complete dissolution and formation of a uniform phase. **Nanoparticle Formation:** The lipid phase was added dropwise into the aqueous phase under constant stirring at 400 rpm and 70°C. This process facilitated the formation of nanoparticles through solvent evaporation and self-assembly mechanisms. Stirring was continued until complete evaporation of ethanol, resulting in the formation of stable carbon dot-loaded nanoparticles.

RESULTS AND DISCUSSION

The synthesis of carbon dots was confirmed by the characteristic colour transition from clear to brown during the pyrolysis process, indicating successful carbonization of the precursor. Controlled heating and gradual cooling ensured uniform particle formation and minimized aggregation, thereby preserving fluorescence properties. The formulation of carbon dot-loaded nanoparticles resulted in a stable dispersion, indicating effective incorporation of carbon dots within the lipid matrix. The use of surfactants such as Span 20 and Tween 20 significantly contributed to nanoparticle stability by reducing interfacial tension and preventing aggregation. Dynamic Light Scattering (DLS) analysis was performed to evaluate the particle size distribution at different dilution levels. The observed particle sizes were as follows: raw sample showed a peak size of 54.18 nm, while 100 dilution exhibited 114.9 nm. Further dilution at 1000 showed an increased particle size of 224.0 nm, and at 3000 dilution, the size was reduced to 199.3 nm. Interestingly, at 5000 dilution, the particle size significantly decreased to 32.78 nm. These variations in particle size with dilution suggest possible aggregation and de-aggregation behaviour of nanoparticles. At lower dilutions, increased particle size may be attributed to clustering effects, whereas higher dilution (5000) indicates better dispersion and reduced aggregation, resulting in smaller particle size. This confirms that dilution plays a critical role in determining the stability and size distribution of the nanoparticle system. Overall, the DLS results support the successful formation of nanosized particles and demonstrate that the developed formulation has potential for efficient drug delivery applications, with size tunability depending on dispersion conditions.



DLS results in 1. Raw, 2. 3000 dilution, 3. 1000 dilution, 4. 5000 dilution



CONCLUSION

This study successfully demonstrates the synthesis of carbon dots using a pyrolysis method and their incorporation into lipid-based nanoparticles. The developed system exhibits good stability and holds significant potential for applications in drug delivery and bioimaging. The integration of fluorescent carbon dots with lipid nanoparticles provides a dual- functional platform for therapeutic and diagnostic purposes. Future work should focus on detailed characterization, drug loading efficiency, release kinetics, and biological evaluation to explore its full potential in clinical applications.

ACKNOWLEDGMENT

The authors would like to express their sincere gratitude to Guru Nanak Institute of Pharmaceutical Science and Technology for providing the necessary facilities to carry out this research work.

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Carbon Quantum Dot as Fluorescent Sensor for Selective Detection And Stability Analysis of a Glp-1 Analog (Liraglutide)

Abhi Malakar, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Liraglutide, a GLP-1 analogue used in the management of type 2 diabetes mellitus, is a peptide-based drug prone to aggregation under varying physicochemical conditions such as pH, solvent environment, and ionic strength. Aggregation can alter its therapeutic performance and stability, making its monitoring critically important.[4] Conventional analytical techniques such as UV spectroscopy, circular dichroism, and chromatographic methods are commonly used for stability studies. However, these methods have limitations including low sensitivity, complex sample preparation, time consumption, and inability to monitor aggregation behaviour in real-time. Fluorescence-based methods using external dyes may suffer from photobleaching, interference, and lack of specificity.[3] CQD-based fluorescence sensing offers a label-free, sensitive, and rapid alternative. However, a major limitation in such systems is nanoparticle aggregation, which significantly affects fluorescence behaviour and analytical reliability. Despite growing interest, limited studies have addressed the role of solvent systems and pH in controlling CQD aggregation for peptide drug analysis.[5] Carbon Quantum Dots (CQDs) are <10 nm carbon nanomaterials with strong fluorescence, high solubility, and good biocompatibility. Their surface functionality enables biomolecular interaction, making them useful for sensing, imaging, and drug delivery. [1, 2]. Therefore, the present study focuses on developing a CQD-based fluorescence sensing system for liraglutide, with particular emphasis on understanding and optimizing solvent-dependent aggregation behaviour to improve detection accuracy and stability analysis.

MATERIALS AND METHODS: Carbon quantum dots (CQDs) were synthesized using lysine and tryptophan via thermal methods and systematically optimized as a fluorescent sensing platform for the selective detection and stability analysis of the GLP-1 analog liraglutide. The synthesized CQDs were characterized using Dynamic Light Scattering (DLS) to assess particle size and dispersion behaviour in different media, where carbonate buffer (pH 9) exhibited optimal stability and was selected for further studies. Fluorescence optimization was performed by varying CQD dilution to identify the ideal working concentration. Liraglutide solutions were then prepared in carbonate buffer and water for injection-based systems to evaluate environmental effects on analyte behaviour. The interaction between CQDs and liraglutide, along with its stability under different conditions, was investigated using UV–Visible and fluorescence spectroscopy, enabling the development of a sensitive and selective nano-enabled fluorescence sensing system.

**RESULTS AND DISCUSSION**

Dynamic Light Scattering (DLS) analysis demonstrated a strong dependence of CQD particle size on the dispersion medium, where Milli-Q water resulted in large hydrodynamic diameters (~133–523 nm) due to severe aggregation, while borate buffer (pH 9) showed partial stabilization (~55–129 nm); in contrast, carbonate buffer (pH 9) produced highly dispersed CQDs with nanoscale sizes (~1.29–4.14 nm), confirming minimal aggregation, although one tryptophan oil bath sample (~68 nm) indicated possible incomplete carbonization or surface heterogeneity. Fluorescence studies revealed concentration-dependent emission, with high intensity at lower dilutions followed by quenching at higher concentrations due to inner filter effects, while higher dilutions provided stable and reproducible signals, establishing the optimal sensing range. UV–Visible spectroscopy of liraglutide showed a characteristic absorbance peak at ~350 nm, attributed to $n \rightarrow \pi^*$ transitions of functional groups and peptide chromophores, with slight medium-dependent variation, leading to its selection as the excitation wavelength. Overall, improved dispersion in carbonate buffer enhanced fluorescence by preventing aggregation-induced quenching, whereas aggregated systems showed unstable signals, confirming that alkaline ionic conditions are critical for maintaining CQD stability and ensuring efficient fluorescence-based sensing of liraglutide.

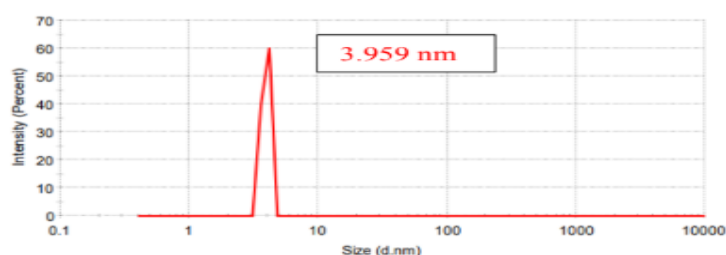


Figure 1. Dynamic light scattering (DLS) number-based size distribution of CQDs measured at 1000× dilution in carbonate buffer solution, demonstrating a narrow particle size distribution with a single dominant peak.

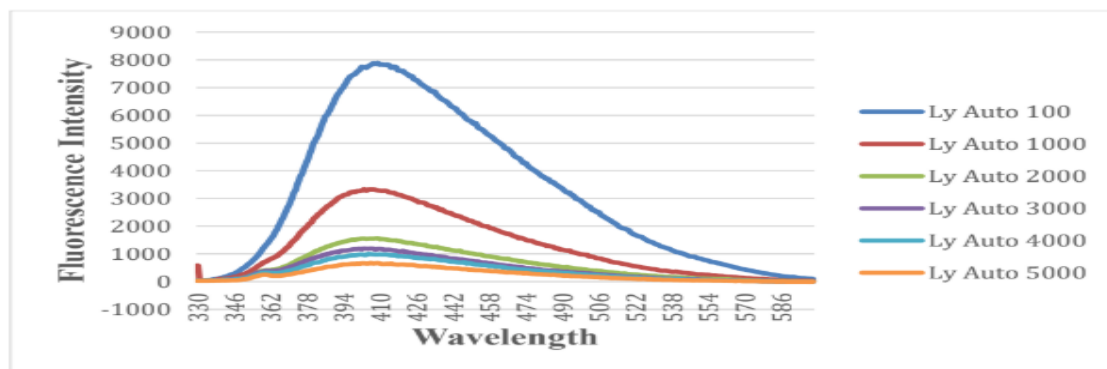


Figure 2. Fluorescence emission spectra of lysine-derived carbon quantum dots (CQDs) synthesized by the autoclave method at different dilutions, showing a prominent emission peak around 400–420 nm and concentration-dependent changes in fluorescence intensity.



CONCLUSION

This study presents a CQD-based fluorescence sensing system for the analysis of liraglutide. CQDs synthesized from lysine and tryptophan exhibited strong fluorescence properties; however, significant aggregation was observed in Milli-Q water, whereas carbonate buffer (pH 9) enabled stable dispersion with particle sizes below 10 nm. UV–Visible analysis revealed a characteristic absorbance peak at ~350 nm, which was selected as the excitation wavelength for fluorescence studies. Overall, the use of a controlled alkaline buffer environment improved nanoparticle stability and fluorescence performance, highlighting the crucial role of pH and solvent conditions in optimizing CQD-based sensing systems.

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Amorphous Carbon-Coated Carbon Nanotubes-Based Hybrid Nanocomposites

Manjeet Kumar, Saket Suman, Sneha Singh, Md.

Nafis, Md. Arman, Ayush Singh Thakur

Department of Computer Science & Engineering, Dr. Sudhir Chandra Sur Institute of
Technology and Sports Complex, 540, Dum Dum, Surer Math, Kolkata-700074

E-mail: manjeet85422@gmail.com

INTRODUCTION

Increasing global need for efficient energy storage systems is leading to intensive research on new types of nanomaterials. Specifically, nanomaterials based on carbon including carbon nanotubes (CNTs) are of great interest because of their exceptional electrical conductivity, mechanical properties, and very high surface area. Hybrid nanocomposites with CNTs and amorphous carbon provide a combination of the structural characteristics of CNTs and disorderliness of amorphous carbon, contributing to better electrochemical properties

MATERIALS AND METHODS: The hybrid nanocomposites were prepared using a chemical vapor deposition (CVD) method, wherein the synthesis of CNTs was performed via thermal decomposition using metal catalysts. The deposition of amorphous carbon on the nanotube structure was done using a pyrolysis process. Techniques used for characterization include: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), X-Ray Diffraction (XRD), Raman Spectroscopy

RESULT AND DISCUSSION

1. SEM and TEM analysis confirmed uniform coating of amorphous carbon over CNTs, forming a porous network structure.
2. Raman spectra indicated the presence of both graphitic (G-band) and disordered (D-band) carbon, confirming hybrid formation.
3. The hybrid nanocomposite exhibited enhanced electrochemical performance with high specific capacitance (~200–250 F/g), excellent charge–discharge stability, and low internal resistance.

Comparing With Conventional Materials: Activated carbon, Pure CNT, Graphene.

Materials	Specific Capacitance (F/g)	Stability	Conductivity
Activated Carbon	~150	Moderate	Low
Pure CNT	~180	Good	High
Hybrid	~250	Excellent	Very High

Table 1: The hybrid nanocomposite exhibits significantly higher capacitance and stability compared to conventional materials due to the synergistic effect of CNTs and amorphous .

Electrochemical characterization proved the following:



1. High specific capacitance 2. Good charging-discharging stability 3. Low internal resistance

The hybrid nanocomposites possessed a higher energy density compared to the CNTs alone, owing to a larger active surface area and easier ion diffusion channels.

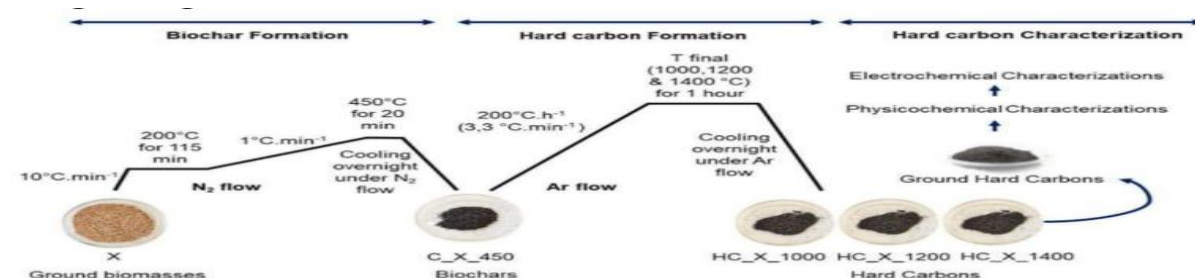


Figure 1: Schematic representation of CNT synthesis via CVD followed by Amorphous carbon coating through pyrolysis

Figure 1: Schematic representation of CNT synthesis via CVD followed by Amorphous carbon coating through pyrolysis

CONCLUSION

Hybrid Nanocomposites Composed of Amorphous Carbon Nanotubes Have Great Promise as Materials for Next Generation Energy Storage Devices. The key discoveries made by researchers include:

1.Superior Electrochemical Behaviour due to Hybrid Nature. **2.** High Conductivity and Stability. **3.** Large Surface Area.

This class of materials has the potential to be applied to the development of effective energy storage systems.

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Process Sensitivity and Reproducibility in Chitosan–TPP Microparticle Systems: A Critical Analysis Of Ionic Gelation Dynamics

Arghyadip Manna, and Dr. Debabrata Ghosh Dastidar*
Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Chitosan–tripolyphosphate (TPP) microparticles prepared by ionic gelation are widely used as simple, scalable, and biocompatible drug delivery systems, where electrostatic interactions between chitosan and TPP lead to rapid particle formation under mild conditions. However, despite this simplicity, many studies report poor reproducibility in key properties such as particle size, morphology, encapsulation efficiency, and drug release behavior. The process is highly sensitive to factors like pH, mixing speed, polymer concentration, and order of addition, where even small changes can significantly affect particle formation and lead to variations between studies and laboratories. This indicates that ionic gelation occurs under non-equilibrium conditions with heterogeneous structure development, raising questions about whether it is a truly controlled process or a kinetically driven and unstable system. This review therefore highlights ionic gelation as a process-sensitive system in which subtle changes in conditions strongly determine structural outcomes and reproducibility.

MATERIALS AND METHODS

This study was carried out as a systematic review using a PRISMA-based framework to ensure a structured and reproducible selection of literature. Relevant articles were searched from PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using keywords related to chitosan ionic gelation, process parameters, and microparticle formation. Only peer-reviewed English-language studies published between 2020 and 2025 were included. Studies focusing on ionic gelation, synthesis conditions, particle formation dynamics, and reproducibility were selected, while unrelated systems, incomplete data, and duplicate studies were excluded. The articles were screened through title, abstract, and full-text review, and data such as synthesis conditions, particle characteristics, and variability in results were extracted. A critical synthesis approach was then used to identify relationships between process and structure, as well as inconsistencies and gaps in the current understanding.

RESULTS AND DISCUSSION

- 1. Sensitivity of Ionic Gelation to Process Parameters:** Ionic gelation is driven by rapid electrostatic interactions and is therefore highly sensitive to process conditions. Factors such as pH, ionic strength, polymer concentration, and mixing conditions directly affect particle formation, including nucleation and growth. Even small changes in pH can alter chitosan protonation and reduce crosslinking efficiency, while stirring speed influences particle size distribution. In addition, the order of addition, such as adding TPP into chitosan or vice versa, can change nucleation behavior and final particle characteristics. As a result, the properties of the particles depend not only on the materials used but also strongly on the processing conditions.
- 2. Lack of Reproducibility as a Fundamental Limitation:** A major issue reported in recent studies is the lack of reproducibility of ionic gelation across different experiments and laboratories. Even when using the same formulation, researchers often obtain different particle sizes, shapes, and drug release profiles. This variation is mainly caused by poor control of local concentration gradients, differences in mixing efficiency, and sensitivity to environmental



conditions. In addition, the absence of standardized preparation protocols makes the results highly dependent on the specific experimental setup. This inconsistency is considered a significant barrier to scaling up and applying this method in industrial production. **3.Non-Equilibrium Nature of Particle Formation:** Particle formation in ionic gelation occurs under kinetically controlled, non-equilibrium conditions where rapid addition of TPP causes localized crosslinking and heterogeneous particle development. This process involves quick nucleation, uneven particle growth, and the formation of density gradients within the particles. As a result, the final structures show significant variability, leading to differences between batches and unpredictable drug release behavior. Therefore, ionic gelation is not a fully controlled synthesis method but rather a kinetically driven self-assembly process. **A. Role of Mixing and Hydrodynamics:** Mixing plays a crucial role in controlling particle uniformity during formation processes. Poor mixing can create localized regions of high TPP concentration, which leads to rapid aggregation and irregular particle formation. In contrast, high shear mixing improves uniformity by ensuring better distribution of components, while controlled addition rates help reduce heterogeneity. Additionally, turbulence significantly influences particle size distribution. Overall, these findings show that hydrodynamic conditions are just as important as chemical composition in determining the final properties of particles. **B. Process–Structure–Function Relationship:** A key insight is that process parameters affect not only how particles form but also important outcomes like drug release and stability. For instance, rapid gelation can create a heterogeneous structure that leads to burst drug release, while controlled gelation forms a more uniform network that supports sustained release. This shows a clear connection between process conditions, the resulting structure, and drug release behavior. However, most current research still treats these factors separately rather than combining them into a single, unified framework. **C. Critical Gap: Absence of Standardized and Predictive Process Models:** Despite extensive research, there is still no reliable predictive model that connects process parameters such as pH, mixing, and concentration with structural outcomes like particle size, porosity, and crosslinking, and further links them to functional performance including drug release kinetics and stability. As a result, most studies depend on empirical trial-and-error optimization rather than a clear mechanistic understanding. This lack of integration limits reproducibility and makes it difficult to design chitosan-based systems in a rational and controlled way.

Table 1. Influence of Process Parameters on Particle Formation and Reproducibility

Table 1. Influence of Process Parameters on Particle Formation and Reproducibility

Process Parameter	Effect on Formation Mechanism	Impact on Reproducibility
pH	Controls chitosan protonation	High sensitivity → variability
Mixing speed	Affects nucleation and growth	Poor mixing → heterogeneity
Addition rate	Determines local concentration gradients	Rapid addition → aggregation
Polymer concentration	Influences viscosity and crosslinking	High variability in structure
Ionic strength	Modulates electrostatic interactions	Alters particle stability

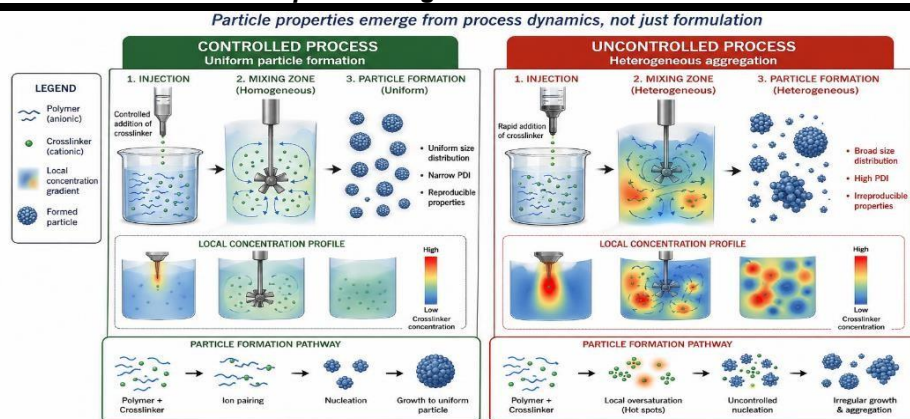


Figure 1: Ionic Gelation Process Sensitivity Model The image I provided is AI generated

CONCLUSION

This review shows that ionic gelation in chitosan–TPP systems depends strongly on the process

conditions, so results are often not reproducible because particle formation is controlled by fast, non-equilibrium kinetics, where mixing, hydrodynamics, and other process parameters greatly affect

structure and function, and due to the lack of standardized methods and predictive models linking process variables to final properties, ionic gelation should be understood as a process-controlled self-assembly system rather than one governed only by formulation composition.

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A Systematic Review of Classical, Artificial Intelligence and Quantum Computing Frameworks in Drug Repurposing: Methodologies, Integration And Translational Challenges (2020–2025)

Aditya Patra, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Drug repurposing has become a viable strategy in drug discovery to reduce time, cost and failure rates by discovering new uses for existing drugs. But while new methods have improved the process, it is still limited by biological complexity and the difficulty of finding relevant drug-disease associations from a vast combinatorial space [1]. Historically, drug repurposing was limited to traditional methods such as structure-based screening, phenotypic data, and hypothesis-driven research. In recent years, drug repurposing has also benefited from the application of artificial intelligence (AI) and machine learning (ML) to enable large- scale, data-driven prediction of drug–target and drug–disease interactions, and quantum computing has been suggested as a future approach to handle molecular complexity via physics-based modelling [2][3]. While all three approaches co-exist, they are typically framed as alternative approaches, rather than different representations of the drug repurposing problem. This begs an important Conceptual question: Do classical, AI and quantum approaches provide different solutions to the same problem, or are they distinct representations of the problem of drug repurposing?

MATERIALS AND METHODS:

A systematic review, following PRISMA guidelines, was used in this study. Studies were sourced from PubMed, Scopus, Web of Science and ScienceDirect with keywords including "drug repurposing computational methods", "AI drug repurposing challenges", and "quantum computing drug discovery". The search was restricted to peer-reviewed journals between 2020-2025. Inclusion criteria were studies that discussed classical computational methods and AI/ML- based drug repurposing frameworks, as well as new quantum or hybrid computational drug repurposing frameworks. Exclusion criteria revolved around descriptive studies without mechanistic and computational insights. A critical synthesis approach was used to assess variations in problem formulation, limitations in methodology, and translation challenges of frameworks.

RESULTS AND DISCUSSION:

A key difference between classical, AI and quantum paradigms is their underlying understanding of the drug repurposing problem. Classical approaches are often hypothesis- driven and utilise preconceived biological assumptions such as structural similarity, pathway analysis and experimental testing. By contrast, AI approaches are data-driven and rely on pattern recognition to detect correlations in large-scale biomedical data, without making assumptions about underlying mechanisms. Quantum computing, in contrast, is a physics- driven approach that seeks to model molecular interactions in a fundamental manner, potentially resolving some of the shortcomings of classical models of chemical interactions [2][3]. These variations indicate that the three paradigms are not just alternative tools but reflect different epistemological foundations in the discovery of new drugs. Whilst AI has been embraced widely, its perceived benefits over classical approaches are questionable. AI has greatly enhanced the speed of drug discovery by incorporating multi-omics data to discover previously unknown relationships in complex data [2]. But its predictive accuracy is inexorably linked to the quality, completeness and biases inherent in the data.



Often, AI does not produce new insights into molecular biology but amplifies existing knowledge, suggesting that its benefits might be more computational than conceptual. This suggests a key constraint: The accuracy of AI-powered repurposing largely depends on data representation rather than the complexity of the algorithm. In all approaches, data are the limiting factor. Traditional approaches are constrained by limited biological understanding and AI frameworks by diverse, biased, and sparse data. Even quantum methods, which are theoretically promising, need high-quality molecular information and are currently confined to proof-of-concept studies [3]. This intersection implies drug repurposing is more a data-limited problem than a purely computational problem, in which better algorithms cannot overcome insufficient biological knowledge. A second key limitation is the lack of translational success of computational predictions. While many studies present potential drug–disease predictions, only a handful are successfully validated [1]. This failure to translate is due not only to inaccurate predictions but also poor validation. The majority of drug repurposing approaches focus on retrospective validation, docking studies or in vitro experiments, without robust prospective validation and clinical implementation. This leads to "virtual" success not translating to clinical success. The combination of classical, AI and quantum techniques is often touted as the solution of the future; however, it is not clear how this will be achieved. Although composite models that employ AI-based predictions in conjunction with classical or quantum-based validations are appealing, there is no integrated pipeline to specify how these models interact during the various phases of drug repurposing. The absence of integration reflects a broader issue: a lack of a systems-level approach to link prediction, validation and clinical practice. This is especially evident with quantum computing. While quantum approaches hold the promise of modelling molecular interactions with an unprecedented level of detail, their current uses are, for the most part, experimental and constrained by technological limitations, scalability and validation [3]. This begs the question about its application to drug repurposing: Is quantum computational methodology solving an existing problem, or is it trying to solve a problem that is not currently limiting for the current approaches? Finally, a key and under-recognised concern is bias towards commonly researched drugs and diseases. AI and classical databases are biased towards knowledge, which can perpetuate established drug–disease associations rather than identifying new therapeutic targets. This implies that existing models may be fine-tuning predictions within the existing biological knowledge space, but may not be broadening our knowledge of disease processes.

Framework	Core Approach	Key Limitation
Classical	Hypothesis-driven	Limited biological knowledge
AI/ML	Data-driven prediction	Data bias and incompleteness
Quantum	Physics-based simulation	Limited practical applicability
Validation	Experimental confirmation	Lack of standardization
Translation	Clinical application	Poor success rate

Table 1. Comparative Limitations Across Drug Repurposing Frameworks

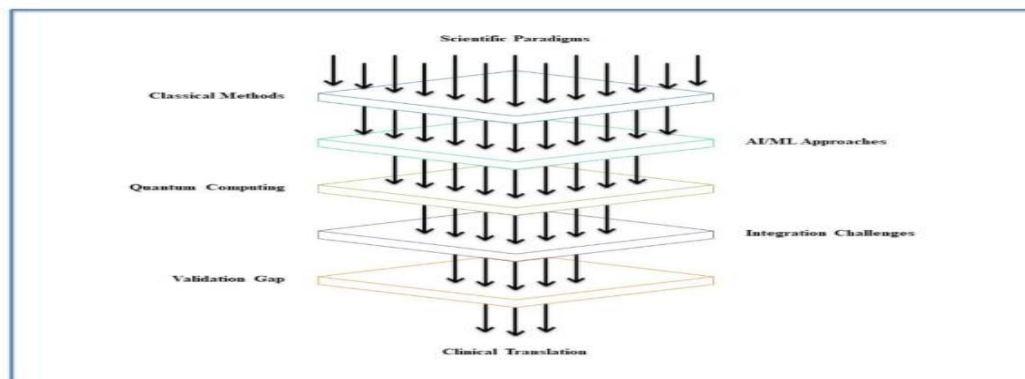


Figure 1: Framework-Gap-Translation Model

CONCLUSION: This review shows that drug repurposing models should not be compared purely by computational power but as a complex interlinked system that is limited by data, biology and translation. Framework Core Approach Key Limitation Classical Hypothesis-driven Limited biological knowledge AI/ML Data-driven prediction Data bias and incompleteness Quantum Physics-based simulation Limited practical applicability Validation Experimental confirmation Lack of standardization Translation Clinical application Poor success rate

Our analysis shows that:

- Traditional, AI and quantum approaches are alternative representations of the problem
- Quantum computing has theoretical benefits but is immature
- The limiting factor is not computational but data, validation and integration

The bottleneck in drug repurposing is not the lack of cutting-edge computational techniques, but rather, the lack of an integrated approach that links data, biology, and clinical validation through classical, AI and quantum approaches.

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Advancements In Paper-Based And Textile-Integrated Flexible Pressure Sensors

Utsav Singha, Shruti Bhattacharyya, Soumarya Ghosh, Parthiv Poddar, Sayan Hazra, Swagata Mandal

Department of Computer Science & Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex, 540, Dum Dum, Surer Math, Kolkata-700074

Email:-utsavsingha289@gmail.com

INTRODUCTION

Flexible pressure sensors represent a critical advancement in human-machine interface (HMI) technology, shifting from rigid components like keyboards toward adaptable, skin-conformable electronics. These sensors, which convert pressure into electrical signals, are essential for health monitoring, electronic skin, and robotics. While synthetic polymers like PDMS have dominated, paper and textile-based substrates offer promising low-cost, sustainable, and breathable alternatives. This paper reviews the integration of paper and textile substrates for high-performance capacitive and piezoresistive sensing.

MATERIALS AND METHOD: The development of these sensors relies on modifying inherently insulating materials like paper and cotton textiles with conductive agents. Common conductive additives include carbon nanotubes (CNT), silver nanowires (AgNW), graphene, and conductive polymers like PEDOT: PSS. The core challenge in flexible pressure sensors is maintaining electrical conductivity while undergoing mechanical deformation.

Active Materials:

Conductive Fillers: The most common approach involves creating composites. You can cite Huang et al. (2019) regarding the use of carbon-based nanomaterials (carbon nanotubes, graphene, and carbon black). These materials form percolation networks that change resistance when pressure is applied, altering the contact area between conductive pathways. **Substrates:** Zhang et al. (2022) highlight that textile-based sensors use natural or synthetic fibers (cotton, nylon, or polyester). The choice of substrate is dictated by the desired "wearability" and breathability.

Fabrication Techniques:

Dip-Coating: This is a low-cost, scalable method where the textile is immersed in a conductive ink. Mishra et al. (2021) note that the number of dipping cycles directly dictates the sensitivity and resistance range. **Micro-structuring:** To achieve high sensitivity, researchers often replicate natural surfaces. By casting a polymer over a flower petal or a lotus leaf and then coating it with a conductive layer, the sensor gains a hierarchical microstructure. This increases sensitivity because the contact area between electrodes changes drastically under even tiny amounts of pressure. **Sensing Mechanisms:** The sensors predominantly utilize piezoresistive (resistance change) or capacitive (capacitance



change) mechanisms. Capacitive sensors, in particular, are favored for their low power consumption and simple structure.

RESULT AND DISCUSSION:

Sensitivity (Gauge Factor): A major finding, as noted by Xu et al. (2024), is that sensitivity is generally a trade-off with the measurement range. Highly sensitive sensors are excellent for detecting pulse or heartbeat but often saturate quickly (cannot measure heavy pressure). **Hysteresis and Response Time:** One of the main "discussions" in recent literature is how to reduce hysteresis (the delay in the sensor returning to its original state). Using porous, elastic sponges (like polyurethane foam) coated with conductive materials is a common solution proposed by Dong et al. (2024) to allow for rapid recovery. **Environmental Stability:** This is a critical discussion point for your paper. Research shows that while these sensors perform well in the lab, they face degradation from moisture and oxidation. Future research needs to focus on encapsulation techniques (thin-film protective layers) to ensure they remain functional after being washed or exposed to sweat.

CONCLUSION

Paper and textile-based flexible pressure sensors provide a sustainable, scalable foundation for the next generation of wearable electronics. Future breakthroughs depend on refining structural design and manufacturing to achieve higher precision and reliability. These sensors are vital for evolving interactive HMIs and advanced medical diagnostics.

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siRNA-Based Gene Silencing in Overcoming Multidrug Resistance: A Critical Analysis Of Mechanistic Targeting And Delivery Limitations

Sunandan Ray, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Multidrug resistance (MDR) is a major challenge in cancer chemotherapy, leading to treatment failure and disease recurrence due to mechanisms such as drug efflux, altered apoptosis, and metabolic changes. Small interfering RNA (siRNA) therapy offers a targeted approach by silencing resistance-related genes like MDR1, enabling precise regulation at the gene level. While studies show that siRNA can enhance drug retention and restore chemosensitivity, its clinical application remains limited. This highlights a key issue: the effectiveness of siRNA therapy is primarily constrained not by its gene-silencing ability, but by challenges in efficient intracellular delivery.

MATERIALS AND METHODS

This study was conducted as a systematic review following a PRISMA-based framework, with literature collected from PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar. The search (2020–2025, English, peer-reviewed) used keywords related to siRNA, MDR, MDR1 delivery, nanocarriers, and delivery barriers. Included studies focused on siRNA-mediated MDR targeting, delivery systems, and mechanistic or translational analyses, while non-MDR therapies, incomplete datasets, and duplicates were excluded. Data extraction emphasized gene targets, delivery strategies, and therapeutic outcomes, followed by critical synthesis to identify mechanistic gaps and translational limitations.

RESULTS AND DISCUSSION

siRNA induces gene silencing via the RNA interference pathway, where it is incorporated into the RNA-induced silencing complex (RISC) to enable sequence-specific degradation of target mRNA. In multidrug resistance systems, this leads to downregulation of drug efflux transporters such as P-glycoprotein, increased intracellular drug accumulation, and restoration of chemosensitivity in resistant cancer cells. Thus, siRNA acts as a highly precise strategy by targeting the genetic basis of resistance rather than its downstream effects.

Table 1. Key Barriers in siRNA-Based MDR Therapy

Barrier Level	Limitation	Impact
Molecular	Instability, enzymatic degradation	Reduced bioavailability
Systemic	Rapid clearance, RES uptake	Poor circulation time
Cellular	Poor membrane permeability	Low uptake
Intracellular	Endosomal trapping	Ineffective gene silencing
Targeting	Limited tumor specificity	Poor clinical translation

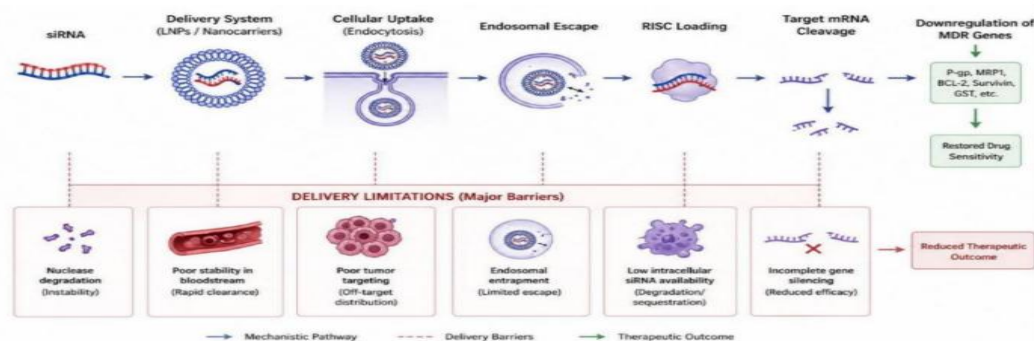


Figure 1. Mechanistic pathway and delivery barriers of siRNA therapeutics. Schematic illustration of the stepwise intracellular journey of siRNA delivered via lipid nanoparticles (LNPs) or nanocarriers. Following systemic administration, siRNA undergoes cellular uptake through endocytosis, escapes from endosomal compartments, and is incorporated into the RNA-induced silencing complex (RISC), enabling sequence-specific target mRNA cleavage and subsequent downregulation of multidrug resistance (MDR)-associated genes (e.g., P-gp, MRP1, BCL-2, surviving, GST), ultimately restoring drug sensitivity. The lower panel highlights major delivery limitations, including nuclease-mediated degradation, poor systemic stability and rapid clearance, inadequate tumour targeting, endosomal entrapment, low intracellular siRNA availability, and incomplete gene silencing, which collectively contribute to reduced therapeutic efficacy.

CONCLUSION

siRNA-based therapy for multidrug resistance is mechanistically effective in silencing resistance-related genes, but its clinical success is primarily limited by delivery challenges. While it demonstrates strong molecular targeting capability, biological barriers significantly restrict intracellular availability, and existing delivery systems, though improving stability, still lack efficient targeting. As a result, translational failure occurs due to multiple interconnected limitations. Therefore, siRNA therapy should be viewed as a delivery-dependent approach, requiring integrated optimization of gene targeting, carrier design, and intracellular transport rather than relying solely on RNA interference.

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pH-Responsive Lysin-Loaded Nanocarriers for Mdr-Infected Wounds: A Critical Analysis Of Targeted Delivery And Translational Limitations

Supravat Pramanik, and Dr. Debabrata Ghosh Dastidar*
Guru Nanak institute of Pharmaceutical Science and Technology
157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074
E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Multidrug-resistant (MDR) wound infections represent a major clinical challenge due to biofilm formation, impaired drug penetration, and increasing resistance to conventional antibiotics. These infections significantly delay wound healing and increase morbidity, highlighting a fundamental limitation of current antimicrobial therapies [4]. Biofilms act as physical and biochemical barriers, restricting drug diffusion and protecting bacteria from antimicrobial agents. As a result, conventional antibiotics often fail to achieve effective concentrations at the infection site. Bacteriophage-derived lysins (Enz biotics) have emerged as a promising alternative due to their rapid and specific bacteriolytic activity, directly targeting the peptidoglycan layer of bacterial cell walls [1]. However, lysins suffer from instability, enzymatic degradation, and poor retention at the wound site. To overcome these limitations, pH-responsive nanocarriers have been developed to exploit the acidic microenvironment of infected wounds, enabling targeted and controlled drug release. Such systems aim to enhance local drug concentration while minimizing systemic exposure.

MATERIALS AND METHODS

This study was conducted as a systematic review using a PRISMA-based analytical framework, with literature collected from PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using search keywords such as “pH-responsive nanocarriers wound infection lysin,” “biofilm targeted nanomedicine MDR wounds,” and “stimuli-responsive antimicrobial delivery systems.” The review was restricted to peer-reviewed articles published between 2020 and 2025, with inclusion criteria focusing on studies involving lysin/phage-based antimicrobial systems, pH-responsive nanocarriers, and MDR wound infection models, while exclusion criteria included non-responsive delivery systems and non-MDR infection studies. A critical synthesis approach was applied to identify mechanistic patterns, delivery limitations, and translational gaps.

RESULTS AND DISCUSSION

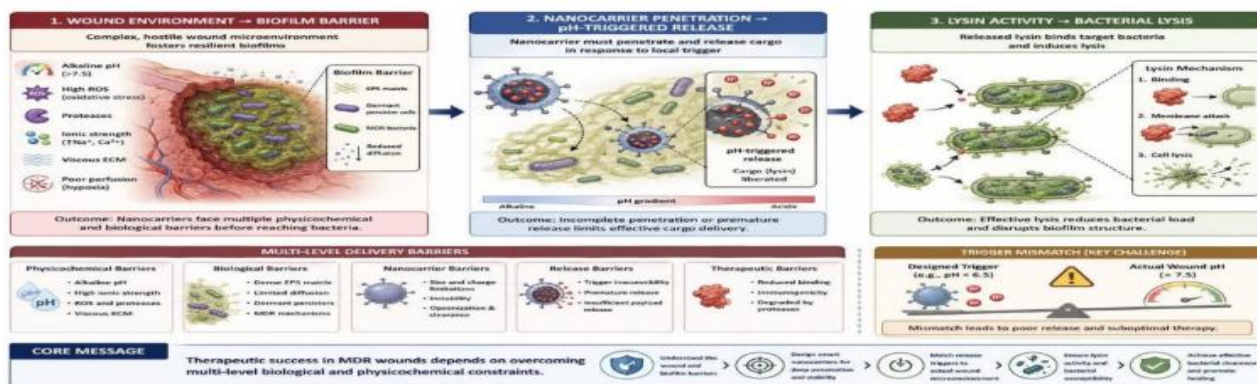
Lysins act by hydrolysing specific bonds in the bacterial peptidoglycan layer, leading to rapid osmotic lysis of bacterial cells, and unlike antibiotics, they exhibit high specificity with low resistance development potential [1]; however, their effectiveness is significantly reduced in biofilm-associated infections due to limited penetration into the extracellular polymeric matrix, enzymatic degradation in biological environments, and short residence time at infection sites, indicating that the limitation of lysins lies not in mechanistic efficacy but in biological



accessibility. To address this, pH-responsive nanocarriers are designed to exploit the acidic environment of infected wounds (pH ~4.5–6.5) using acid-labile linkages, protonation-induced swelling, and charge-switching mechanisms, remaining stable at physiological pH (~7.4) and releasing lysins under acidic conditions, thereby enabling site-specific drug activation, reduced systemic toxicity, and enhanced therapeutic efficiency [2][5]. These nanocarriers improve lysin performance by protecting them from proteolytic degradation, increasing retention at the wound site, and enhancing penetration into biofilms, with systems such as hydrogels, liposomes, and polymeric nanoparticles demonstrating improved antibacterial activity and accelerated wound healing in preclinical models [1], although effective delivery requires maintaining lysin activity, ensuring controlled release, and achieving sufficient biofilm penetration. Despite these advantages, a critical limitation arises from the heterogeneity of wound pH, which varies spatially and temporally depending on infection severity and healing stage, leading to variable acidity, gradual pH gradients, and dynamic changes that cause incomplete activation, premature release, and reduced targeting specificity, highlighting a mismatch between designed triggers and biological reality. Furthermore, translational barriers such as instability of protein-based therapeutics, difficulty in large-scale production, lack of standardized formulation protocols, and limited in vivo and clinical validation, along with challenges in integrating these systems into clinically acceptable wound dressings, hinder clinical application. Overall, therapeutic failure occurs across multiple levels—molecular (lysin instability), carrier (formulation and release control), and biological (wound heterogeneity and biofilm barrier)—indicating that effective therapy requires integrated optimization across all levels.

Table 1. Key Determinants and Limitations of pH-Responsive Lysin Nanocarriers

Parameter	Functional Role	Limitation
Lysin activity	Rapid bacterial lysis	Instability in vivo
Nanocarrier design	Protection and delivery	Complex formulation
pH responsiveness	Targeted release	Variable wound pH
Biofilm penetration	Improves efficacy	Limited diffusion
Release kinetics	Sustained delivery	Difficult to control

**Fig 1: Multi-Level Delivery Model for MDR Wounds**

CONCLUSION

Organized by: Department of Basic Science & Humanities,
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex (SurTech), (Autonomous), Kolkata



This review demonstrates that pH-responsive lysin-loaded nanocarriers represent a promising but delivery-constrained strategy for treating MDR wound infections, revealing that lysins provide highly effective antibacterial mechanisms, nanocarriers enhance stability, retention, and targeting, and pH-responsive release enables site-specific therapy; however, biological variability and formulation challenges limit clinical translation, indicating that lysin-based nanocarrier systems should be redefined as multi-level therapeutic platforms where success depends on integrating molecular stability, carrier design, and environmental responsiveness rather than relying solely on antibacterial mechanisms.

ACKNOWLEDGMENT

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pH-Responsive Nanomaterials in Tumor Microenvironment Wounds: A Critical Analysis Of Targeted Delivery And Translational Limitations

Manjar Alam,, and Dr. Debabrata Ghosh Dastidar*

Guru Nanak institute of Pharmaceutical Science and Technology

157/F Nilgunj Road, Pani Hati, Sodepur, Kolkata – 700074

E-mail: debabrata.ghoshdastidar@gnipst.ac.in*

INTRODUCTION

Conventional chemotherapy remains limited by non-specific drug distribution, systemic toxicity, and poor selectivity toward tumor tissues, resulting in significant damage to healthy cells and reduced therapeutic efficiency. This highlights a fundamental challenge in cancer therapy: the inability to achieve spatially selective drug delivery at the tumor site. The tumor microenvironment (TME) provides a potential solution due to its distinct physicochemical characteristics, particularly slightly acidic extracellular pH (≈ 6.5 – 7.0) compared to normal physiological pH (~ 7.4) [1]. This acidity arises from altered tumor metabolism, including enhanced glycolysis, lactate accumulation, and impaired clearance of acidic metabolites [1]. Based on this difference, pH-responsive nanomaterials have been developed to enable triggered drug release in tumor-specific environments. Recent literature reports a wide range of pH-responsive systems, including polymeric nanoparticles, liposomes, metal–organic frameworks, and inorganic nanocarriers, which are designed to remain stable in circulation and undergo structural transformation under acidic conditions [2]. However, despite extensive research and promising in vitro results, clinical translation remains limited.

MATERIALS AND METHODS

This study was conducted as a systematic review following a PRISMA-guided framework to ensure a transparent, structured, and reproducible selection process. Relevant literature was identified through comprehensive searches of PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using keywords related to pH-responsive nanomaterials, tumor microenvironment, and acid-triggered drug release. Only peer-reviewed English- language articles published between 2020 and 2025 were included. Studies focusing on pH-responsive drug delivery systems, tumour targeting, and mechanistic drug release were selected, while unrelated systems, incomplete data, and duplicates were excluded. The selection involved screening titles, abstracts, and full texts, followed by extraction of key data such as nanoparticle design, pH-triggering mechanisms, drug release profiles, and in vivo outcomes. A critical synthesis approach was applied to identify mechanistic trends, inconsistencies, and key limitations affecting clinical translation.

RESULTS AND DISCUSSION: Mechanisms of pH-Responsive Drug Release pH-responsive nanomaterials function through specific physicochemical mechanisms that enable structural changes in acidic environments. These include protonation of ionizable groups, cleavage of acid-labile bonds, and charge conversion that destabilizes the nanocarrier. Such changes lead to swelling, disassembly, or rupture of nanoparticles, allowing controlled drug release.



These systems are typically designed on a threshold-based activation principle, where slight pH variations trigger significant structural responses.

Dependence on Subtle pH Gradients: A key limitation of pH-responsive systems is that tumour acidity in vivo is relatively weak and poorly defined. Unlike ideal experimental conditions with clear and uniform pH differences, actual tumours exhibit only small pH variations (about 0.5–1 unit), along with significant spatial heterogeneity and temporal changes during progression. Due to metabolic gradients and irregular vascularization, pH can vary widely across different tumour regions, leading to inconsistent activation of pH-sensitive systems. This creates a fundamental challenge in achieving reliable and predictable drug release in clinical settings.

Passive vs Active Responsiveness

Most pH-responsive systems function through passive responsiveness, relying on environmental acidity to trigger drug release. However, recent studies indicate that these systems often lack precise activation thresholds, clear selectivity between tumour and normal tissues, and consistent control under physiological conditions. As a result, they are considered fundamentally limited, as they depend on passive environmental sensing rather than incorporating active targeting strategies.

Discrepancy Between In Vitro and In Vivo Performance:

A major challenge in pH-responsive drug delivery is the gap between in vitro success and in vivo performance. Under controlled laboratory conditions, these systems show efficient drug release, clear pH-triggered behaviour, and high targeting specificity. However, in vivo environments introduce complexities such as protein adsorption (corona formation), multiple biological barriers, and variable pH microenvironments, all of which significantly diminish their effectiveness in clinical applications. **Lack of Defined Activation Thresholds** Another key limitation of pH-responsive systems is the lack of well-defined activation thresholds. While most designs assume stability at pH 7.4 and activation around pH 6.5, real biological conditions show significant overlap between normal and tumor pH levels. As a result, small fluctuations can cause premature drug release, while insufficient acidity may fail to trigger activation, leading to unpredictable and inconsistent drug delivery outcomes.

Critical Gap: Absence of Predictive Design Framework: Despite extensive research, there remains no robust quantitative framework that directly links material pH sensitivity with tumor pH variability to predict drug release efficiency. As a result, most pH-responsive systems are developed empirically, without adequately incorporating biological variability into their design, limiting their reliability and translational potential.



Table 1. Key Limitations of pH-Responsive Nanomaterials in Tumor Targeting

Parameter	Ideal Assumption	Actual Biological Reality	Impact
Tumor pH	Strongly acidic	Slightly acidic (6.5–7.0)	Weak triggering
@pH uniformity	Homogeneous	Highly heterogeneous	Inconsistent activation
Activation threshold	Well-defined	Overlapping with normal tissue	Poor selectivity
Responsiveness	Sharp transition	Gradual response	Reduced efficiency
In vitro vs in vivo	Similar conditions	Highly complex environment	Translational failure

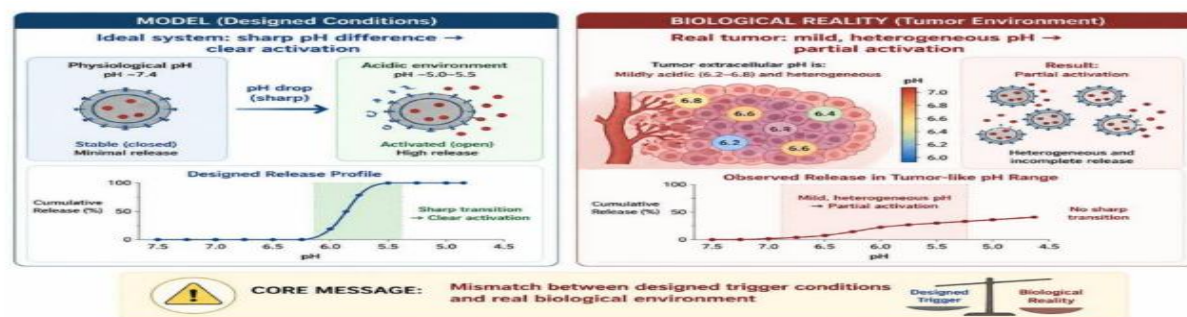


Figure 1: pH-Triggered Release vs Biological Reality

CONCLUSION

This review highlights that pH-responsive nanomaterials are a promising yet fundamentally constrained approach for tumour-targeted drug delivery. Drug release in these systems is driven by pH-induced structural changes, but their effectiveness is limited by the weak and heterogeneous nature of tumour acidity, which restricts selective activation. Most systems depend on passive responsiveness, reducing targeting efficiency, and their strong in vitro performance often fails to translate reliably in vivo. A key limitation is the lack of predictive frameworks that integrate material properties with biological variability. Therefore, pH-responsive drug delivery should be viewed as a context-dependent strategy, where success depends not only on material design but also on overcoming tumour microenvironment complexity, emphasizing the need for multi-stimuli or active targeting approaches for better clinical outcomes.

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Hybrid Nanostructured Catalysts For Sustainable Hydrogen Production Systems

Md Faizan Salim, Md Sajid Raza Khan, Soha Dhauria, and Md Miftahur Rahman

Department of Computer Science & Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,
540, Dum Dum, Surer Math, Kolkata-700074

Email: - faizansalim690@gmail.com, miftahzeya456@gmail.com

INTRODUCTION

The escalating global energy demand and the environmental crisis caused by fossil fuel combustion have accelerated the transition toward carbon-neutral energy carriers. Green hydrogen (H₂) is regarded as the most promising alternative due to its high gravimetric energy density and zero-carbon emission profile when produced via water electrolysis powered by renewable sources like solar or wind energy. Water splitting consists of two half-cell reactions: the Hydrogen Evolution Reaction (HER) at the cathode and the Oxygen Evolution Reaction (OER) at the anode. While precious metals such as Platinum (Pt) for HER and Iridium/Ruthenium (Ir/Ru) for OER remain the performance benchmarks, their high cost and scarcity limit large-scale commercialization.

MATERIALS AND METHODS: This literature survey identifies several classes of Earth-abundant materials that have shown significant promise as electrocatalysts. Key materials discussed in the selected research include: **Transition-Metal Compounds:** Oxides (TMOs), phosphides (TMPs), sulfides (TMSs), nitrides (TMNs), and carbides (TMCs). **Layered Double Hydroxides (LDHs):** Particularly NiFe-LDH, which exhibits exceptional OER activity due to its unique electronic structure and high surface area. **Hybrid Nanostructures:** Composite materials such as NiFe-LDH grown on conductive substrates like nickel foam or defective graphene (DG) to improve charge transfer kinetics. **2D Nanomaterials:** Copper oxide (CuO) nanosheets and molybdenum disulfide (MoS₂) nano boxes incorporated with nickel/cobalt. **Methods (Working Principle)** The fundamental principle of electrochemical water splitting involves the dissociation of water molecules using electrical energy. □ **HER Mechanism:** Occurs via the Volmer-Heyrovsky or Volmer-Tafel pathways, where protons are adsorbed onto the catalyst surface and reduced to form H₂ gas. **OER Mechanism:** A more complex four-electron transfer process involving the Adsorbate Evolution Mechanism (AEM) or Lattice Oxygen Mechanism (LOM). It is kinetically more sluggish than HER, requiring higher overpotentials. □ **Hybrid Strategy:** By nano structuring these materials, researchers increase then electrochemical surface area (ECSA) and optimize the binding energy of reaction intermediates, thereby lowering the overpotential required for the reactions. **3. RESULTS AND DISCUSSION** A comparative analysis of recent literature reveals that hybrid nano structuring significantly outperforms bulk counterparts. For instance, NiFe-LDH integrated with defective graphene (NiFe-LDH NS@DG) demonstrates a low OER overpotential of 210 mV at 10 mA/cm² and a HER overpotential of 115 mV at 20 mA/cm². Transition metal- based core-shell structures (e.g., Pt/Ni or Pt/Cu) also enhance mass activity by protecting the transition metal core while utilizing a small amount of precious metal on the surface.



Table 1: Comparative Performance of Selected Electrocatalysts from Literature

Catalyst type	substrate	Overpotential (OER)	Overpotential (HER)
NiFe-LDH NS@DG	Defective Graphine	210 mV @ 10 mA/cm ²	115 mV @ 20 mA/cm ²
CuO Nanosheets	Stainless Steel	250 mV @ n10	-
Ni-Mo/Ni-Fe	Ni-Mo Interface	-	High Activity in 1M NaOH
NiFeRu-LDH	Nickel Foam	Enhanced Stability	

The discussion focuses on the synergistic effects of hybrid designs, where the interaction between different phases (e.g., metal and support) facilitates faster charge transfer and provides more active sites for the reaction.

CONCLUSION

Hybrid nanostructured catalysts are central to the development of sustainable green hydrogen production systems. This survey underscores that while noble metals are the standard, Earth-abundant transition metal hybrids—especially those utilizing LDH structures and nano structuring techniques—offer a viable path toward cost-effective electrolysis. Future research should focus on long-term stability under industrial conditions and the integration of these catalysts into large-scale alkaline water electrolyzers to meet global energy demands sustainably.

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Nanostructured Electrocatalysts for Efficient Electrochemical Water Splitting Systems

Souvik H., Abir M., Gourab P., Ranit M., Sohani D. A.

Department of Computer Science & Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,
540, Dum Dum, Surer Math, Kolkata-700074

Email: - souvikh564@gmail.com

INTRODUCTION

Hydrogen is emerging as a clean and sustainable energy carrier due to its high energy density and zero carbon emissions during use. However, most hydrogen production today relies on fossil fuels, which contributes to environmental pollution. Electrochemical water splitting offers a greener alternative by using electricity from renewable sources to produce hydrogen. The efficiency of this process depends heavily on electrocatalysts that accelerate the reactions involved. Recently, nanostructured electrocatalysts have gained significant attention due to their superior properties. Their extremely small size provides a high surface-to-volume ratio, increased active sites, and enhanced charge transfer, making them highly effective in improving reaction efficiency. This study focuses on the role of nanostructured electrocatalysts in enhancing the performance of electrochemical water splitting.

MATERIALS AND METHODS

This work is based on a review of recent research on nanostructured electrocatalysts used in water splitting. The study includes-

- i) Analysis of nanomaterials such as nanoparticles, nanowires, and nanosheets
- ii) Comparison of catalyst materials including noble metals (Pt, Ir) and transition metals (Ni, Co, Fe)
- iii) Evaluation of how nano structuring improves catalytic activity, conductivity, and stability
- iv) Overview of electrochemical water splitting reactions (HER and OER) as the application area

RESULTS AND DISCUSSION:

Nanostructured electrocatalysts enhance the performance of electrochemical water splitting primarily by modifying surface and electronic properties at the nanoscale. Unlike bulk materials, nanostructures exhibit a significantly higher surface-to-volume ratio, which increases the number of active catalytic sites available for reactions. One of the key advantages of nano structuring is the reduction in overpotential. Due to improved surface interactions between the catalyst and reaction intermediates, nanomaterials facilitate faster adsorption and desorption processes, thereby accelerating reaction kinetics. This directly improves the efficiency of both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER).

Hydrogen Evolution Reaction (HER):



Oxygen Evolution Reaction (OER):





Table 1. Comparison of Different Types of Electrocatalysts for Electrochemical Water Splitting.

Catalyst type	Examples	Advantages	Limitations
Noble Metals	Pt, Ir	Very high activity, low overpotential	Expensive, scarce
Transition Metals	Ni, Co, Fe	Low cost, abundant	Moderate activity
Metal Compounds	Oxides, Sulfides	Good stability, tunable properties	Lower conductivity
Nanostructured Catalysts	Nanoparticles, Nanowires	High surface area, enhanced kinetics	Complex synthesis

Different catalyst types show varying performance when engineered at the nanoscale, as summarized in Table 1. Noble metals such as platinum and iridium demonstrate excellent catalytic activity due to optimal binding energies with hydrogen intermediates. However, their high cost and scarcity limit large-scale applications. To address this, transition metal-based catalysts (Ni, Co, Fe) are widely studied, and their performance can be significantly enhanced through nano structuring. Nano structuring also improves electrical conductivity and charge transfer efficiency. For example, reducing particle size shortens electron transport pathways; while creating porous or hybrid structures enhances electrolyte accessibility. These factors collectively contribute to improved catalytic activity and stability. Among the two reactions involved in water splitting, OER remains the major challenge due to its complex multi-step mechanism and higher energy requirement. Nanostructured catalysts help mitigate this limitation by providing optimized active sites and facilitating intermediate reaction steps more efficiently. Overall, the integration of nanotechnology with catalyst design enables the development of cost-effective and high-performance electrocatalysts, making electrochemical water splitting more viable for sustainable hydrogen production.

CONCLUSION: Nanostructured electrocatalysts play a crucial role in improving the efficiency of electrochemical water splitting. Their high surface area, enhanced catalytic activity, and improved charge transfer make them highly effective for hydrogen production. The use of nano structuring allows cost-effective materials to achieve better performance, reducing dependence on expensive noble metals. Future research should focus on scalable synthesis methods, long-term stability, and integration with computational tools for optimized catalyst design.

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Bimetallic Nanocatalysts for High Efficiency Hydrogen Evolution Reaction

Nilanjan Jana, Arbaj Hussain, Gourav Saha, Suraj Sk
Dr. Sudhir Chandra Sur Institute of Technology and Sports Complex,
540, Dum Dum, Surer Math, Kolkata - 700074
E-mail- nilanjanjana5367@gmail.com

INTRODUCTION

The increasing demand for clean and sustainable energy has spurred interest in hydrogen as an alternative fuel. Hydrogen is a promising energy source because it is environmentally friendly and produces only water when used in fuel cells. The Hydrogen Evolution Reaction (HER) is one of the most effective methods for hydrogen production, occurring during water electrolysis. However, HER is a slow electrochemical process that needs catalysts to speed up its reaction rate and efficiency. Traditionally, noble metals like platinum serve as catalysts due to their great activity, but their high cost and limited availability limit widespread use. To address these issues, researchers have developed bimetallic nanocatalysts. These catalysts combine two different metals at the nanoscale, resulting in better catalytic activity, lower costs, and improved stability due to synergistic effects. Thus, bimetallic nanocatalysts offer a promising solution for enhancing HER efficiency and supporting sustainable hydrogen energy technology

MATERIALS AND METHODS

The chemicals and materials used to prepare bimetallic nanocatalysts include metal salts such as nickel (Ni), cobalt (Co), and platinum (Pt), along with a reducing agent like sodium borohydride (NaBH_4). Water and ethanol serve as solvents, while carbon black, graphene, or carbon cloth function as supporting materials. Nafion solution acts as a binder, and the electrolyte can be either acidic (H_2SO_4) or alkaline (KOH). The bimetallic nanoparticles are made using the chemical reduction method, where metal salt solutions are first mixed in the desired ratio. A reducing agent is then added while stirring continuously, leading to the formation of nanoparticles. These nanoparticles are collected, washed, centrifuged, and dried. For electrode preparation, a catalyst ink is made by mixing the catalyst with Nafion and ethanol. This ink is then drop-cast onto a glassy carbon electrode and dried before testing. To study the material properties, different characterization techniques are employed, such as SEM/TEM for morphology, XRD for crystal structure, and EDX for chemical composition. Finally, the electrochemical performance is assessed using Linear Sweep Voltammetry (LSV), Tafel slope analysis, Electrochemical Impedance Spectroscopy (EIS), and Cyclic Voltammetry (CV).

RESULTS AND DISCUSSION

The synthesized bimetallic nanocatalysts showed significantly better catalytic performance for the Hydrogen Evolution Reaction (HER). Compared to single-metal catalysts, they demonstrated lower overpotential, higher current density, and a smaller Tafel slope, indicating faster hydrogen production and improved reaction kinetics. This enhanced performance mainly results from the synergistic effect between the two metals, which boosts hydrogen adsorption and speeds up electron transfer. Structural analysis confirmed that the nanoparticles are evenly distributed and have a high surface area, offering many active sites for the reaction. The EIS results also revealed lower charge transfer resistance, while stability tests showed excellent long-term durability of the catalyst.



CONCLUSION

Bimetallic nanocatalysts are very effective materials for boosting the Hydrogen Evolution Reaction (HER). They provide better catalytic activity, improved stability, and are more affordable, making them suitable for sustainable hydrogen production. The enhanced performance mainly stems from the synergistic effect between the two metals, which plays a crucial role in raising catalytic efficiency. As a result, bimetallic nanocatalysts outperform traditional single-metal (monometallic) catalysts.

ACKNOWLEDGMENT

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Mutation-Specific Modulation of Docetaxel Binding to β -Tubulin: A Comparative Multi-Target Docking Analysis

Soham Singha, Debabrata Ghosh Dastider*

Guru Nanak Institute of Pharmaceutical Science and Technology 157/F Nilgunj Road, Panihati, Sodepur, Kolkata-700114

*debabrata.ghoshdastider@gnipst.ac.in

INTRODUCTION

Microtubules are essential cytoskeletal structures responsible for maintaining cellular architecture and mediating mitotic progression through dynamic polymerization–depolymerization cycles. The β -tubulin subunit plays a central role in regulating these dynamics via conformational transitions, particularly within the M-loop region. Microtubule-stabilizing agents such as taxanes bind to the taxoid pocket of β -tubulin and promote microtubule stabilization by locking the M-loop in an extended conformation, thereby preventing depolymerization. Docetaxel, a semi-synthetic analogue of paclitaxel, exhibits structural modifications including a tert-butyl carbamate group and hydroxyl substitution, which are known to influence binding interactions and pharmacological behavior. Despite its improved clinical performance, resistance remains a significant limitation, primarily arising from β -tubulin isotype variation and point mutations within the taxoid binding region. The β III-tubulin (TUBB3) isotype is associated with intrinsic resistance due to altered pocket geometry and increased flexibility. Additionally, mutations such as A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I introduce structural perturbations affecting ligand binding either directly (steric/electrostatic) or indirectly (allosteric and dynamic effects). This study evaluates the mutation-specific impact on docetaxel binding across wild-type, TUBB3, and mutant β -tubulin variants using a multi-target docking approach, emphasizing comparative changes in binding affinity.

MATERIALS AND METHODS

Docetaxel was docked against eleven β -tubulin targets, including wild-type, β III-tubulin (TUBB3), and nine mutant variants (A187T, A233T, A250V, D199N, F272V, R284N, R308C, S174A, and T276I), using the GIRL server multi-target docking platform. Ligand conformations were generated using ETKDGV3 followed by UFF energy minimization. Molecular docking was performed using the SMINA engine with an exhaustiveness parameter of 8, generating multiple binding poses within an energy range of 3 kcal/mol. Ensemble docking was employed to account for protein conformational variability, and the best docking score per target was selected. Docking scores (kcal/mol) were used as the primary metric to evaluate ligand–protein interactions and to compare the influence of structural mutations and isotype variation.

RESULTS AND DISCUSSION

1.1 Docking Score Variation Across Targets

The docking results for docetaxel (Page 1–2 of report) show the following trend:



Compared to paclitaxel, docetaxel exhibits overall **reduced binding affinity**, but demonstrates a **narrower variation across mutants**, indicating altered interaction dependence.

1.2 Effect of β III-Tubulin (TUBB3) Isotype : Docetaxel binding decreases from -8.73 kcal/mol (wild-type) to -6.68 kcal/mol in TUBB3. This reduction is more pronounced relative to paclitaxel, indicating that docetaxel is more sensitive to isotype-driven structural changes.

Mechanistically:

- TUBB3 introduces increased pocket flexibility
- Hydrophobic complementarity is reduced
- Induced-fit stabilization becomes energetically unfavorable

Thus, docetaxel experiences a higher **entropic penalty**, resulting in decreased binding affinity.

1.3 Mutation-Specific Effects on Docking

(i) Direct Pocket Disruption

- **A250V** (-6.45 kcal/mol): Steric hindrance at pocket floor leads to displacement of docetaxel, similar to paclitaxel but with slightly greater sensitivity due to altered side-chain accommodation.
- **F272V** (-6.48 kcal/mol): Loss of aromatic interaction weakens hydrophobic anchoring. These mutations produce consistently reduced docking scores, indicating compromised binding stability.

(ii) M-Loop Perturbations

- **T276I** (-6.43 kcal/mol): Shows one of the lowest binding affinities, indicating that docetaxel is highly sensitive to M-loop rigidity changes.
- **R284N** (-6.48 kcal/mol): Loss of electrostatic interactions destabilizes ligand positioning.

Compared to paclitaxel, docetaxel exhibits **less tolerance to M-loop perturbations**, suggesting greater reliance on local conformational flexibility.

(iii) Core Structural Mutations

- **A233T** (-6.50 kcal/mol): Induces pocket instability through internal structural rearrangement.

The effect is similar to paclitaxel; however, docetaxel shows slightly reduced binding, indicating weaker adaptability to fluctuating pocket geometry.

(iv) Allosteric Mutations

- **A187T** (-7.86 kcal/mol): Retains relatively strong docking affinity, indicating minimal direct disruption of the binding pocket.

S174A, D199N, R308C (~ -6.46 to -6.49 kcal/mol): Affect surface and inter-dimer interactions, indirectly reducing binding efficiency

These mutations highlight that **binding affinity may remain moderate while functional stabilization is compromised**.

1.1 Comparative Mechanistic Insight

A key observation is that docetaxel exhibits:



- Lower absolute binding affinity compared to paclitaxel
- Reduced variability across mutations
- Increased sensitivity to M-loop perturbations

This suggests that docetaxel relies less on strong hydrophobic anchoring and more on **distributed interactions**, making it:

- Less affected by single-point steric disruptions
- More affected by global conformational instability

1.2 Figures and Tables

Table 1. Docking score summary across β -tubulin variants

Mutation	Location	Docking Score (kcal/mol)
WT	Native	-8.73
TUBB3	Isotype	-6.68
A187T	Allosteric	-7.86
A233T	Core	-6.50
A250V	Pocket floor	-6.45
D199N	Surface	-6.46
F272V	M-loop	-6.48
R284N	M-loop	-6.48
R308C	Surface	-6.48
S174A	Interface	-6.49
T276I	M-loop	-6.43



Figure 1. Structural representation of β -tubulin showing taxoid binding pocket and mutation sites [Adapted From: doi: [10.1038/sj.onc.1206934](https://doi.org/10.1038/sj.onc.1206934)]

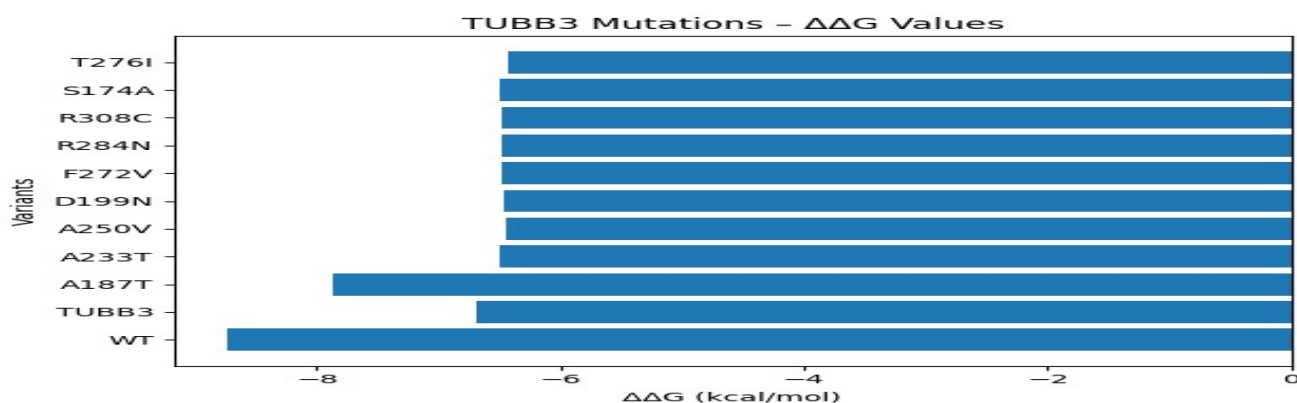


Figure 2. Comparative docking score distribution of docetaxel across wild-type, TUBB3, and mutant variants.



CONCLUSION

The present study demonstrates that docetaxel binding to β -tubulin is significantly influenced by both isotype variation and mutation-specific structural perturbations. Compared to paclitaxel, docetaxel exhibits lower overall binding affinity but shows a more uniform response across mutations, suggesting a distinct interaction profile. Mutations affecting the binding pocket (A250V, F272V) reduce affinity through steric and hydrophobic disruption, while M-loop mutations (T276I, R284N) significantly impair stabilization. Allosteric mutations (A187T) retain docking affinity but may compromise functional outcomes.

These findings indicate that docetaxel exhibits a different resistance interaction pattern compared to paclitaxel, emphasizing the importance of mutation-specific analysis in understanding taxane resistance and guiding future drug design strategies.

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Amorphous carbon nanotubes- copper ferrite hybrid: for enhanced electrochemical performance in neutral electrolyte

Supratim Maity^{1*}, Biplab K. Chatterjee¹, Kalyan K. Chattopadhyay¹

¹Thin Film & Nanoscience Laboratory, Department of Physics, Jadavpur University, Kolkata-32

*Corresponding Author's E-mail: msupratim@yahoo.co.in

INTRODUCTION

Efficient electrical energy storage devices are highly required for sustainable green energies. In this regards supercapacitors are electrochemical energy storage device with high power density. Supercapacitors have some advantages due to its fast charging-discharging rate, long cycling life, light weight, small size and safe operation. Supercapacitor can supply high electrical energy instantly which makes them potential candidates hybrid electric vehicles, aeronautics for regenerative braking and burst mode power delivery.

In this work we have synthesized copper ferrite decorated amorphous carbon nanotubes via simple solvothermal procedure in search of supercapacitor application in neutral solution.

MATERIALS AND METHODS

Copper ferrite (CuFe_2O_4) nanosphere attached amorphous carbon nanotube (aCNT) has been synthesized by simple solvothermal procedure in presence of aCNT at 200°C for 24 h [1]. Prior to the solvothermal procedure, aCNTs are synthesized by simple chemical reaction between ferrocene and ammonium chloride at 230°C in an air oven [2]. Structural and morphological characterization of as synthesized hybrid sample by X-ray diffraction (XRD) and field emission scanning tunneling microscopy (FESEM) study. XRD pattern [Fig. 1(a)] confirms the pure phase formation. Formation of CuFe_2O_4 spheres on the wall of the aCNT surface is clearly observed from the FESEM image [Fig. 1(b)]. The outer diameter of the aCNT is ~100-120 nm and the diameter of CuFe_2O_4 spheres is ~100 nm.

RESULTS AND DISCUSSION

Electrochemical performances of these nanostructures are measured in three electrode set up. 1M Na_2SO_4 is chosen as electrolyte. Comparative cyclic voltammogram of bare CuFe_2O_4 and CuFe_2O_4 -aCNT is shown in Fig. 1(c). From cyclic voltammetry (CV) graph, it is calculated that our CuFe_2O_4 -aCNT sample exhibits ~25.5 mF/cm^2 specific capacitance at 100 mV/S scan rate which is almost double than that of bare CuFe_2O_4 .





Fig. 1: (a) XRD pattern; (b) FESEM of CuFe₂O₄ -aCNT & (c) Comparative CV study of bare CuFe₂O₄ and composite system

CONCLUSION

In summary supercapacitor property of CuFe₂O₄ -aCNT is investigated in neutral solution. CuFe₂O₄ -aCNT hybrid is successfully fabricated with pure phase via a simple solvothermal procedure. As obtained results proclaim that this CuFe₂O₄-aCNT nanostructures may be a promising positive electrode for high performance electrochemical storage device in a low cost manner.

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Porosity-Driven Diffusion In Chitosan Microparticles: Structural Determinants of Drug Release Kinetics And Transport Efficiency

Souvik Sahoo and Debabrata Gosh Dastidar

Guru Nanak Institute of Pharmaceutical Science and Technology

157/F, Nilgunj Road, Panihati, Khardaha, West Bengal, 70114

*debabrata.goshdastidar@gnipst.ac.in

INTRODUCTION

Chitosan-based microparticulate systems are widely explored for controlled drug delivery due to their tenable structural properties and ability to modulate drug release kinetics. Among the various structural parameters, porosity has emerged as a critical yet under-theorized determinant of drug transport behavior. While conventional studies emphasize crosslinking density and particle size, increasing evidence suggests that internal pore architecture plays a dominant role in governing diffusion pathways and release kinetics. Drug release from chitosan systems is typically described as a combination of surface release, diffusion through the swollen matrix, and polymer erosion. However, these mechanisms are strongly influenced by the microstructure of the carrier, particularly pore size, connectivity, and distribution [1]. High porosity has been associated with enhanced drug mobility and accelerated release, whereas dense, low-porosity systems exhibit restricted diffusion and sustained release profiles. Despite this understanding, current literature largely treats porosity as a secondary structural feature rather than a primary design variable. Furthermore, conflicting observations—where increased porosity does not always correlate with faster release—indicate that the relationship between porosity and diffusion is non-linear and poorly understood.

This leads to a critical research question: Is drug release in chitosan microparticles governed by porosity alone, or by the complex interaction between pore structure, diffusion pathways, and polymer dynamics?

This review critically evaluates recent literature (2020–2025) to establish porosity as a key structural determinant of diffusion-controlled drug release, while identifying limitations in current mechanistic interpretations.

MATERIALS AND METHODS

This study was conducted as a systematic review using a PRISMA-based analytical framework to ensure transparency and reproducibility. A comprehensive literature search was performed across PubMed, Scopus, Web of Science, ScienceDirect, and Google Scholar using combinations of keywords such as “chitosan microparticles porosity drug release,” “porosity diffusion polymer drug delivery,” and “microstructure drug transport chitosan.” The search was restricted to peer-reviewed articles published in English between 2020 and 2025. Studies were selected based on predefined inclusion and exclusion criteria, where inclusion focused on research addressing porosity, microstructural characteristics, and drug release mechanisms in chitosan-based systems, while exclusion criteria eliminated unrelated delivery systems, incomplete data, and duplicate publications. Articles were systematically screened through title, abstract, and full-text evaluation. Relevant data were extracted, including porosity characteristics, fabrication methods, diffusion models, and release kinetics, and a critical analytical synthesis approach was applied to identify mechanistic patterns, inconsistencies, and existing research gaps.

RESULTS AND DISCUSSION

1.1 Role of Porosity in Drug Transport Mechanisms

Drug release from chitosan microparticles is governed by multiple mechanisms, including surface desorption, diffusion through the swollen matrix, and polymer erosion. Among these, diffusion through the porous network is a



dominant pathway, particularly in early and intermediate release phases

[1]. Porosity directly affects drug mobility, diffusion pathway length, and the rate of solvent penetration within the matrix. Highly porous systems allow faster drug transport due to interconnected pathways, while dense systems resist diffusion and lead to slower, sustained release. Studies also show that porosity not only increases drug movement but can change the overall transport mechanism [2].

1. Structural Complexity of Porous Networks

Porosity is not a single property but a combination of pore size, connectivity, tortuosity, and spatial variation, which together control drug transport. These factors affect how easily molecules move through the matrix. Even highly porous systems can show slow drug release if pores are poorly connected or highly tortuous. Studies also show that porous and non-porous microparticles made from the same material behave differently, proving that microstructure—not just composition—controls drug release [2].

2. Non-Linear Relationship Between Porosity and Release

A major limitation in current studies is the assumption that porosity and drug release have a simple linear relationship. In reality, this relationship is non-linear and depends on multiple factors. Higher porosity can increase diffusion, but it may also increase the length of diffusion pathways. Swelling or structural changes can block pores and reduce transport. Therefore, higher porosity does not always mean faster drug release.

3. Interaction Between Porosity and Swelling: Porosity cannot be considered independently of swelling behaviour, as hydration induces structural expansion in chitosan that dynamically alters pore geometry and connectivity. During this process, swelling may expand pores and enhance diffusion, collapse pore structures and restrict transport, or generate transient, dynamic pathways that lead to time-dependent release profiles. This interplay demonstrates that porosity is not a static attribute but an evolving property that changes throughout the release process; consequently, drug transport becomes inherently time-dependent, governed by continuous structural transformations within the polymer matrix.

Critical Gap: Lack of Predictive Microstructure–Diffusion Models Despite extensive research, no quantitative framework yet links porosity parameters—such as size, connectivity, and tortuosity—with diffusion coefficients and drug release kinetics. Most studies rely on empirical models without mechanistic integration, limiting the ability to design microparticles with predictable release profiles.

Table 1. Influence of Porosity Characteristics on Drug Release Behaviour

Porosity Parameter	Structural Effect	Impact on Drug Release
Pore size	Determines diffusion channel width	Larger pores → faster release
Pore connectivity	Controls pathway continuity	High connectivity → efficient transport
Tortuosity	Defines pathway complexity	High tortuosity → slower diffusion
Porosity (%)	Overall void fraction	Moderate porosity → optimal release
Structural stability	Resistance to collapse	Stable pores → consistent release

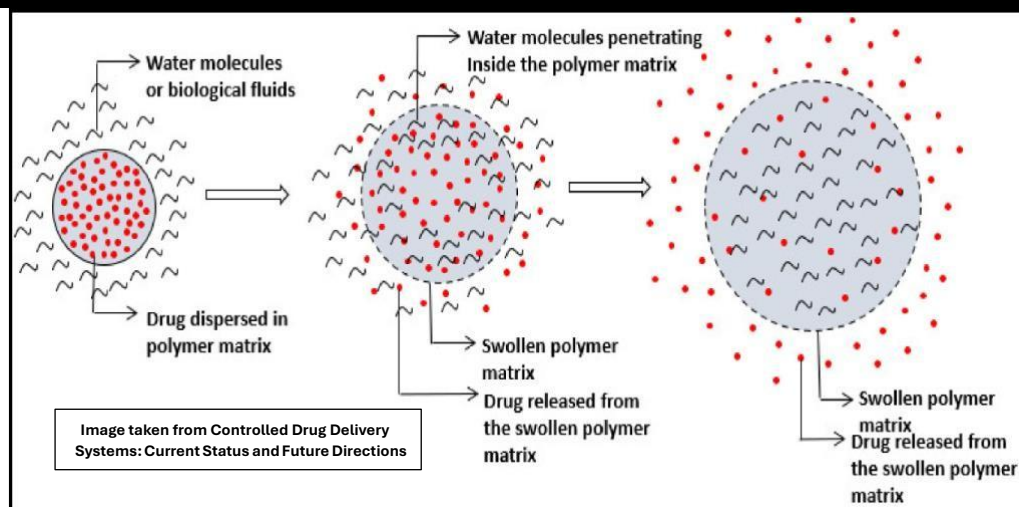


Figure 1: Porosity–Diffusion Interaction Model

2. CONCLUSION

This review shows that drug release in chitosan microparticles is mainly controlled by porosity-driven diffusion, where internal structure plays a key role. Porosity determines diffusion pathways and release rate, but release depends on overall structure, including pore connectivity and tortuosity. Swelling further changes pore structure over time, making drug transport dynamic. Therefore, the relationship between porosity and drug release is non-linear and depends on conditions. A major limitation is the lack of predictive models linking structure to release. Thus, porosity should be viewed as a dynamic property that must be carefully controlled to achieve predictable drug delivery.

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“Two- Dimensional Materials for Electrochemical Hydrogen Evolution Reaction(HER)”

Hanzalah Ejaz, Sudeshna Bhattacharjee, Alquama Ahmad, Anubrihi Banerjee, Sthiti Goswami, Subhanita patra
Department of Computer Science and Engineering, Dr. Sudhir Chandra Sur Institute of Technology and Sports
Complex, 540, Dum Dum, Surer Math, Kolkata – 700074.

E-mail: info.hanzalahejaz@gmail.com

ABSTRACT

This review evaluates the potential of 2D materials as inexpensive electrocatalysts for the Hydrogen Evolution Reaction (HER). It is based on the structure and electrochemical activity of such types of materials as transition metal dichalcogenides (TMDs), MXenes, and doped graphene. This review highlights the mechanisms involved in HER, including the Volmer-Heyrovsky mechanism and the Volmer-Tafel mechanism. It examines how phase engineering and edge site activation increase charge transfer efficiency, emphasizing the significance of 2D materials in achieving environmentally friendly hydrogen. Conclusion: Although 2D materials can be scaled up compared to precious metals, stability is still an issue.

INTRODUCTION

The global inclination towards sustainable energy sources has rendered green hydrogen a key energy carrier in the mission of attaining carbon neutrality. The electrochemical process of water splitting involves OER and HER, and serves as an effective method for generating hydrogen energy. Though Pt is currently regarded as the best performing HER catalyst due to its zero overpotential, the prohibitive cost and unavailability make it impractical to use on an industrial scale. This has led to interest in employing two-dimensional (2D) materials. TMDs, MXenes, and graphene-based hybrids are known to have a large surface to volume ratio, numerous edge sites, and controllable electronic configurations. This review discusses the reaction mechanism of HER and evaluates the activity of different 2D electrocatalysts.

Materials for HER

The primary materials discussed in this survey include:

- **Transition-Metal Dichalcogenides (TMDs):** Specifically Molybdenum Disulfide (MoS_2), which possesses a layered structure where metallic edge sites are highly active for hydrogen adsorption.
- **MXenes:** Two-dimensional transition metal carbides and nitrides (e.g., $\text{Ti}_3\text{C}_2\text{T}_x$) characterized by high metallic conductivity and hydrophilic surfaces.
- **Graphene-based Materials:** Doped graphene (e.g., N-doped or S-doped) and its hybrids with transition metals, which provide excellent electron transfer pathways and structural stability.

Methods and Working Principle

The reaction for HER in both acidic and basic media is known to take place via a process involving the



successive reduction of protons on the surface of the catalyst. The effectiveness of such reactions is measured in terms of the overpotential (η), which is defined as the additional voltage required above the theoretical value to initiate the reaction. There are two major routes for reaction to take place:

1. **Volmer Step (Adsorption):** A proton from the electrolyte is reduced and adsorbed onto an active site ($H^+ + e^- + * \rightarrow H^*$).
2. **Heyrovsky Step (Electrochemical Desorption):** An adsorbed hydrogen atom combines with another proton and electron to form H_2 ($H^* + H^+ + e^- \rightarrow H_2$).
3. **Tafel Step (Chemical Desorption):** Two adsorbed hydrogen atoms combine directly to form H_2 ($2H^* \rightarrow H_2$).

RESULTS AND DISCUSSION

Review of the existing literature suggests that the effectiveness of the catalytic performance of 2D materials is heavily dependent upon the density of active sites and the conductivity of the material. Whereas the pristine 2H-MoS₂ acts as a semiconductor, 1T metallization and doping with transition metals like nickel (Ni) and cobalt (Co) can reduce the overpotential substantially. However, MXenes exhibit fast electron transfer reactions due to their inherent metallic properties but are highly susceptible to surface chemistry ($-OH$, $-F$, $-O$).

The results suggest that while 2D materials currently require higher overpotentials than Pt, their low cost and durability make them viable for industrial-scale water electrolysis, especially when combined in heterostructures.

CONCLUSION

Two-dimensional materials represent a revolutionary category of electrocatalysts for the production of hydrogen energy. In view of methods including heteroatom doping, phase tuning, and nanoengineering, the catalytic efficiency of molybdenum disulfide and MXene can be dramatically improved to match the effectiveness of precious metals. Further study must focus on the stability of these compounds in an aggressive electrolyte to facilitate the shift from thermolysis to electrolysis of hydrogen.

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Optimization of Sodium Chlorite-Assisted Cellulose Extraction from Mercerized Bamboo Fiber

¹ Sayantan Mandol, ¹ Arijit Das, ² Ananya Barman, ² Tanmoy Dutta*, ² Jit Chakraborty, ² Trina Dutta

¹Department of Computer Science,

²Department of Chemistry

JIS College of Engineering, Kalyani, West Bengal, India

* To whom correspondence should be addressed: E-mail: *dutta.tanmoy88@gmail.com

ABSTRACT

Bamboo is a fast-growing renewable lignocellulosic material with strong potential as a sustainable source of cellulose for value-added applications. In this study, bamboo strips were first mercerized using 20% caustic solution to improve fiber accessibility and facilitate the removal of non-cellulosic components. The mercerized bamboo fibers were then subjected to cellulose extraction using sodium chlorite (NaClO_2) at different concentrations, namely 1.5%, 1.75%, 2.0%, and 2.25%, with the aim of identifying the most effective condition for obtaining cellulose-rich material with improved physicochemical properties. The extracted samples were characterized using dynamic light scattering (DLS), X-ray diffraction (XRD), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and scanning electron microscopy (SEM) to evaluate particle behavior, crystallinity, thermal stability, and surface morphology. The study was designed to standardize an efficient cellulose extraction condition from mercerized bamboo fiber and to obtain material with high microcrystalline cellulose content suitable for further industrial and research applications.

Keywords: Microcrystalline cellulose (MCC), Optimum concentration, NaClO_2 , thermal stability, crystallinity

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- Plant growth chamber, Water Bath, Laboratory chiller, N2 Container
- Water Distillation Apparatus, Conductivity meter, Viscometer
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- JASCO UV VIS spectrophotometer
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- JASCO FTIR
- JASCO RAMAN spectrometer
- JASCO Digital Polari meter

Brand:  Brookhaven
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- Particle Size Analyzer,
- Zeta Potential Analyzer,
- Molecular Weight Analyzer,
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- Static Light Scattering,
- Differential Refractometer,
- Sample Filtration System,
- Dielectric Constant Meter

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Brand: 

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