Centre for Functional Materials
VIT Vellore

40 YEARS OF TRANSFORMING LIVES

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# IC-FMFT 2025

# Book of Abstracts

INTERNATIONAL CONFERENCE ON FUNCTIONAL MATERIALS FOR FUTURE TECHNOLOGY
IC-FMFT 2025
VIT VELLORE
2025

## 2nd INTERNATIONAL CONFERENCE ON FUNCTIONAL MATERIALS FOR FUTURE TECHNOLOGY

05-07 NOVEMBER

VIT VELLORE, INDIA

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# IC-FMFT 2025
# ORGANIZING COMMITTEE

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**Dr. G Viswanathan**
Founder and Chancellor, VIT

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Vice President , VIT

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Director and Professor, CFM, VIT

**Dr. Palanisami N.**
Professor, CFM, VIT

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Professor, CFM, VIT

**Dr. Kaleemulla S.**
Professor, CFM, VIT

**Dr. Ramesh M Thamankar**
Professor, CFM, VIT

**Dr. Ankur Rastogi**
Assistant Professor, CFM, VIT

**Dr. Atul Thakre**
Assistant Professor, CFM, VIT

**Dr. Amlan Das**
Assistant Professor, CFM, VIT

# Preface

The future of technology depends on our ability to design new materials with specific, exceptional properties. To get there, we need a deep understanding of these materials from both a scientific and engineering standpoint. This is why fostering a continuous exchange of ideas between researchers in science, engineering, and industry is essential.

Keeping this in mind, the Centre for Functional Materials (CFM) at VIT Vellore is organizing on the ***"2nd International Conference on Functional Materials for Future Technology (IC-FMFT 2025)"*** **from November 05 to 07, 2025, at the Vellore Institute of Technology**. This is to help make this important connection. It is meant to be a platform to students, researchers, and professors to hear from and talk to recognized scientists from all around the world.

We are excited to host **distinguished speakers** from India and various other countries, all bringing a wide range of scientific expertise in materials and devices. They will be sharing their knowledge and experience through a series of talks, offering a fantastic chance for students and faculty to engage, build networks, and spark new collaborations across different disciplines. This conference is not just about listening, it is also about sharing. We are providing opportunities for students and researchers to showcase their own work through both poster and oral presentations. This book is a consolidation of **over 160 abstracts** from various themes like Functional Materials and Devices, Functional Polymeric Materials, Magnetic Materials and Spintronics, New Materials for Energy, Quantum Materials and Computation, Organic Electronics, and Optoelectronics.

This event has drawn sponsorship from various industries. The best presentations will be recognized with **awards from** the ***Royal Society of Chemistry***, the ***American Chemical Society***, and ***Wiley***. Furthermore, ***IOP Publishing*** will be recognizing the best female and male researchers.

Following the conference, the submitted manuscripts will undergo a due peer-review process, and accepted papers will be published in various reputed journals from Wiley Publications, such as *Small Methods, Particle & Particle Systems Characterization, ChemistrySelect,* and *Physica Status Solidi*, as well as in Springer's *Journal of Electronic Materials*.

# Messages

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**Dr. G. VISWANATHAN**
**Founder & Chancellor**
Former Member of Parliament
Former Minister, Govt. of Tamil Nadu
President, Education Promotion Society for India, New Delhi

## MESSAGE

I am extremely happy that you are participating in the second edition of the International Conference on Functional Materials for Future Technology (IC-FMFT 2025) organized by the Centre for Functional Materials (CFM), VIT University, Vellore during November 5-7, 2025. The scientific purpose of this conference is to bring the experts and the students from diverse fields of science and technology under one roof, thus creating the platform for sharing their research experiences and expertise.

I am sure that this conference will provide all our earnest and enthusiastic students an opportunity to interact with scientists and academics from different universities and institutes from India and abroad. The meeting will enable the participants to foster professional collaborations with universities across the world. Such events pave way for the flow of fresh ideas and inventions, ultimately contributing tremendously to our nation's prosperous developments in science and technology in the days to come.

I am glad that this conference serves as the next eye-opener for fruitful discussions among the experts and the students. We have invited professors of repute from different countries to this conference to share their knowledge with all of us. We have also invited experts from a number of leading national institutes, including IITs, CSIR labs, and DAE. There are several speakers attending this event, and I am quite confident that their speeches will make a whale of difference in the emerging fields and that the participants will benefit a lot.

I appreciate the organizers for providing students and researchers a good opportunity to showcase their works through posters and oral presentations. A devoted group of faculty members from the Centre for Functional Materials deserve appreciation for making the Conference grander with the help of generous sponsors.

I would like to thank all the speakers and the participants for their involvement. This book is a potpourri of the abstracts sent by the speakers and the participants.

I convey my best wishes to all of you, and I wish that the days that you spend here during the event would be productive and fruitful.

With best wishes,

**Dr. G. Viswanathan**
Founder & Chancellor

October 27, 2025

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**Mr. Sankar Viswanathan**
**Vice–President**

**MESSAGE**

It is my immense pleasure to invite all the distinguished speakers and all earnest participants from across the globe to the second edition of International Conference on Functional Materials for Future Technology (IC- FMFT 2025). The goal of this conference is to bring under one roof all scientists and industrialists by creating the platform for them to share and transform their experience and expertise with each other on scientific projects in the days to come.

Young researchers and students can showcase their research works during this event. I am confident that this conference will give all the participants an opportunity to meet specialists from a wide range of scientific and technological fields, thus paving way for innovations and upgradation of further skills and knowledge.

In this three- day scientific gathering, we have various sessions with invited speakers from all over the world sharing their professional perspectives, knowledge, and present their works. I encourage all the students, the researchers and all other participants to interact with the field experts and benefit a lot.

Active participation interwoven with involvement by the delegates and the students is highly appreciated.

Let's work together to convert our nation into an epicentre of science and technology.

With best wishes,

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**Dr. SEKAR VISWANATHAN, PhD**
**Vice President**


## MESSAGE

I am delighted that you will be taking part in the International Conference on Functional Materials for Future Technology (IC- FMFT 2025) organised by the Centre for Functional Materials (CFM), VIT Vellore. The conference is keen on giving students and young researchers a chance to meet and talk with scientists and professors from different universities and institutes of varied expertise in India and from other countries.

I am sure that the three-day conference will bring out the best in the students and scholars. You will also hear from some of the best scientists and technologists in different fields.

The Centre for Functional Materials (CFM) has highly skilled faculty members who are incharge of the conference. It would be an opportunity to the young researchers to explpre the expertise of CFM and make new acquitences that steer into a greater collaboration. I also want to congratulate everyone who gave an oral or poster presentation and everyone who could bag a price at the conference.

I hope that everyone will have three days of productive scientific conversation that will assist our society move forward in science and technology.

With all my best wishes,

Sekar Viswanathan

Vellore – 14
27th October 2025

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**Dr. Sandhya Pentareddy**
**Executive Director, VIT Vellore**

MESSAGE

Welcome to the International Conference on Functional Materials for Future Technology (IC-FMFT 2025). I am delighted that the Centre for Functional Materials (CFM) at VIT Vellore is hosting this event and excited to welcome all the delegates, participants, academicians, and students.

This conference will bring specialists and researchers together to share their knowledge, ideas, and new discoveries on a common platform. It is a valuable chance for students and young researchers to meet and talk directly with scientists and professors from India and other countries. It's also how we pass knowledge on to the next generation of scientists and engineers.

I am happy to share that that organizes have invited 40 renowned specialists. They will cover topics that are essential for future technology, including Functional Materials and Devices, Magnetic Materials and Spintronics, New Materials for Energy, Quantum Materials and Computation, and Organic Electronics.

Young researchers will also be showing their own work through oral/poster presentations and "best presentation" prizes from publishers like RSC, ACS, and Wiley are planned to encourage them to do even better in the future.

On behalf of the organizers and the CFM faculty, I express a warm welcome to all the delegates, speakers, and participants who accepted our invitation to come and make the conference a success. I hope everyone has three days of productive scientific endeavous that will shape a future ready society.

Best wishes.

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**Ms. Kadhambari S. Viswanathan**
**Assistant Vice-President, VIT Vellore**

## MESSAGE

I am delighted that the Centre for Functional Materials is organizing the second International Conference on Functional Materials for Future Technology (IC-FMFT 2025) at VIT, Vellore. I would like to extend a warm welcome to all the delegates, participants and students who are here for this conference.

This conference includes 40 invited talks from renowned scientists joining us from India and other countries. These lectures will cover the most essential themes for future technology such as Functional Materials and Devices, Magnetic Materials and Spintronics, New Materials for Energy, Quantum Materials and Computation, and Organic Electronics. These are some of the emerging topics that are not only intriguing from a basic science standpoint but are also indispenasble for the prosperity of future technology.

I wish all the particpants the best of luck and truly hope this conference gives you an opportunity to interact with the filed experts and benefit out of their exepreince and expertise.

On behalf of the organizers, I would like to thank all the delegates who accepted our invitation to be here and to make this conference a grand success. The conference provides the right platform for all the attendees to share their ideas and transform knowledge among academic institutions in the days to come.

Best wishes,

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**Dr. V. S. Kanchana Bhaaskaran**
**Vice Chancellor**

## Message

Science and engineering work together to make the world a better place. To have a developed society, we all need to know about the latest scientific and technical advances. In this way, science and technology conferences are quite helpful since they bring together specialists from different fields to talk and exchange their ideas and new things. They will also pass on their knowledge to the next generation of scientists and engineers by doing this. I am very happy that the Centre for Functional Materials (CFM) at VIT Vellore is organizing this conference here.

I welcome all the delegates who have accepted our invitation to be part of this conference. I like to thank all the speakers from India and other countries who will present talks on topics like Quantum Materials, New Energy Materials, Functional Materials and Devices, Optoelectronics, and Magnetism and Spintronics. I am sure that the participants will learn a lot from these lectures and be encouraged to pursue great things.

The young researchers will show their work during the conference via oral and poster presentations. The best oral and poster presentation prizes from RSC, ACS, and Wiley publications will encourage them to do even better in the future. I am glad that the organizers have made it possible for publications in a number of scientific journals.

On behalf of the faculty at the Centre for Functional Materials (CFM), I want to greet all the delegates who have accepted our invitation to come here and make the conference a great success.

28/10/25

**Dr. V.S. Kanchana Bhaaskaran**
Vice-Chancellor

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**PARTHA SHARATHI MALLICK, PhD.,**
**PRO-VICE CHANCELLOR**

## MESSAGE

I welcome you all to the 2nd International Conference on Functional Materials for Future Technology (IC-FMFT 2025) organised by Centre for Functional Materials, Vellore Institute of Technology, Vellore.

I thank all the speakers and participants from India and abroad for accepting our invitation. They will share their expertise in the conference in wide range of areas of functional materials. This conference will create an opportunity for students, research scholars and research professors to showcase their research outcome, ideas through posters and oral presentations.

I thank all sponsors and well-wishers who contributed significantly to this conference. In this conference, the participants will speak on Quantum Computation, Magnetic and Spintronics Devices, Optoelectronics Devices and Energy.

I am sure the conference will bring collaborations in these areas among the researchers of VIT and other organisations.

With best wishes,

Partha Sharathi Mallick

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Dr. T. Jayabarathi,
Registrar.

## MESSAGE

I am delighted that the Centre for Functional Materials is organising an International Conference on Functional Materials for Future Technology (IC-FMFT 2025) in VIT Vellore. I welcome all the delegates, participants, and students to this conference. There will be 40 invited talks at this conference, given by specialists from India and other nations. The most essential themes for future technology are covered in the invited lectures. Some are Functional Materials and Devices, Magnetic Materials and Spintronics, New Materials for Energy, Quantum Materials and Computation, and Organic Electronics. These topics are intriguing from a basic science point of view and also crucial for technology.

Well-known scientific journal publishers offer awards for research students in the form of best posters and oral presentations at the conference. I wish everyone who is taking part good luck and hope that this conference allows you to network and catalyse your research career.

I want to greet all the delegates who have accepted our offer to be here and make this conference a success on behalf of the organisers. I welcome the people from different institutes who will be attending this conference.

This conference is also a chance to share ideas and collaborate more effectively among institutes. I am confident that this conference will create an atmosphere where people can share their new ideas to improve the scientific community and society.

Best wishes,

T. Jayabarathi
Registrar

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Dr Madhuri W
Director, Centre for Functional Materials,

## MESSAGE

It is with great pleasure and pride that I welcome you to the 2nd edition of the International Conference on Functional Materials for Future Technology, conducted by the Centre for Functional Materials, VIT, Vellore. This conference stands as a testament to the growing global interest in the transformative potential of functional materials and their pivotal role in shaping the technologies of tomorrow.

The Book of Abstracts you hold in your hands is more than a compilation of research summaries—it reflects the vibrant intellectual energy and collaborative spirit that define our scientific community. From advanced nanomaterials and smart polymers to energy-harvesting systems and bioinspired materials, the contributions featured here represent the cutting-edge innovation and interdisciplinary exploration.

This year's conference brings together researchers, academicians, scientists from renowned national international research institution, and young scientists from across the country to exchange ideas, foster partnerships, and inspire new directions in functional materials. The diversity and depth of the abstracts submitted highlight not only the ingenuity of the contributors but also the urgency and relevance of their work in addressing global challenges—from sustainable energy and environmental stewardship to healthcare and next-generation electronics.

I extend my heartfelt gratitude to all the authors for their valuable contributions, to the reviewers for their meticulous evaluations, and to the organizing committee for their tireless efforts in bringing this event to fruition. Let this conference and its proceedings serve as a catalyst for continued discovery, dialogue, and development in the field of functional materials.

Wishing you all an engaging and fruitful conference experience.

Warm regards,

# Programme Schedule

**Day-1, November 05, 2025**

| **Time/Venue** | **Ambedkar Auditorium** | |
|---|---|---|
| 08:00 am – 09:30 am | **Registration** | |
| 10:00 am – 10:30 am | **Inauguration Session** | |
| 10:30 am – 11:00 am | Photo Session, Tree plantation followed by the High Tea | |
| **Session Chair** | **Dr. Madhuri W.** | |
| 11.00 am – 12.00 pm | **Plenary Lecture, Dr. Satoru Yoshimura** | |
| 12:00 pm – 01:00 pm | **Keynote by Dr. Parthiban Ramasamy, Eric Schmid Institute Austria** | |
| 01.15 pm – 02.15 pm | **Lunch Break** (@Foodys) | |
| | **Technical Sessions** | |
| **Session Chair** | **Dr. B. B. Lahiri** | **Dr. Akshay Singh** |
| | **Session-1 (VOC Gallery-1)** | **Session-2 (Ambedkar Auditorium)** |
| 02:30 pm – 03:00 pm | **Dr. K. Ramesha, CECRI, Kariakudi**<br>Battery Storage: Material Innovations and Challenges | **Dr. Ramakanta Naik, IOC Bhubaneswar**<br>Metal (Bi, La, Ni)-doped CdTe Nanomaterials for Optoelectronic and Photodetector Applications |
| 03:00 pm – 03:30 pm | **Dr. Jathish Kumar, IISER Tirupati**<br>Chiral Light Emitting Nanomaterials: From Fundamentals to Applications | **Dr. Sunil Singh Kushvaha, NPL Delhi**<br>Heterojunction of GaN and topological insulator $Bi_2Se_3$ for Optoelectronics devices |
| 03:30 pm – 04:00 pm | **Dr. Pratap Vishnoi, JNCASR, Bengaluru**<br>From Visible to Near Infrared: Emission Engineering in Lead-free Low-Dimensional Hybrid Metal Halide Perovskites | **Dr. B. B. Lahiri, IGCAR, Kalpakkam**<br>Magnetic fluid hyperthermia: recent insights from numerical modelling and future challenges |
| 04:00 pm - 04:15 pm | **Tea Break** | |
| **Session Chair** | **Dr. Sunil Singh Kushvaha** | **Dr. Ankur Rastogi** |
| **Time/Venue** | **Session-3 (VOC Gallery-1)** | **Session-4 (Ambedkar Auditorium)** |
| 04:15 pm – 04:45 pm | **Dr. Srinath, University of Hyderabad**<br>Spin-phonon coupling, magneto-caloric effect and critical phenomena in $Ga_{1-x}Al_xFeO_3$ orthoferrite | **Dr. François Courvoisier, University of Franche Comte, France**<br>Ultrafast laser-induced extrusion of nano-rods |
| 04:45 pm – 05:15 pm | **Dr. Kiran Kumar M, BARC, Mumbai**<br>High Temperature Oxidation of Zr Alloys and Development of Accident Tolerant Fuel Cladding Approaches | **Dr. R. Jayavel, Anna University**<br>Two Dimensional Functional Nanostructures for Sustainable Energy Storage Applications |
| 05:15pm – 05:45 pm | **Dr. P. D. Babu, BARC, Mumbai**<br>Incommensurate Magnetic Structure of $Ho_3Co$ and its magnetism under high pressure | **Dr. Aravinda Babu, DMRL** |
| 06:00 pm – 07:30 pm | **Cultural Event** (@Foodys) | |
| 07:30 pm onward | **Dinner** (@Foodys) | |

## Day-2, November 06, 2025

| | | |
|---|---|---|
| **Session Chair** | **Dr. S. Srinath** | **Dr. P. D. Babu** |
| **Time/Venue** | **Session-5 (VOC Gallery-1)** | **Session-6 (TT513)** |
| 09:00 am – 09:30 am | **Dr. Abdul Azeem, NIT Warangal**<br>A sustainable approach for developing supercapacitor electrodes from industrial waste for energy storage applications | **Dr. K. G. Suresh, IIT Bombay**<br>Recent studies on spintronic and topological aspects of certain Heusler alloys |
| 09:30 am – 10:00 am | **Dr. Narayanasamy Vijayan, NPL Delhi**<br>Melt-Grown Single Crystals: Growth Dynamics and Functional Properties for Optical and Thermoelectric Applications | **Dr. Ashis Kumar Panda, CSIR-National Metallurgical Laboratory**<br>Journey of Rapidly Quenched Magnetic Materials to Sensors for Industrial Applications |
| **Session Chair** | **Dr. Ezhil Vizhi R** | |
| 10.00 am – 11.00 am | **Keynote by Dr. M. S. R. Rao, IIT Madras (VOC Gallery-1)**<br>Diamond: The most versatile ultra wide bandgap quantum material for many technological applications | |
| | **Tea Break** | |
| 11:15 am – 12:45 pm | **Poster presentation at Foodys** | |
| 12.45 pm – 01.45 pm | **Lunch Break** (@Foodys) | |
| **Time/Venue** | **Session-7 (VOC Gallery-1)** | **Session-8 (VOC Gallery-2)** |
| **Session Chair** | **Dr. Manish Kumar Mishra** | **Dr. Parthiban Ramasamy** |
| 02:00 pm – 02:30 pm | **Dr. Shweta Agarwala, Ahmedabad University**<br>From Green Materials to Biodegradable Devices: Steps towards responsible innovation | **Dr. P. Savaranan, DMRL Hyderabad**<br>Permanent Magnetic Thin Films: Prospects for Micromagnetic Devices |
| 02:30 pm – 03:00 pm | **Dr. Akshay Singh, IISc Bengaluru**<br>Wafer-scale growth of 2D magnetic materials, and creating single photon emitters in 2D semiconductors | **Dr. Subramanian Venkatachalam, IIT Madras**<br>Magnetoelectric composites for multifunctional applications |
| 03:00 pm – 03:30 pm | **Dr. G. L. Samuel, IIT Madras**<br>Advanced Manufacturing Techniques for Surface Functionalization | **Dr. Binay Kumar, Delhi university**<br>Flexible Piezoelectric Nanogenerators for Green Energy Harvesting and Sensor Applications |
| 03:30 pm – 03:40 pm | **Tea Break** | |
| **Session Chair** | **Dr. Arivarasu M** | **Dr. Annamalai Senthil** |
| 03:40 pm – 05:40 pm | **Oral Presentation – 1 (VOC Gallery-1)** | **Oral Presentation – 2 (VOC Gallery-2)** |
| Session Chair | **Dr. Atul Thakre** | |
| 05:40 pm – 06:40 pm | **Industry interaction** (Jasco, Metrohm, JetSpin, Ant Ceramics) | |
| 07:30 pm onward | **Dinner** (@Foodys) | |

## Day-3, November 07, 2025

| **Time/Venue** | **Ambedkar Auditorium** | |
|---|---|---|
| **Session Chair** | **Dr. Ramesh M. Thamankar** | |
| 09:00 am – 10:00 am | **Keynote: Dr. R. Ramesh, Rice University, USA (Online)** | |
| **Session Chair** | **Dr. Palanisami N** | **Dr. Ramesh M. Thamankar** |
| **Time/Venue** | **Session -9 (VOC Gallery-1)** | **Session -10 (Ambedkar Auditorium)** |
| 10.00 am – 10.30 am | **Dr. Mahesh Peddigari, IIT Hyderabad**<br>Artificial relaxor ferroelectric behavior in aerosol deposited films: Emerging pathway for high energy density capacitors | **Dr. Bruno Peixoto de Oliveira, Universidade Federal do Cariri (UFCA), Brasil**<br>Biomass-based carbon dots: sensing and bioimaging applications |
| 10.30 am – 11.00 am | **Dr. Vanchiappan Aravindan, IISER Tirupati**<br>From Dead Li-ion Batteries to High Performance Na-ion Batteries via Solvent-co-Intercalation | **Dr. Neeraj Sharma, University of New South Wales, AU**<br>Understanding batteries & battery materials |
| | **Tea Break** | |
| 11:15 am – 11:45 pm | **Dr. K. Sethuraman, CUTN, TamilNadu**<br>Chemical Spray Pyrolysis – A Versatile Technique for Semiconductor Thin Film Preparation | **Dr. Rohini Dattatraya Kitture, Deputy Editor Small AND Physical Sciences Portfolio** |
| 11:45 am – 12:15 pm | **Dr. Manish Kumar Mishra, NCL Pune**<br>Engineering Motion in the Solid State: Dynamics of Smart Crystalline Materials | **Dr. K. Prabhakar, University of Pusan, South Korea**<br>Intrinsic Versus Extrinsic Electrocatalyst Activity in Water Splitting |
| 12:15 pm – 12:45 pm | **Dr. Abha Mishra, IISc, Bengaluru**<br>$MoS_2$-graphene interface for molecular sensing and switching | **Dr. Sayani Majumdar, Tampere University, Finland**<br>Capacitive In-Memory-Computing: A Device to Systems Level Perspective on the Future of AI Hardware |
| 12.45 pm – 01.45 pm | **Lunch Break** (@Foodys) | |
| **Session Chair** | **Dr. Kaleemulla S** | **Dr. Amlan Das** |
| **Time/Venue** | **Session -11 (VOC Gallery-1)** | **Session -12 (Ambedkar Auditorium)** |
| 02:00 pm – 02:30 pm | **Dr. Emila Panda, IIT Ghandhinagar** | **Dr. Sumeet Walia, RMIT, AU**<br>Ultra-thin materials for next-generation electronics and optoelectronics technologies |
| 02:30 pm – 03:20 pm | **Oral Presentation – 3 (VOC Gallery-1)** | **Oral Presentation – 4 (Ambedkar Auditorium)** |
| 03:50 pm – 04:30 pm | **Valedictory Function (Ambedkar Auditorium)** | |
| 04:30 pm – 05:00 pm | **High Tea** | |

**Day -2 Oral Presentation-1 VOC Gallery-1**

| Time | Abstract ID | Presenter | Title |
|---|---|---|---|
| 03:50 pm – 04:00 pm | OPT082401 | Prabhukrupa Chinmaya Kumar | $V_2O_9Te_2$ Nanorods Prepared via Microwave Method for Photodetection and NLO Applications |
| 04:00 pm – 04:10 pm | OPT100209 | Muthuvelan Venkatramani | Probing the relaxation pathways of Yellow and Narrow Red Emitting Carbon Dots by Femtosecond Transient Absorption Spectroscopy |
| 04:10 pm – 04:20 pm | OPT102103 | Tamanna Jindal | Spectral Response of Different Fluorescent Colors under UV Excitation |
| 04:20 pm – 04:30 pm | FMD100801 | Anuradha Bharat Bansode | Fabrication and Characterization of $Fe_3O_4$ Dispersed PEDOT:PSS Field Effect Transistor |
| 04:30 pm – 04:40 pm | FMD101504 | Girish Chandrashekar | Quantum Conductance in $MoO_3/TiO_2$ Heterojunction Memristors: Crafting Controlled Analog-to-Digital Transition for Multilevel Memory Applications |
| 04:40 pm – 04:50 pm | MMS100104 | Inchara M | Enhancement of the Magnetoimpedance ratio of $Co_{77}S_{i5}Cu_1Nb_2B_{15}$ ribbons with the Permalloy coating |
| 04:50 pm – 05:00 pm | MMS100303 | Dr Suganya Velliyan | Microwave-assisted polyol synthesis of porous $Fe_3O_4$ nanoparticles with tuneable size and enhanced magnetization |
| 05:00 pm – 05:10 pm | MMS101601 | Mallikarjun R | Fabrication and Characterization of Benzaldehyde Molecular Schottky Junction with Magnetic Electrode |
| 05:10 pm – 05:20 pm | NME100211 | Mudda Deepak | Nanostructured $Li_4Ti_5O_{12}$–$TiO_2$ Dual-Phase Electrodes Synthesized via Sol–Gel Method for Enhanced energy storage applications |
| 05:20 pm – 05:30 pm | OEL101102 | Meenu Maria Sunny | Bio-Derived Neuromorphic Device using Aloe vera for Energy-Efficient Computing Exhibiting Activity Dependent Synaptic Plasticity |
| 05:30 pm – 05:40 pm | OEL101503 | Vishwas Dahyabhai Patel | Optoelectronic simulation and optimization of all perovskite tandem solar cells employing electrodeposited copper oxide as hole transport layer |

**Day -2 Oral Presentation-2 VOC Gallery-2**

| Time | Abstract ID | Presenter | Title |
|---|---|---|---|
| 03:50 pm – 04:00 pm | FMD101002 | Dr. Sivagami K | Plastic waste-derived activated porous carbon through thermochemical conversion: A circular pathway towards sustainable carbon black feedstock |
| 04:00 pm – 04:10 pm | FPM100302 | Dr. Sreekanth M S | Multifunctional Polyvinyl Alcohol based Nanocomposites for water induced Shape Memory and Flexible Electronics |
| 04:10 pm – 04:20 pm | FPM091702 | Dr. Barnali Dasgupta Ghosh | PVDF Composites: An Excellent Piezoelectric Energy Harvesting and Storage Material for Wearable Devices |
| 04:20 pm – 04:30 pm | FPM092502 | Dr. Amilan Jose Devadoss | Ruthenium Nitrosyl Complexes based functional soft nanomaterials for Cancer Therapy |
| 04:30 pm – 04:40 pm | FPM100101 | Dr. Parvez Alam | SH-Wave Propagation in a Functionally Graded piezoelectric Plate Clamped Between a Temperature-Dependent Layer and a Microstructurally Coupled Substrate |
| 04:40 pm – 04:50 pm | FPM100208 | Dr. Sumangala T. P. | Layer-by-layer deposition of polyurethane/reduced Graphene Oxide/PANI composites for electromagnetic interference shielding application |
| 04:50 pm – 05:00 pm | NME100301 | Dr. Uma Sathyakam P | Electrochemical Simulation of SnSe coated Porous Nickel Electrodes for Supercapacitors |
| 05:00 pm – 05:10 pm | NME101704 | Dr. R. Vidya | Microbial fuel cell from Coconut water |
| 05:10 pm – 05:20 pm | MMS100102 | Dr. Ketaki C Patankar | Investigations of magnetic properties of Holmium-doped cobalt–zinc ferrite |
| 05:20 pm – 05:30 pm | MMS070803 | Dr. Ravi Chinnappan | Engineering Ferromagnetism in Wide Band Gap w-AlN for Spintronic Applications: Insights from DFT Calculations |

**Day -3 Oral Presentation-3, VOC Gallery-1**

| Time | Abstract ID | Presenter | Title |
|---|---|---|---|
| 02:30 pm – 02:40 pm | OPT100902 | Shyam Krishnan N | Role of Topology in Nanopillars and Its Effects on Performance on CdS/CdTe Solar Cells |
| 02:40 pm – 02:50 pm | OPT101603 | Ravindra Kumar Nitharwal | Oxygen defect-induced polarons and electron-phonon interactions in $MoO_{3-x}$ nanostructures |
| 02:50 pm – 03:00 pm | OPT101607 | Bhargav Midathani | Systematic Tuning of Optoelectronic Properties in Lead-Free Metal Halide Materials for Solar-Blind Ultraviolet Photodetectors |
| 03:00 pm – 03:10 pm | FMD102904 | Dr. Avanish Babu T | Hybrid Microwave Sintered Multifunctional Multiferroics as Energy Harvester and Flexible Screen Printed Absorption Dominant Energy Shields: ML Driven Composition Prediction |
| 03:10 pm – 03:20 pm | FMD102903 | Dr. Vaishnavi Khade | Fabrication and Comparison of Flexible Electromagnetic Interference Shields with Simulation and Experimentation: Screen Printed Bulk Metallic Glass Verses Nanocrystalline Ferrite for Electromagnetic Interference Shielding |
| 03:20 pm – 03:30 pm | NME102006 | Dr. Amiruddin R | Development of Direct Current (DC) Biomechanical Energy Harvesters Using p-Zno:N Nanowires / Organic Polymer Bilayers |

**Day -3 Oral Presentation-4, Ambedkar Auditorium**

| Time | Abstract ID | Presenter | Title |
|---|---|---|---|
| 02:30 pm – 02:40 pm | NME102001 | Dr. Samir Ranjan Meher | First principles investigation of doping induced band gap engineering in $BaZrS_3$ perovskites for solar cell applications |
| 02:40 pm – 02:50 pm | NME102005 | Dr. Vasu Kuraganti | Doped $WS_2$ and $MoS_2$ semiconductors as ferromagnetic spin catalysts for overall water splitting |
| 02:50 pm – 03:00 pm | NME102008 | Dr. Paskalis Sahaya Murphin Kumar | Cadmium Sulfide Nanourchins Constructed with g-$C_3N4$ for Millimolar Photocatalytic $H_2O_2$ Production within a Few Minutes. |
| 03:00 pm – 03:10 pm | OPT100214 | Dr. T. Prakash | Numerical Simulation on UV Light Intensity Dependent Complex Impedance Spectroscopy of $SnO_2$ using SCAPD 1D |
| 03:10 pm – 03:20 pm | FMD102905 | Dr. N. Varalaxmi | Impedance spectroscopic studies of the electric conduction in polycrystalline in Ferrites materials |

**Day -2 Poster Presentation Schedule**
**11:15 am - 12:45 pm**
**Venue Foodys**

| S.No. | Abstract ID | Presenter | Title |
|---|---|---|---|
| 1 | FMD080701 | Sathyajith Sathyanesan | Investigation of the influence of coating cycles and dipping time on ZnS thin films deposited by the SILAR method using an in house developed Arduino Uno-based low-cost coating machine. |
| 2 | FMD082101 | Kajol Sahoo | Double-encapsulated red-emitting formamidinium lead halide perovskite nanocrystals for fluorescent sensing and lighting applications |
| 3 | FMD092201 | Dr Ketaki Ketan Patankar | Memristor for next-generation surveillance system: A Review |
| 4 | FMD100106 | Gomathipavithra R | Exploring the structural and electrical properties of $Bi^{3+}$ modified $AgNbO_3$ Lead-free Ceramics |
| 5 | FMD100107 | Esakkiappan Natarajan | Structural and magnetoelectric coupling in $Sc^{3+}$, $Sm^{3+}$ co-substituted BFO BTO ceramics |
| 6 | FMD100202 | Govindaraji D | Structural and Electrical properties of metal ions doped $NaNbO_3$ lead free ceramics |
| 7 | FMD100206 | Gokul Das | Mechanochemical Synthesis of Complex Ceramic Oxides: A Sustainable Route to High-Performance Functional Materials |
| 8 | FMD100216 | Nikunj Dharmendrabhai Pandya | Growth and Complex Impedance Studies of Ni Mixed Co Levo Tartrate Crystals |
| 9 | FMD100217 | Delli Babu P | In-situ Chemically Reduced Graphene Oxide and PANI for Resistive Gas Sensing: Toward FET-Based Sensor Platforms |
| 10 | FMD100502 | Amal Banerjee | Numerical Estimation of Aluminum Gallium Nitride – Gallium Nitride Interface Two\|Three Dimensional Electron\|Hole Gas(2DEG\|3DEG, 2DHG\|3DHG) Properties |
| 11 | FMD100601 | Yazhini D | CdSe-Doped Bimetallic ZIF-67-Derived Electrode Materials for High-Performance Supercapacitor |
| 12 | FMD101001 | Mubeena Shaik | Flexible Electrospun PVDF/BCZT Nanofiber Composite for Efficient Piezoelectric Energy Harvesting |
| 13 | FMD101404 | Sarala Shanthi Shanthi.J | Impact of Electron Irradiation on the Capacitance and Frequency Response of GaN MOSFETs at Elevated Temperatures |
| 14 | FMD101505 | Bhaskaraiah M | Impact of antimony substitution on the structural and functional properties of $CuFeS_2$ nanoparticles synthesized by a hydrothermal route |
| 15 | FMD101602 | Jenish Mugilan | Fabrication and Study of PVA–PEG Blend Nanocomposite Solid Polymer Electrolytes Incorporating ZnO Nanofillers |
| 16 | FMD101605 | Sahana C S | Room temperature photoinduced resistance response of LPCMO thin films |
| 17 | FMD101702 | Navya Kukreja | Optimization of $CsPbBr_3$ perovskite nanocrystals featuring enhanced stability and optical efficiency |
| 18 | FMD101706 | Ashly Sunny | Emulating Ebbinghaus forgetting curve via characterization of excitatory synaptic transmission in a ZnO-based optoelectronic synapse with ultra-low power consumption |
| 19 | FMD101801 | Gangadhar Mahar | Agro-industry waste derived akermanite a photo catalyst for industrial wastewater purification |
| 20 | FMD101901 | Hajira S | Tuning ZIF-8 with Different Electrolyte Concentrations for Enhanced Supercapacitor Performance at Multiple Potential Windows |
| 21 | FMD101903 | Gopika Lal | Investigation of Structural and Optical Properties of Unique MOF-5 Synthesized via Facile Chemical Precipitation Method |

**Day -2 Poster Presentation Schedule**
**11:15 am - 12:45 pm**
**Venue Foodys**

| S.No. | Abstract ID | Presenter | Title |
|---|---|---|---|
| 22 | FMD101905 | Padma Uthirapandi | Metal Oxide Based Ferroelectric Random Access Memory (FeRAM) for Neuromorphic Computing Applications |
| 23 | FMD101906 | Yokesh S | Synthesis and Characterization of Semi Organic Single Crystal DL-Malic Acid Strontium Nitrate (DLMSN) |
| 24 | FMD102002 | Agesthian Suresh K | Self-rectifying second-order memristive behavior in PLD deposited tungsten oxide thin films |
| 25 | FMD102007 | Debadrita Dasgupta | Tunable polyaniline–polyvinyl pyrrolidone composite for flexible and biodegradable acetone vapor sensing application |
| 26 | FMD102009 | Allam Vasundhara | Enhanced Crystallization behavior in GaSb/$Sb_2Te_3$ Heterojunction Phase Change Materials |
| 27 | FMD102010 | Sreekar Sagar U S | Vanadium Oxide Thin Films for Neuromorphic Memory and Computing Applications |
| 28 | FMD102016 | Sanjay Paul C | Effect of Titanium doping on the physical properties of Nickel Oxide thin films for Electrochromic smart windows applications |
| 29 | FMD102017 | Vilya K | Tuning blue hue of $V_2O_5$/$MoO_3$/$V_2O_5$ electrochromic trilayer film prepared by thermal evaporation |
| 30 | FMD102203 | Dr. Thenmozhi Kathavarayan | $Co_3O_4$/$Ti_3C_2T_x$ MXene composite as catalase mimetic nanozyme towards selective electrochemical detection of $H_2O_2$ |
| 31 | FMD102301 | Sruthi Vadakke Purakkal | Atomically dispersed iron catalyst-based catalase nanozyme for distinctive determination of hydrogen peroxide |
| 32 | FMD102403 | Ankita Manjunath Joshi | Enhancing GaN HEMT Performance through AlGaN Barrier Thickness and Aluminum Composition Engineering |
| 33 | FMD102501 | Amala Sweety V | Ferrocene-Anisole-appended centrosymmetric push-pull Barbiturate and Thiobarbiturate dyes for Non-Linear Optics |
| 34 | FMD102502 | Rajesh Kumar Sekar | Ferrocenecarboxylates and Nitro Phenanthroline-Based Monomeric and dimeric Zn (II) and Cd (II) Complexes: Structural, Electrochemical, Luminescence and Nonlinear Optical Properties |
| 35 | FMD102503 | Satishkumar G | The effect of aluminium doping in magnetite spinel on the catalytic wet peroxide oxidation of antibiotics in batch and continuous reactors |
| 36 | FMD102601 | Venkatesh M | Effect of Ni-doping on $SnO_2$ Nanoparticles for the Scrutinization of Physico-Chemical Properties for Gas Sensing Applications |
| 37 | FMD102602 | Mariammal V | Biosensing Structure-Based Design of Metal–Carbamate Complexes as Cholinesterase Inhibitors for Alzheimer's Disease |
| 38 | FMD102701 | P. Poongothai | Environmentally Friendly Hydrometallurgical Approach for Sequential Precipitation of Critical Metals from Spent LIBs |
| 39 | FMD102702 | Shakina J Selva | Understanding the Impact of Activation Methods on Biomass-Based Hard Carbon Anodes in Sodium-Ion Batteries |
| 40 | FMD102901 | A. Priyadharshini | Synthesis, Growth and Characterizations of third order NLO single crystal :2- Amino-5-chloropyridinium 4–hydroxybenzoate (ACH) |
| 41 | FMD102902 | C. Pavithra | Synthesis and Characterization of Barium Nickel Titanium Oxide by Sol-gel Method |
| 42 | FMD102903 | Dr. Vaishnavi Khade | Fabrication and Comparison of Flexible Electromagnetic Interference Shields with Simulation and Experimentation: Screen Printed Bulk Metallic Glass Verses Nanocrystalline Ferrite for Electromagnetic Interference Shielding |
| 43 | FMD102906 | Dr. D. Zarena | Expression, purification and biophysical Characterization of the Conopeptide Mo1692 from Conus monile |

**Day -2 Poster Presentation Schedule**
**11:15 am - 12:45 pm**
**Venue Foodys**

| S.No. | Abstract ID | Presenter | Title |
|---|---|---|---|
| 44 | FMD291007 | Deepa John | Photophysical Properties of Aurone Derivatives: Solid-State Fluorescence and Solvatochromic Effects |
| 45 | FMD291008 | A. Divya | Synthesis and Characterisation $Zn_{1-x}Fe_xTiO_3$ (x=0.2,0.4,0.6,0.8) by Sol Gel Method Energy Storage Application |
| 46 | FPM080702 | Vijayakumar Krishnan | 2D FEM-based study on the performance of XLPE insulation material in Submarine power cable systems |
| 47 | FPM092202 | Dhanush P C | Ionic Transport and Structural Analysis of Zinc Chloride doped í-Carrageenan Solid Polymer Electrolytes for Energy Storage Devices |
| 48 | FPM092501 | Vishnu C V | Hybrid approach to enhancing PMMA radiation shielding using $WO_3$ and BaO modifiers. |
| 49 | FPM093001 | Dr. Sathyaraj Weslen Vedakumari | Quercetin-loaded chitosan microneedle patches for efficient wound management – Preparation, characterization, and in vivo evaluation |
| 50 | FPM100103 | Sameera Shabnum S | CuFeZnO Trimetallic Nanoparticles decorated on Reduced Graphene Oxide: A Multifaceted Nanocomposite for Sustainable Environmental and Healthcare Applications |
| 51 | FPM100215 | Kapileshwar Srikanth | Performance Analysis and Comparative Study of Additively Manufactured Scintillators with BC408 for Cosmic Ray Detection |
| 52 | FPM100701 | Divyarajashree B | New Palladium-Loaded Functionalized Polyurethane Foams and Their Applications in Catalytic C-C Coupling Reactions |
| 53 | FPM101604 | Sandhiya Ezhumalai | Sodium Ion Conducting Biopolymer Electrolyte from Eucalyptus Gum and Chitosan Blended Polymer Electrolyte for Solid State Energy Device |
| 54 | FPM101902 | Rohan Rajendra Gharad | Self-Assembled NDI Amphiphiles as Esterase Mimics in Aqueous Media |
| 55 | FPM102703 | Pauline Ida. P | Investigations on plasticized Solid Biopolymer Electrolytes developed for sustainable Na-ion Capacitor |
| 56 | MMS101101 | Shridhar N Mathad | Green synthesis of Mg-Zn Nanoferrites using Lemon extract; Modification in dielectric and magnetic properties by Co-substitution |
| 57 | MMS101403 | Subashini A | One-Pot Hydrothermal Synthesis and Characterization of Silver Nanoferrites ($AgFe_2O_4$) |
| 58 | MMS101501 | Harekrushna Behera | Tailoring Mn Substitution in $SmCo_5$ for Enhanced $(BH)_{max}$ Using Mechanical Milling |
| 59 | MMS101502 | Gnanavel Selvanantham | Electronic, Magnetic and Spin Orbit Coupling Properties of Antisite Defect Induced Monolayer 2H-$MoS_2$ for Spintronics Applications |
| 60 | MMS101701 | Anjana Vinod | Structural, Microstructural, and Magnetic Properties of Melt Spun Ribbons of $LaFe_{13-x}Si_x$ Alloys |
| 61 | MMS101703 | Arya Rose Thomas | Microwave-Assisted Synthesis of Cobalt Ferrite: A Fast and Efficient Route to Tailor Magnetic and Dielectric Properties |
| 62 | MMS101802 | M. Hariharan Nil Nil | Studies on the influence of neodymium-doped strontium hexaferrite/cobalt-zinc ferrite nanocomposites for microwave absorption properties in the X-band region. |
| 63 | MMS102014 | Aiswarya R Prasad | Structural and Magnetocaloric Investigation of $L_{21}$-Ordered $Co_2MnAl$ Exhibiting Griffiths Singularity |
| 64 | MMS102015 | Sreelakshmi E | Griffiths Singularities and Long-Range Ferromagnetic Ordering in Half-Heusler CoMnAl Alloy |
| 65 | NME081501 | Banaja Dandasena | Hydrothermally synthesized Cobalt-doped $VS_2$ for Supercapacitor application |

**Day -2 Poster Presentation Schedule**
**11:15 am - 12:45 pm**
**Venue Foodys**

| S.No. | Abstract ID | Presenter | Title |
|---|---|---|---|
| 66 | NME092901 | Mohamed Sufiyan K T | Hybridizing NiFe-LDH and MXene nanosheets for high performance energy storage application |
| 67 | NME092902 | Swathi Muraleedharan | Unravelling the effect of addition of inorganic electroactive additives to Triazolium Ionic Liquid- making them into Ternary and Quaternary ions electrolytes for EDLC applications |
| 68 | NME100105 | Vannala Guruprasad | Hydrothermal synthesis of $CoMn_2O_4$ Nanostructers as Efficient Electrode Materials for Next-Generation Supercapacitors |
| 69 | NME100201 | Pratheeksha D | Exploring the amino acid–ionic liquid systems through Machine Learning Approaches |
| 70 | NME100207 | Reema Sagitha Sikkandar | Hydrogen Storage Capacity of $BaCdH_3$ Perovskite Hydride: Theoretical Analysis |
| 71 | NME100210 | Varsha K | Influence of protonation states on the excited state dynamics of chlorophyll a |
| 72 | NME100213 | Suguna P | Synthesis of 211 MAX phases by a probe sonication approach |
| 73 | NME100501 | Abhishek Kumar Singh | Fabrication of an exfoliated h-BN-$Bi_2S_3$ hybrid supercapacitor device for superior electrochemical performance |
| 74 | NME100504 | Nagendra K | Electrical properties of sodium ion conducting boro tellurite glasses: Materials for battery applications |
| 75 | NME101705 | Dr. Senthilkumar Sellappan | Electrochemical Synthesis of $WSe_2$ Featuring Abundant Selenium Vacancies towards Efficient Electrocatalytic Hydrogen Evolution |
| 76 | NME101904 | P S Vignesh Pillai | Formability-Microstructure-Performance Linkages in Lightweight Alloys for Energy-Efficient Transportation: A Materials-Centric Review of Hydroforming as a Validation Platform |
| 77 | NME102003 | Hema Palani | Impact of Electrolyte Concentration on Electrochemical Performance of Lanthanum Ferrite ($LaFeO_3$) Perovskites for Aqueous Based Supercapacitors |
| 78 | NME102004 | Ibhanan Saini | Sustainable Intelligence:A survey on ultra low powered embedded systems and their enabling technologies |
| 79 | NME102006 | Amiruddin R | Development of Direct Current (DC) Biomechanical Energy Harvesters Using p-Zno:N Nanowires / Organic Polymer Bilayers |
| 80 | NME102012 | Arul Britto Kavin | Efficiency enhancement of Chalcogenide based Thin Film Solar Cells |
| 81 | NME102102 | Hari Prasath S | An Extensive Investigation on the Structural, Morphological, Dielectric and Ferroelectric Properties of Nd Doped $BiFeO_3$-$BaTiO_3$ Solid Solutions |
| 82 | NME102201 | Basil Chacko | Effect of $ZnSO_4$ and $Zn(CF_3SO_3)_2$ on dendrite formation in Aqueous Zinc Ion Batteries |
| 83 | NME102303 | Usha Ramani M | Sustainable and Low-Cost Catalytic Conversion of Carbon Dioxide and Hydrogen into formic acid Using a Copper Complex as a Green Catalyst |
| 84 | NME102401 | Dr Edinsha Gladis E H | Greener synthesis of water-soluble nanosized copper(II) complex with 1,10-Phenanthroline derivatives as catalyst for the production of hydrogen |
| 85 | OEL100503 | Ravi C | Photophysical, Solvatochromic, and Electronic Structure Studies of fluorescent Azo-Anthracene dye for dye-sensitised solar cell Applications |
| 86 | OEL101301 | Sreelakshmi B | Natural Dye based memristor and Ion Incorporation: Towards Sustainable Neuromorphic Devices |

**Day -2 Poster Presentation Schedule**
**11:15 am - 12:45 pm**
**Venue Foodys**

| S.No. | Abstract ID | Presenter | Title |
|---|---|---|---|
| 87 | OPT091701 | Swikruti Supriya | Controlled hydrothermal synthesis of La-doped CdTe nanomaterial for enhanced optoelectronic applications |
| 88 | OPT100203 | Mohammed Khimani | Dielectric, Impedance, Modulus Spectroscopy Studies of KDP – $K_2SO_4$ Composite Crystal System |
| 89 | OPT100205 | Nithish Sriram K | First principles study of electronic structure and optical response of $Cu_2O$: Effects of group-III doping and Cu vacancy – DFT+U study |
| 90 | OPT100212 | M. Dhanush | Temperature Dependent Complex Impedance Spectroscopy of $SnO_2$ using SCAPS 1D |
| 91 | OPT101001 | Vithaldas Vallabhdas Raja | Visible blue and NIR emission in Nd3+ singly doped $CaZrO_3$ perovskite |
| 92 | OPT101003 | Giri Ram N | Studies on excitonic absorption and polarization property of perovskite 2-D nanoplatelets with varying thicknesses |
| 93 | OPT101401 | Mohammedasif R | V-Shaped Nano Groove Design for Enhanced Efficiency in CdS/CdTe Nanowall Solar Cells |
| 94 | OPT101603 | Ravindra Kumar Nitharwal | Oxygen defect-induced polarons and electron-phonon interactions in $MoO_{3-x}$ nanostructures |
| 95 | OPT101606 | Sarojini N | Polyaniline Incorporation as a Strategy to Suppress Surface and Grain Boundary Defects in $MAPbI_3$ Perovskite Thin Films |
| 96 | OPT102101 | Siva Venkata Pranietaa Ratna Jonnadula | Thermodynamic Stability and Phase Transition Map of Mixed-Anion Chalcogenide-Halide Perovskites via DFT Simulation |
| 97 | OPT102402 | Dr K Nagashri | Development of Novel 1,10-Phenanthroline-Based Ligands and Metal Complexes for High-Performance Organic Light Emitting Diode |
| 98 | QMC101402 | Paul Monson | The stability of micro-mechanically exfoliated 2D layered magnetic material Chromium Chloride |
| 99 | QMC102202 | Geethapriyanga D | Computational, Spectroscopic and Docking Investigation of 5-(2-Methoxy-Phenylamino)-3-Phenyl-Thiazolidine-2,4-Dione by employing DFT Methods – Anti-diabetic agent |
| 100 | QMC102302 | Dr. Joseph J | Greener, sustainable and affordable bio integrated Quantum sensor enabled by seaweed for climate monitoring device with dual carbon dioxide capture and sensing capabilities |

# Themes

1. Functional Materials and Devices
2. Functional Polymeric Materials
3. Magnetic Materials and Spintronics
4. New Materials for Energy
5. Organic Electronics
6. Optoelectronics
7. Quantum Materials and Computation

# Contents

# ABSTRACTS

# Plenary Lecture

# Development of ferromagnetic and ferroelectric thin films with excellent magnetic properties and their application to newly proposed high-performance magnetic devices

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## Abstract

Magnetization reversal method using an electric field is a future technology for high performance magnetic devices with lower power consumption. Ferromagnetic and ferroelectricity (multiferroic) materials with magneto-electric effect have been receiving greater attention for this method. The doped $BiFeO_3$ (pure $BiFeO_3$ is typical material with antiferromagnetic and ferroelectricity) were reported as multiferroic material with clear ferromagnetic and dielectric hysteresis in room temperature. Although the excellent magnetic properties such as high saturation magnetization, perpendicular magnetic anisotropy, and high Curie temperature are needed to realize the high performance magnetic devices, the magnetic properties of previous $BiFeO_3$-based thin films are not sufficient for application to the magnetic devices. To realize excellent magnetic properties, pulsed DC reactive sputtering method and various substitution elements were investigated in this study. As the results, the new multiferroic thin films with high saturation magnetization, perpendicular magnetic anisotropy, high Curie temperature, and function of magnetization reversal by applying electric field was obtained. By using these multiferroic thin films, we are proposing new "magnetization transfer by electric field application" type magnetic memory with very high capacity and low power consumption (figure1), and new "MOKE amplification by magnetization transfer with electric field application" type display device for 3D with high brightness and low power consumption (figure2), and also we are demonstrating the device operation.

**Keywords:** Multiferroic thin films, Magnetization reversal, Magnetization transfer, Magnetic Devices

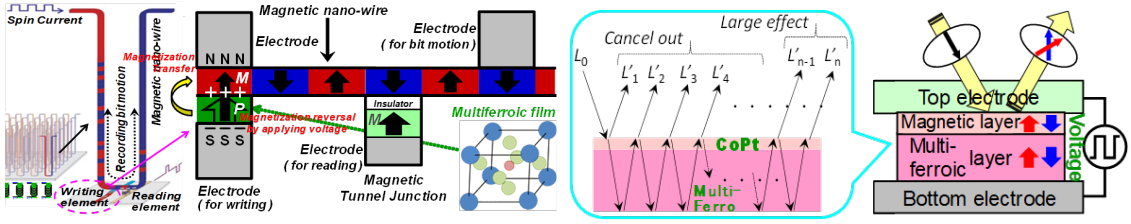


**Figure:** (a) Very high capacity and low power consumption magnetic memory with using "magnetization transfer by electric field application". (b) High brightness and low power consumption 3-D display device with using "MOKE amplification by magnetization transfer with electric field application".

# Keynote Lectures

## Synthesis and characterization of soft magnetic metallic glass nanoparticles via laser ablation

Parthiban Ramasamy[1,*], Laszlo Sajti[2], Christoph Gammer[1], Rainer Lechner[3], Ivan Skorvanek[4], Devinder Singh[1], Jurgen Eckert[1,5]

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**Abstract**
Metallic glass nanoparticles (MG NPs) are highly promising materials for various industrial and technological applications, where the distinct mechanical[1] or catalytic[2] properties of each constituent metal are combined within a single nanoparticle[3-5]. Laser ablation in liquid (LAL) for metallic glasses is challenging, particularly when the metallic glass crystallizes even at high cooling rates. In this research, metallic glass nanoparticles are prepared from two different glass-forming alloys $Fe_{82}Si_5B_{10}P_3$ and $Fe_{75}Co_8Si_4B_{13}$, in water and in two organic solvents, ethanol and acetone. An in-depth analysis of the structure and elemental distribution of the obtained nanoparticles, down to the single-particle level, was conducted using advanced transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) methods. This analysis revealed an amorphous phase and the presence of oxide layers. Additionally, in-situ carbonization through the decomposition of solvents further stabilizes the alloy system, enabling the successful achievement of the amorphous phase in the NPs. The carbon-rich molecules in solvents enhance the relative fraction of MG-NPs, and the completion kinetics of oxygen lead to the formation of Fe oxide. Further magnetic measurements confirmed the contribution of MG and Fe oxide NPs to the magnetism. This work presents a novel approach to producing magnetic MG-NPs for advanced multifunctional applications.

**References:**

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# Diamond: The most versatile ultra wide bandgap quantum material for many technological applications

M.S. Ramachandra Rao

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India Centre for Lab-grown Diamond (InCent-LGD)
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**Abstract**

Our group focusses on the physics, doping and electronic correlations, defect-engineering and applications of thin films and nano-structures of TMOs and diamond. During the past two decades, we have been focusing on utilizing diamond, the most versatile ultra-wide bandgap material for many technological applications. Diamond is a fascinating allotrope of carbon that offers half a dozen different applications and its lattice is amenable to doping. Diamond, despite being one of the most resistive materials, is driven to a semiconducting to superconducting state by boron doping and boron doped diamond (BDD) is considered as the most useful next generation granular superconductor useful for quantum-interface devices requiring high kinetic inductance. We have also demonstrated the use of boron doped diamond electrodes in the waste-water treatment. We are focusing on the quantum applications of diamond using nitrogen and other dopants. I will give a summary of our research and development journey of diamond.

**Keywords:** Quantum Material, Diamond, Ultra-wide bandgap, Semiconducting state, Superconducting state, Boron-doped diamond

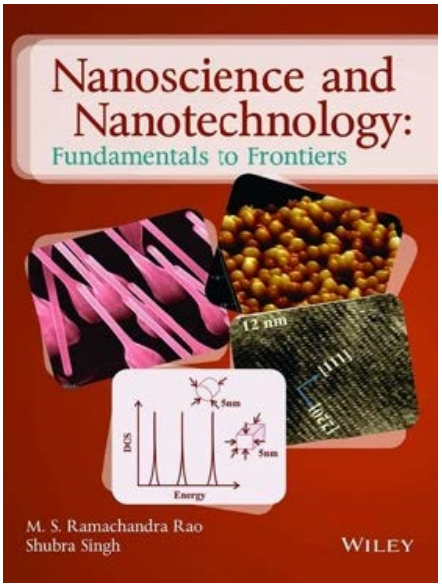


**Figure:** Book: "Nanoscience and Nanotechnology; Fundamentals to Frontiers"

# Energy: the true final frontier

R. Ramesh

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**Abstract**

More than five decades ago, President Kennedy exhorted the nation to rise up and meet the biggest challenges of that period, amongst them being the Race to the Moon, that led to the establishment of NASA and the Apollo program. In one of the most stirring presidential speeches, he urged the nation to "ask not what the country can do for you, but what you can do for the country". It is quite likely that we, as a nation (and the world), are once again at crossroads, from many perspectives. I will use Energy as a "Clear and Present" example of where we, as scientists, engineers, young and not-so-young, need to rise up and meet the challenges that we are faced with. Energy and Water are perhaps the most pressing issues of our generation. I will argue that Materials are the most strategic enablers of both fields. A few years ago, I had the opportunity to serve the nation in the role of the founding Director of the DOE Sunshot Initiative, which was designed to bring solar electricity down to grid parity. The huge impact of Sunshot and more generally Solar, is already being felt with prices of solar electricity dropping rapidly. More recently, I had the opportunity to help shape the "Earthshots", aimed at solving the biggest problems in Energy and Climate Change. In this talk, I will attempt to take you through from the "Macro", global energy economics down to what fundamental materials physics can do to help solve the key problems in Energy Efficient Electronics.

# Invited Talks

## Battery storage: material innovations and challenges

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**Abstract**

Li-ion batteries possess a number of desirable features, including high energy density, high power density, energy efficiency and long cycle life. With such attractive performances, the Li-ion technology has captured the portable electronic market, invaded the power tool equipment market, and penetrated the EV market. Research directions are towards increasing the Li-ion battery energy density, to lower its cost, improve its safety and make it more sustainable and 'greener'. A substantial segment of the battery materials community is moving toward developing electrode materials on the basis of the abundance and availability of the relevant chemicals. In addition to the Li-ion chemistry, Na-ion chemistry is also interesting and could be used in batteries due to the ample availability of Na, unlike Li resources. New technologies such as Li-Air, Lithium-Sulphur, Solid State Batteries are emerging but currently in the R & D stage. Lithium-ion battery technology has been at the forefront of energy storage research at CSIR-CECRI. CSIR-CECRI is involved in developing cutting-edge technology in the area of Li-ion batteries and Sodium-ion batteries and creating crucial IPR in these forefront areas of research. The greater vision is to assist the nation's aspirations towards developing efficient energy storage technologies required for utilizing the renewable energy, to reduce carbon emissions, to achieve carbon neutrality and to achieve sustainable development goals (SDGs).

**Keywords:** Li-ion Battery, Battery Technology, Sodium-ion Battery

# Metal (Bi, La, Ni)-doped CdTe nanomaterials for optoelectronic and photodetector applications

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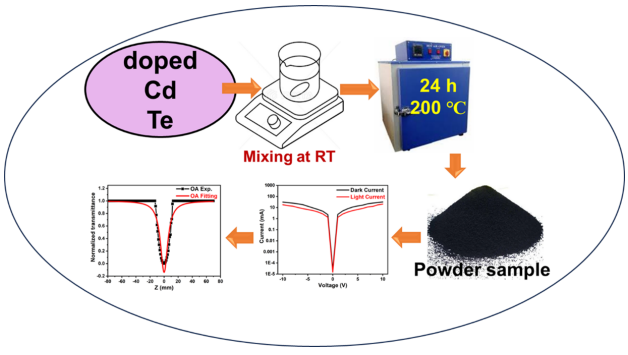
**Abstract**

The hydrothermal synthesis route was effectively employed to fabricate a series of metal-doped CdTe nanomaterials. Among the prepared samples, one served as the pristine (undoped) CdTe, while the remaining samples contained varying concentrations of metal dopants to systematically study their influence on the structural, optical, and electronic characteristics of CdTe. The XRD patterns confirmed the formation of a single-phase cubic structure of CdTe, with no detectable impurity peaks. A noticeable shift of diffraction peaks toward higher or lower 2Θ angles was observed, indicating lattice distortion and successful substitution of Cd atoms by the dopant ions within the CdTe crystal lattice.

Raman spectroscopy provided additional evidence of structural modification, revealing characteristic CdTe vibrational modes and slight peak shifts associated with the phonon confinement effect and dopant incorporation. TEM images further validated the crystalline nature of the samples and revealed well-defined lattice fringes, allowing precise measurement of interplanar spacings consistent with the cubic CdTe phase. The XPS analysis confirmed the presence and oxidation states of Cd, Te, and the dopant metal, providing insights into the surface chemical composition and the alteration of the local electronic structure due to metal inclusion.

Optical characterisation using UV-Vis spectroscopy demonstrated a clear tunability of the direct bandgap with increasing dopant concentration, attributed to quantum confinement effects and band structure modification induced by metal incorporation. The photo response studies under illumination showed a significant enhancement in photocurrent, indicating improved charge carrier separation and transport efficiency. Time-dependent current (I-T) measurements further exhibited faster rise and decay times with optimised dopant levels, suggesting superior photo-switching behaviours. The derived photo response parameters, such as responsivity (R) and detectivity (D*), also showed considerable improvement, highlighting the enhanced photodetection capability of the doped samples. Moreover, nonlinear optical (NLO) investigations using the Z-scan technique revealed pronounced values of the nonlinear absorption coefficient ($\beta$) and nonlinear refractive index ($n_2$), confirming strong optical nonlinearity. These findings suggest that metal-doped CdTe nanomaterials hold significant promise for next-generation optoelectronic and photonic applications, including photodetectors, optical switches, and laser protection devices.

**Keywords:** Hydrothermal synthesis, Metal-doped CdTe, Direct optical bandgap, Optoelectronics



# Chiral light emitting nanomaterials: from fundamentals to applications

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**Abstract**

Chirality is ubiquitous in nature and chiral molecules/materials are finding application in diverse fields. This field of research has gained revived interest after the observation of optical activity in nanomaterials. Nanoscale chirality is considered as an effective strategy to generate materials with enhanced optical activity. Chiral nanomaterials are synthesized by adopting majorly three approaches: (i) the synthesis of intrinsically chiral nanoparticles in solution, (ii) chiral induction in achiral nanoparticles using chiral ligands, and (iii) template assisted methods using chiral/helical templates. Investigations on molecular chirality using circular dichroism (CD) spectroscopy has been an active research topic over the past few decades due to their application in catalysis and pharmaceuticals. Recently, research interest has focused attention on chiral light emitting molecules and materials due to their vast application in field of display devices, data encryption, chiral biosensing and bioimaging. A relatively new technique that investigates the excited state optical activity in molecules and materials is circularly polarized luminescence (CPL). Our recent attempts on the synthesis of chiral emissive nanomaterials, and the investigations on their ground and excited state optical activity using CD and CPL spectroscopy will be discussed in the talk. CPL is a relatively new technique that has gained tremendous attention due to its relevance to both fundamental and applied research. Working in this direction, we have recently demonstrated CPL organic molecular systems as well as nanomaterials. A correlation between the optical activity in molecules to that similar effect in nanomaterials will be discussed. Our recent attempts towards understanding the fundamentals of optical activity in nanomaterials and the correlation of the observed spectral properties to the conventional organic systems will be discussed briefly. The potential applications of the molecular/nanomaterial systems will form the topic of discussion during the presentation.

**Keywords:** Nanoscale chirality, Circularly polarized luminescence, Photonic materials, Light emitting nanomaterials

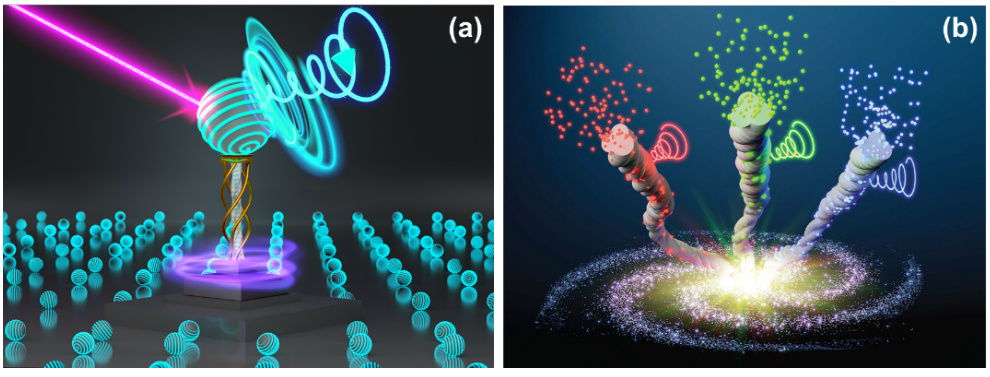


**Figure:** Scheme illustrating the chiral light emission achieved in nanomaterials through (a) structural symmetry breaking and (b) host-guest interactions.

# Heterojunction of GaN and topological insulator $Bi_2Se_3$ for optoelectronics devices

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**Abstract**

Ultraviolet (UV) radiation has a variety of impacts, affecting human health, agricultural productivity, and the integrity of materials across diverse environments. In the modern era, self-powered UV photodetectors provide detection of UV radiation enabled by the photovoltaic effect without any power consumption. Heterojunction-based on wide band gap GaN and topological insulators (TIs) $Bi_2Se_3$ materials have shown great potential in various fields, including electronics, photonics, and quantum sensing[1-2]. Over the past decades, significant efforts have been made to explore the stable III-nitrides compound semiconductor materials and GaN-based devices have been widely adopted and commercialized successfully, as GaN possesses chemical inertness, high electron mobility, a wide energy band gap (3.4 eV), high breakdown voltage, sustainable nature in harsh environments, etc. Here, topological $Bi_2Se_3$ thin films were deposited using the magnetron sputtering technique on GaN/sapphire (0001) substrate for multifunctional study of magneto-transport under 2 K to 100 K temperature, self-powered broadband high-responsive UV photodetection, and ultrafast charge carrier dynamics properties. A variety of optoelectronic devices have been designed and fabricated with unique morphology exhibiting higher photocurrent generation and significantly enhanced responsiveness optical illumination. The developed device taps the broad wavelength range from deep UV to the NIR spectrum and able to work without any external bias. The magneto-transport analysis reveals weak antilocalization in $Bi_2Se_3$/GaN, confirming the presence of topological surface states. Transient absorption spectra of the $Bi_2Se_3$/p-GaN heterojunction reveal oscillations attributed to the Se-Se interface, along with a notably faster carrier lifetime from the visible to near infrared spectrum region. The UV-A responsivity of $1.1 \times 10^4 A/W$, $\sim 1.2 \times 10^3$ fold higher than pristine p-GaN/sapphire was obtained at 5 V. The strong built-in electric field and high-mobility surface states in the $Bi_2Se_3$/GaN heterojunction facilitate efficient charge separation and rapid transport, enabling self-powered operation, superior photodetection performance, and providing valuable insights for the design of next-generation high-performance photodetectors.

**Keywords:** $Bi_2Se_3$, GaN, Topological Insulators, Photodetectors

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# From visible to near infrared: emission engineering in lead-free low-dimensional hybrid metal halide perovskites

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**Abstract**

Recently, lead-free low-dimensional metal halide perovskites have become an important class of light-emitting materials. In contrast to their three-dimensional analogues, two-dimensional layer, one-dimensional chain, or zero-dimensional molecular halide perovskite materials exhibit pronounced quantum confinement and enhanced exciton binding energies, leading to bright, tunable emission across a wide spectral range. Systems incorporating metal cations with isoelectronic configurations to $Pb^{2+}$, such as $Bi^{3+}$, $Sb^{3+}$ and $In^{3+}$, have attracted considerable research and technological interest in resent years. However, achieving precise control over their chemical composition, and consequently their optical properties, remains a significant challenge. Tuning the chemical composition and structural dimensionality has been of great interest to us because this allows access to a wide variety of structures and the exploration of diverse optical phenomena. Over the past few years, our group at JNCASR Bangalore has focused on the solution-based, low-temperature synthesis of hybrid halide perovskites with precise control over their compositions and atomic-level structures. During this talk, I will disucss the structure and electronic characteristics of low-dimensional halide perovskites, which make them potential candidates for light-emitting applications. Specifically, we have developed antimony(III)-doped $(MA)_4InCl_{(7-x)}Br_x$ and $(MA)_4InBr_{(7-x)}I_x$ as molecular emitters, along with one-dimensional $(MA)_2NaInX_6$ (X = Cl or Br; MA = $CH_3NH_3^+$). The doped samples show high emission quantum yield up to 93% with a color purity up to 94%. Furthermore, by taking advantage of the structural flexibility of the perovskite framework and the templating influence of organic ammonium cations, we have developed new bimetallic gold-iodide-based two-dimensional hybrid halide double perovskites, $(H_2DAC)_2AuSbI_80.5H_2O$ and $(H_2DAC)_2AuBiI_8H_2O$ ($H_2DAC$ = *trans*-1,4-diammoniumcyclohexane), which exhibit near-infrared light emission at low temperatures, and hold potential for NIR optoelectronic applications.

**Keywords:** Perovskites, Emission engineering, Low-dimensional materials

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## Magnetoelectric composites for multifunctional applications

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**Abstract**

Magnetoelectric composites, in comparison to the single phase magnetoelectric (ME) compounds, are promising materials for practical applications. Among the different composite formations, layered composites are preferable due to easy fabrication and testing. The important applications for these composites are magnetic energy harvesting and magnetic field sensing. It is reported that as a sensor, ME composites are better than many of the existing sensors that operate at room temperature. In fact, ME sensor is preferable to its SQUID counterpart due to its room temperature operation.

It is also well known that ferromagnetic resonance (FMR) falls in the microwave frequency range. The study of FMR provides the basic information about the anisotropic field and environmental conditions. It is also possible to control this ferromagnetic resonance by an externally induced strain thereby giving an opportunity to develop microwave devices.

In this talk, a few magnetoelectric laminate composites will be presented for use as energy harvesters and magnetic sensors apart from a special mention about the possible development of tunable microwave devices.

**Keywords:** Piezoelectric, Magnetoelectric composite, Magnetic Field Sensor, Energy Harvesting, Tunable Microwave Filter

# Spin-phonon coupling, magneto-caloric effect and critical phenomena in $Ga_{1-x}Al_xFeO_3$ orthoferrite

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**Abstract**
Due to the interplay between the spin degrees of freedom, lattice dynamics and electric polarization, $GaFeO_3$ orthorhombic perovskite presents a unique opportunity to probe into the complex physical phenomena such as the spin-phonon coupling (SPC), multiferroic orders and the coupling between them. To this end, the thermally-induced shifts in the wavenumbers corresponding to the positions of the Raman-active (RA) peaks, the magneto-caloric effect and critical phenomena near the ferromagnetic (FM)–paramagnetic (PM) phase transition in the orthoferrite compound $Ga_{1-x}Al_xFeO_3$ have been extensively investigated. Several unambiguously identified RA modes are shown to provide clear evidence for SPC. The isothermal magnetic entropy change,-$\Delta S_M$ (T), peaks at $T^{pk}$, which is close to the Neel temperature ($T_N$). Like $T_N$, $T^{pk}$ increases linearly with the Al concentration (x). In this work, the existence of a universal $\Delta S_M/\Delta S_M^{pk}$ curve and the validity of the Banerjee criterion assert that the ferrimagnetic-PM and the FM-PM phase transitions occurring at $T_N$ and curie temperature ($T_C$), respectively, in the present case, are of second order. These transitions are characterized by the mean-field critical exponents.
In this talk, after the brief introduction to multiferroics the structural, magnetic, dielectric properties of Al substituted $GaFeO_3$ with emphasis on Spin-phonon coupling, magnetocaloric effect and critical phenomena will be presented.

**Keywords:** Functional materials, 2D Nanostructures, Energy storage, Supercapacitors

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# Ultrafast laser-induced extrusion of nano-rods

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**Abstract**

Ultrafast near-infrared laser pulses can trigger highly localized material transformations through nonlinear mechanisms initiated by multiphoton ionization. Controlling the pulse in space, time, or polarization allows a fine control over the light-matter interaction. Until now, most ultrafast laser applications have focused on ablative or bulk-modification processes.

In this talk, we will report a fundamentally different femtosecond-laser phenomenon that is neither ablative nor subtractive. A single pulse can drive the a translation of material over several micrometers, forming positive surface features, as first shown in [1].

This effect arises from the generation of a nanometer-thick cylindrical melt inside sapphire by a 100 fs radially polarized zero-order Bessel beam with a hollow elongated focus. The resulting pressure gradients expel material outward, creating nanopillars about 800 nm in diameter and in excess of 10$\mu$m high.

Three distinct regimes were identified and analyzed by Transmission Electron Microscopy (TEM), revealing that the material is, in all cases, a single-crystal. The underlying mechanisms range from pure material displacement to liquid jetting followed by capillary breakup and resolidification, producing wavy pillars up to 15$\mu$m high.

Fundamentally, this demonstrates that ultrafast pulses can generate extreme temperatures over $\sim$ 50nm scales. Practically, it provides a fast route to fabricate ordered nanopillar arrays for metamaterial, photonic, phononic, or micro-mechanical applications.

This project has received funding from H2020 European Research Council (ERC) under grant agreement 682032-PULSAR, the European Union's Horizon 2020 research and innovation program under grant agreement No 825246 kW-flexiburst, the French Agence Nationale de la Recherche, projects DENSE (ANR-21-CE08-0005) and EQUIPEX+ SMARTLIGHT platform (ANR-21-ESRE-0040), the EIPHI Graduate School (ANR-17-EURE-0002). This work was also supported by the French Renatech network, MIMENTO technological facility, and the Région Bourgogne Franche-Comté.

**Keywords:** Ultrafast near-infrared laser, Laser, Femtosecond-laser, Nanorods, Highly-localized material transformations

**References:**

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# Flexible piezoelectric nanogenerators for green energy harvesting and sensor applications

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**Abstract**

Piezoelectric nanomaterials can be used to generate electric energy by utilizing natural mechanical forces like foot stroke, vehicle motion, wind/water flow, finger tapping bending or twisting of body part. With higher piezoelectric coefficient of synthesized materials, better sensitivity and range of the energy harvesting devices are possible which can be utilized in energy application, sensors and medical devices.

In the present work, we have synthesized many high performance piezoelectric systems and used them to fabricate flexible nanogenerators. Nanomaterials of advanced piezoelectric materials like alkali based NKLN and BZN:KNN[1,2], lead based PMN-PT[3], doped/hybrid ZnO[4] systems and rare earth doped ZnS[5] nanoparticles were synthesized using low temperature chemical route and hydrothermal processes. They are characterized for crystallographic, electrical, mechanical, optical, etc. properties. These nanoparticles are used to fabricate thick tapes with PDMS as binder and then flexible nanogenerators are developed. The piezoelectric output efficiency were studied by applying tapping force of varying value and frequency. It has been further demonstrated that the green energy can be generated by simple finger tapping and bending of knees or even the force exerted by the vocal cord while speaking which has great potential in medical applications[5,6]. It has been established that these nanogenerators are suitable for practical wearable electronic devices.

**Keywords:** Magnetic, Rapid quenching, Melt-spinning, In-water quenching, Amorphous, Ribbons, microwires, Magnetostrictive, Giant magneto-impedance

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# Two dimensional functional nanostructures for sustainable energy storage applications

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**Abstract**

Two dimensional (2D) functional nanostructures are emerging futuristic materials for sustainable energy storage applications because of their unique properties with excellent functionality. The study of decorating the 2D nano sheets with inorganic functional materials such as metals, metal oxides and metal sulfides is now becoming a promising and challenging area for energy storage devices. In this study, reduced graphene metal-oxide composites with $SnO_2$, $CeO_2$, have been synthesized by homogeneous co-precipitation method. Multi-layered composite structures with 1 D carbon nanotubes integrated with 2 D graphene structures with the addition of 3 D bulk nanoparticles were prepared with improved properties. The structural properties of natural graphite, graphene oxide, graphene-metal oxide composites were studied. The prepared composite structure has been subjected to optical, electrical, and electrochemical property studies. The electrochemical properties of graphene-metal oxide composites reveal that these materials can be effectively used for supercapacitor application with improved specific capacitance, higher power density, energy density and cyclic stability. Coin cell supercapattery device using nickel cobaltite nanostructures as a cathode material has been developed for energy storage applications Heterostructures of different 2D materials have also been fabricated to improve the electrochemical performance. The structural aspects of graphitic carbon and reinforced carbon fibres have also been explored for energy storage applications.

**Keywords:** Functional materials, 2D Nanostructures, Energy storage, Supercapacitors

## Incommensurate Magnetic Structure of $Ho_3Co$ and its magnetism under high pressure

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**Abstract**
Intermetallic compounds of rare-earth and transition metal elements have been widely studied, however the rare-earth rich compounds of the type $R_3T$ have received relative less attention. These compounds, which crystallize in the orthorhombic $Fe_3C/Al_3Ni$ type structure, exhibit highly complex magnetic behaviour, multiple magnetic transitions as function of temperature and magnetic field. In this talk, the magnetic behaviour of $Ho_3Co$ that was investigate using AC & DC magnetization, heat capacity and temperature and field dependent neutron diffraction will be presented. Highly complex incommensurate magnetic structure of $Ho_3Co$ determined from neutron diffraction will be presented. Its magnetic behaviour under high pressure will also be presented along with magnetocaloric effect under pressure of $Ho_3Co$ and $Tb_3Co$.

**Keywords:** $Ho_3Co$, $Tbo_3Co$, Magnetic Materials, Magnetocaloric effect, Neutron diffraction, High pressure

# A sustainable approach for developing supercapacitor electrodes from industrial waste for energy storage applications

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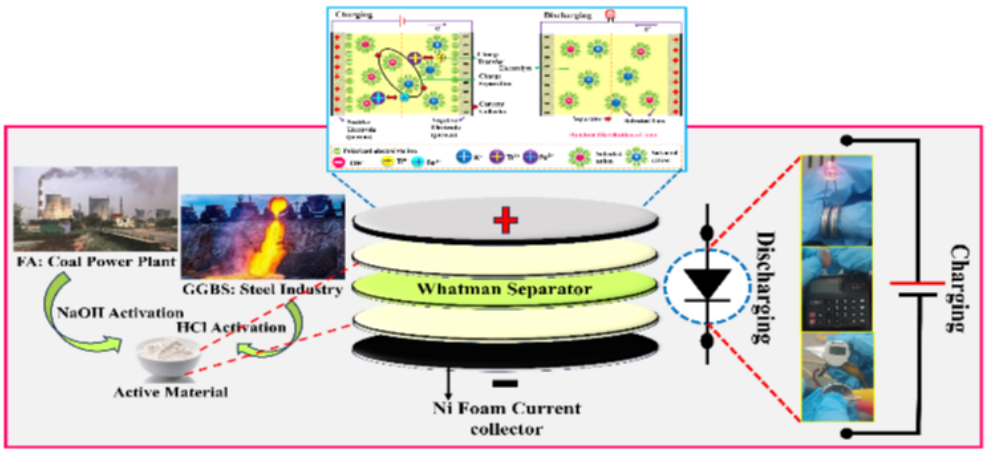
**Abstract**

The main aim of this work can be summarized by the catch-phrase "waste to wealth. The investigation for environmentally friendly energy systems is of prime importance in reducing the environmental impact caused by the widespread use of fossil fuels across the world. The revolutionary technologies must be developed to create energy storage devices with increased capacity, cost-effective, and longer lifetimes.

In this study, industrial waste materials such as fly ash (FA) and ground granulated blast furnace slag (GGBS) were used as precursor materials for synthesizing active electrode material via the sol-gel technique. A series of samples were prepared by varying the FA-to-GGBS weight ratio (0.2 to 5), and the crystallization temperature of the synthesized materials was optimized through sintering at different temperatures (700, 850, 900, 950, 1000, and 1100°C). Material characterization revealed that the sample with an FA-to-GGBS ratio of 1 primarily consists of Akermanite ($Ca_2MgSi_2O_7$) as the major phase and diopside ($Ca(Mg, Fe)Si_2O_6$) as a minor phase, with an optimal crystallization temperature of 950°C. The synthesized material was coated onto nickel foam and tested in a three-electrode system, demonstrating excellent pseudocapacitive behavior due to the presence of trace transition metal oxides ($Fe_2O_3$, $TiO_2$). To further enhance the electrochemical performance, different basic aqueous electrolytes (KOH and NaOH) were tested To improve adhesion between the active material and the current collector, Nd: YAG laser irradiation was applied to different current collectors, including copper sheets, graphite sheets, stainless steel, and nickel foam, with varying laser pass spacings. The material coated on Ni foam electrode exhibited 97.25% capacitance retention after 3000 charge-discharge cycles, with a decent energy density of 29.73 $Whkg^{-1}$ and a power density of 524.95 $Wkg^{-1}$. Furthermore, a symmetric coin-cell supercapacitor device was fabricated, successfully powering red LEDs, a digital watch, and an electronic calculator. This study presents a promising approach for converting industrial waste into cost-effective, high-performance electrode materials for real-world supercapacitor applications.

**Keywords:** Biowaste, Energy Storage, Supercapacitor, Fly ash, Ground granulated blast furnace slag



## Recent studies on spintronic and topological aspects of certain Heusler alloys

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**Abstract**

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

# Melt-grown single crystals: growth dynamics and functional properties for optical and thermoelectric applications

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**Abstract**

In the current technological world, a wide range of advanced devices—ranging from integrated circuits to sensor-based systems—depend heavily on high-quality electronic and optical components. Most of these components are fabricated from single crystal wafers, which are precisely cut from defect-free bulk single crystals. However, the growth of large, defect-free single crystals is a highly challenging and time-consuming task, as it requires stringent control over several growth parameters such as temperature gradient, thermal field stability, pulling rate, and rotation speed. The presence of even minor defects such as dislocations, inclusions, or compositional inhomogeneities can significantly alter the electrical, optical, and thermoelectric performance of the materials. Therefore, the optimization of growth parameters and innovative design of growth systems are essential to minimize these defects and achieve superior crystal quality. In this talk, I will present our recent efforts on the growth of high-temperature single crystals such as lithium niobate ($LiNbO_3$), bismuth silicon oxide ($Bi_{12}SiO_{20}$), lithium fluoride (LiF), and bismuth telluride ($Bi_2Te_3$), and discuss their structural, optical, and thermoelectric properties for various device applications. These materials are of particular interest due to their diverse functionalities—$LiNbO_3$ is widely used for nonlinear optical and piezoelectric applications; $Bi_{12}SiO_{20}$ serves as an excellent photorefractive material; LiF is useful for UV optical components; and $Bi_2Te_3$ is a well-known thermoelectric material for energy conversion. At CSIR–National Physical Laboratory (NPL), we have successfully grown several of these crystals using both melt growth and slow evaporation solution growth techniques. We have also developed an in-house single-zone furnace equipped with a seed rotation mechanism to enable controlled, defect-minimized crystal growth. For the vertical Bridgman technique (VBT), specially designed ampoules were fabricated to enhance crystal nucleation and stabilize the solid–liquid interface during the growth process. Comprehensive characterization of the grown crystals was carried out using X-ray diffraction, UV–Vis–NIR spectroscopy, and thermoelectric measurements to study their structure–property relationships. In a few cases, the growth process was further refined by systematically modifying parameters such as the temperature profile, cooling rate, and ampoule geometry to improve crystal perfection. The detailed results, including the correlation between growth conditions and material performance, will be presented during the conference, highlighting the potential of these melt-grown single crystals for future optoelectronic and thermoelectric applications.

# Journey of rapidly quenched magnetic materials to sensors for industrial applications

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**Abstract**

In recent years, the field of sensor research has undergone an exciting transformation, focusing increasingly on innovative functional materials like rapidly quenched magnetic alloys. This paradigm shift is driving the development of advanced smart sensors and portable sensing devices. These rapidly quenched magnetic materials have emerged as highly potential sensor materials due to their exceptional low field sensitivity, ease of large-scale production, and with a scope for device miniaturization

At CSIR-National Metallurgical laboratory (N.M.L), Jamshedpur, India, the research focus is on development of magnetic sensors using the materials prepared in the laboratory. In this quest, rapid quenching techniques like melt spinning, in-water quenching have been adopted to develop amorphous / nanostructured sensor materials in the form of ribbons and wires respectively. The presentation would address the electromagnetic sensing devices developed by CSIR-NML in collaboration with M/s. Accelor Microsystems, Mohali, Punjab and coined as ***'MagStrics'*** and ***'MagRays'***. The device ***'MagStrics'*** is based on the magnetostrictive properties of amorphous / nanostructured ribbons which is used for the detection of defects in pipes using guided wave technique. The methodology of low magnetic field detection is adopted in ***'MagRays'*** using Giant magneto-impedance (GMI) properties of amorphous microwires and has been deployed for evaluation of damage in petroleum reactor steels and also for weld assessment. The GMI sensor has shown potential scope for detection of stray magnetic materials which is undesirable in cement industry raw materials.

**Keywords:** Magnetic, Rapid quenching, Melt-spinning, In-water quenching, Amorphous, Ribbons, microwires, Magnetostrictive, Giant magneto-impedance

# From green materials to biodegradable devices: steps towards responsible innovation

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**Abstract**

The electronics industry is a major contributor to global carbon emissions and e-waste, posing serious environmental and health challenges. As demand for electronic devices surges, aligning the sector with the United Nations Sustainable Development Goals (SDGs) is both urgent and essential. Our research addresses this challenge by developing a novel library of sustainable electronic materials through green chemistry principles. These materials are designed to replace conventional toxic, non-biodegradable components commonly found in electronic devices. These materials are formulated into functional inks suitable for printing on unconventional substrates, enabling low-energy and scalable fabrication of electronic devices. The developed material platform is particularly suited for healthcare applications, where we are advancing biodegradable devices for muscle atrophy monitoring, wound healing, and eczema treatment. By bridging sustainable materials innovation with functional electronics, our work paves the way for the next generation of transient and eco-friendly electronic systems.

**Keywords:** Green Materials, Biodegradable Devices, Sustainable Electronic Materials

# Permanent magnetic thin films: prospects for micromagnetic devices

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**Abstract**

The rapid surge in the discovery of new magnetic phenomena has made the study of magnetic films a vibrant area of contemporary research. A notable recent advancement in this field is the development of magnetic micro-electro-mechanical-systems (MagMEMS), wherein electro-dynamic or electro-magnetic transduction mechanisms generate forces and torques essential for energy conversion. Compared to electrostatic actuators, micro-actuators based on magnetic actuation principles offer several advantages, including low operating voltage, reduced power consumption and higher actuation forces.

The successful realization of such devices depends on three key aspects: (i) the selection of magnetic materials suitable for the intended function, (ii) the optimization of the film deposition process and (iii) precise micro-patterning and integration. From an application perspective, the thickness of magnetic films typically ranges from a few micrometers down to several tens of nanometers for sensor applications, whereas actuator devices often require substantially thicker films, up to several tens of micrometers.

A major research programme has been initiated at DMRL to develop and qualify thin films of permanent magnetic materials, particularly Sm-Co alloys, for device-level applications. Various deposition techniques, including e-beam evaporation, magnetron sputtering and sol-gel spin coating have been explored for the synthesis of Sm-Co based magnetic thin films. Their structural, magnetic and functional performance characteristics are being systematically evaluated for eventual integration into micromagnetic devices. The present contribution highlights the associated challenges and demonstrates proof-of-concept Sm-Co permanent magnetic thin films for sensors / actuator applications.

**Keywords:** Permanent magnetic films, Sm-Co, Sol-gel spin coating, Sputtering

# Wafer-scale growth of 2D magnetic materials, and creating single photon emitters in 2D semiconductors

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**Abstract**

Two-dimensional magnetic materials (2D-MM) are critical for spintronic and quantum devices, but large-area growth remains unsolved. First, I will discuss the development of a generalized vapour deposition approach of synthesizing wafer-scale, epitaxial 2D-MM ($CrCl_3$) films. To achieve this milestone for air-sensitive 2D-MM, we demonstrate several innovations concerning light management during synthesis, carrier-gas purity, and precursor delivery. We also uncover the atomic-scale origin of substrate-dependent growth via state-of-the-art machine learning-enabled simulations. Selective-area synthesis and large-scale transfer of these 2D-MM are shown, which will enable spintronic devices. In the second part of the talk, I will briefly discuss our group's work on creating single photon emitters in monolayer $MoS_2$ by just using ultralow electron beam accelerating voltages (< 5 kV). We understand the physical origin of these peaks and their spin nature, and also find long-term spectral stability.

**Keywords:** 2D materials, Magnetic materials, Semiconductors, Quantum technology

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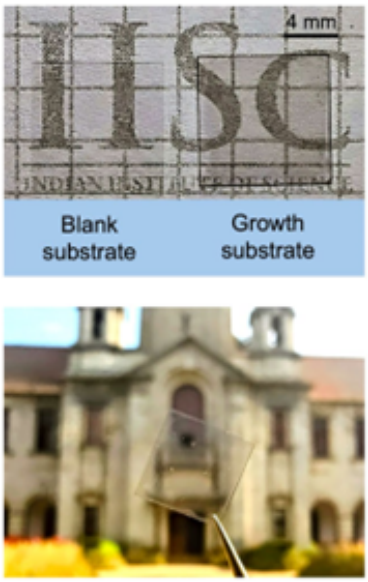


**Figure:** Large scale growth of 2D-magnetic material $CrCl_3$

# High temperature oxidation of Zr alloys and development of accident tolerant fuel cladding approaches

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**Abstract**

Zirconium (Zr) alloys have long been the material of choice for nuclear fuel cladding due to their favourable neutronic properties and mechanical performance under normal operating conditions. Development of fuel cladding materials that are more resistant than zirconium (Zr) alloys to accident conditions in nuclear reactors has been of interest since 1980s. However, the Fukushima Daiichi nuclear accident underscored the vulnerability of Zr-based claddings to rapid oxidation and hydrogen generation under high-temperature steam environments. This has prompted global efforts to develop accident tolerant fuel (ATF) cladding solutions for enhanced reactor safety under design-basis and beyond-design basis accident scenarios. During loss of coolant accident (LOCA), steam / air oxidation of Zr alloys (up to ~1200°C) and consequent hydrogen generation is a major concern for all reactor types.

This talk will provide a comprehensive overview of the high-temperature oxidation behavior of Zr alloys, elucidating the underlying mechanisms and factors that influence their oxidation kinetics and failure modes. It will then present the concept of ATF and the multiple approaches being adopted worldwide to develop ATF clad materials with an emphasis on their potential to enhance high-temperature performance and safety margins. These approaches include development of newer materials and surface modifications /coatings on existing Zr alloys.

The talk will also highlight our recent research advancements in this area, including experimental investigations into uncoated, coated and modified Zr-based claddings and their oxidation behavior under simulated accident conditions. The qualification criteria for any such current or future development of ATF clad in (a) normal operating and (b) simulated LOCA conditions shall be highlighted. The presentation is intended to offer relevant insights into the effectiveness and limitations of different ATF strategies, and contribute to the broader understanding of material behavior in extreme environments.

## Advanced manufacturing techniques for surface functionalization

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**Abstract**

Next generation manufacturing techniques focuses mainly in developing qualitative products in a sustainable way. Hence, qualitative machining techniques are the need of the time, as there is an increase in customer demand for customised multi-functional controlled surfaces having intricate geometric features, spanning from macro to nano scale.

Though there exists different non-traditional manufacturing processes, laser based technology has gained wide acceptance owing to its unique capability to process any material within short span of time with higher dimensional control. Lasers are currently applied in many important fields such as aeronautic, semiconductor, astronautic, automobile, marine etc. Ultra-fast lasers are the recent classification of laser based manufacturing technology, which allows more precise control over feature dimension due to non-thermal ablation characteristics.

Additive manufacturing also known as three dimensional printing is the another most fascinating area of research, which is currently revolutionizing both academia and industries owing to its unique capability to manufacture complex controlled geometries. Though the 3D printing technology has emerged from past 30 years, with the recent advancements in ultra-precision manufacturing and digital technologies, additive manufacturing are now even capable to perform down scale manufacturing with ultra high precision.

This talk will be covering the overall aspect of technological advancements happened in the area of surface functionalisation, mainly giving emphasis on the technology ultra short pulse laser micromachining and 3D printing.

# Biomass-based carbon dots: sensing and bioimaging applications

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## Abstract

Carbon quantum dots (CQDs) are fluorescent nanomaterials with exceptional optical properties, high biocompatibility, and versatile surface chemistry, enabling their use in bioimaging, chemical sensing, photovoltaics, and drug delivery. This study investigates the influence of key synthesis parameters on the optical performance of CQDs derived from chitosan and evaluates pequi *(Caryocar coriaceum)* almond as a sustainable carbon precursor for CQD fabrication. Chitosan-based CQDs were synthesized via hydrothermal treatment, yielding quantum efficiencies between 1.16% and 7.07%, with bright blue fluorescence. A factorial design was applied to assess the impact of synthesis variables, revealing that the interaction between synthesis time and molar ratio significantly enhanced quantum yield. Spectroscopic characterization confirmed the presence of carbonyl groups, which facilitated binding to ergosterol in *Candida albicans* membranes, promoting cellular internalization. These CQDs exhibited multicolor fluorescence (blue, green, and red) under variable excitation, validating their application as bioimaging agents for fungal cells. In parallel, CQDs were synthesized from pequi almond using a green hydrothermal approach. The resulting nanomaterials displayed ultra-small sizes (0.5–1.5 nm) and an outstanding quantum yield of 39%, surpassing typical values reported for CQDs from natural sources. These pequi-derived CQDs (PQ-CDs) were employed as fluorometric sensors for Cu(II) and Fe(III) ions. Fluorescence quenching was proportional to ion concentration, indicating effective analyte interaction. The sensor demonstrated high sensitivity and selectivity toward Cu(II), with a limit of detection (LOD) of 0.84 mg·L$^{-1}$—well below the regulatory threshold of 5 mg·L$^{-1}$ for copper in alcoholic beverages. For Fe(III), the LOD was 0.03 mg·L$^{-1}$, significantly lower than the maximum permissible concentration in drinking water. Figure 1 highlights the fluorescence and applications of CQDs from chitosan and pequi almond.

These findings confirm the dual functionality of CQDs as bioimaging probes and selective sensors for heavy metals. PQ-CDs proved effective for copper detection in **cachaca** (Brazilian sugarcane spirit) and for iron detection in water samples, demonstrating strong analytical performance in real-world matrices.

This work underscores the importance of precursor selection and synthesis optimization in tuning CQD photophysical properties. The integration of biomass-derived materials such as pequi almond aligns with green chemistry principles, offering a cost-effective and eco-friendly route to high-performance CQDs. The versatility of these nanomaterials opens avenues for their application in biomedical diagnostics and environmental monitoring platforms.

**Keywords:** Carbon dots, Bioimaging, Fluorometric sensor, Pequi almond, Chitosan

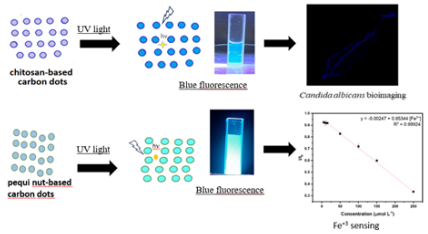


**Figure:** Fluorescent carbon quantum dots (CQDs) from chitosan and pequi almond under UV light. Chitosan-based CQDs were applied in *Candida albicans* bioimaging, while pequi-derived CQDs served as $Fe^{3+}$ sensors, showing strong fluorescence quenching with high sensitivity ($R^2$ = 0.9941).

# Artificial relaxor ferroelectric behavior in aerosol deposited films: Emerging pathway for high energy density capacitors

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**Abstract**

Relaxor ferroelectrics (RFEs) are being actively investigated for energy storage applications due to their large electric-field-induced polarization with slim hysteresis and fast energy charging-discharging capability. These distinctive features of RFEs originate from the nanoscale complex polar states and local structural heterogeneity driven by cation disorder in a specific composition. In the classical RFEs described in literature, most of the work focuses on dopant engineering for inducing the relaxor behavior in ferroelectrics. Here, we report a facile approach for the artificial engineering of relaxor ferroelectric behavior by controlling the volume fraction and dimensions of nanograins in normal dielectric system via aerosol deposition. Artificially tailored relaxor ceramic thick films demonstrated ultrahigh breakdown strengths up to 560 MV/m and reduced hysteresis with large unsaturated polarization ($\sim 100\mu C/cm^2$). A phase-field model in conjunction with high-resolution electron microscopy was utilized to provide a fundamental understanding of the nanograin engineered ceramic thick films. A record-breaking energy storage density over $120 J/cm^3$ with an efficiency over 70% was achieved. The comprehensive results and fundamental analysis provided a feasible approach for the design of high-performance materials with high breakdown strength, reduced hysteretic behavior, and enhanced polarization.

**Keywords:** Aerosol deposition, Energy storage density, Relaxor ferroelectric, Breakdown strength

## Understanding batteries & battery materials

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**Abstract**

A large fraction of world-wide research focuses on making better battery materials, hence better batteries to meet the demands of current and emerging applications. This talk will focus on two critical aspects of work undertaken in my group. The first part will focus on understanding the impact of a materials' atomic scale structure and its evolution on battery performance. The second part will focus on our more recent work on developing sustainable battery materials and developments in battery and battery materials recycling/re-use. A large proportion of the function of batteries arises from the electrodes, and these are in turn mediated by the atomic-scale perturbations during an electrochemical process (e.g., battery use). My group uses a combination of techniques, *ex situ*, *in situ* and *operando* to understand how atomic scale evolution impacts performance. In particular, the *operando* work results in an atomic level "video" of device function which can be directly correlated to performance parameters such as energy density, lifetime (or degradation), rate capability and safety. Examples using *operando* neutron and synchrotron powder diffraction to probe lithium- and sodium-ion battery materials and ex situ solid-state NMR to probe lithium-sulfur battery materials will be discussed.

The notion of sustainability in battery materials and processes will also be explored in this talk – how green can we make the batteries of the future? Can we design battery materials to be completely sustainable? Can we avoid using toxic chemicals in the production of electrodes? Can we be clever about recycling? Various examples will be given in this space which will hopefully encourage further ideas and research collaborations. Overall, this presentation will provide a flavor of the work being undertaken in my group and provide opportunities for further discussion and engagement. I will also showcase the work that is being done to bring the Australian and UNSW-based battery community and enthusiasts together to build better batteries and battery materials here in Australia!

**Keywords:** Sustainability, Crystal chemistry, in-operando studies, Recycling

# From dead Li-ion batteries to high performance Na-ion batteries via solvent-co-intercalation

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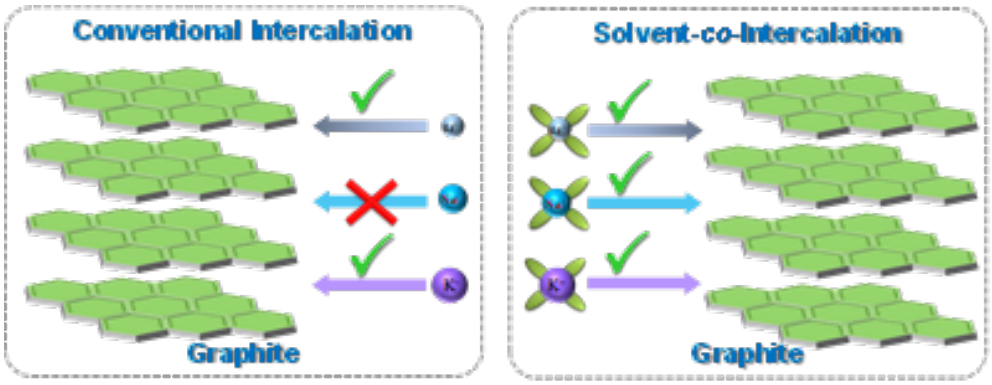
**Abstract**

Sodium-ion batteries (NIBs) are emerging as a promising energy storage technology and a potential alternative to the current state-of-the-art lithium-ion batteries (LIBs). Unlike lithium, sodium cannot be efficiently intercalated into graphite to form the binary graphite intercalation compound ($LiC_6$) due to thermodynamic instability, particularly in the presence of ester-based solvents. In this study, we demonstrate the effective recovery of both the graphite anode and the polypropylene (PP) separator from spent LIBs. We then utilize ether-based solvents to enable reversible Na-ion intercalation into the recovered graphite through a solvent-co-intercalation mechanism. This approach facilitates the formation of a stable ternary graphite intercalation compound, ensuring high reversibility of Na-ion storage. The NIB full cells are assembled using carbon-coated $Na_3V_2(PO_4)_3$ as the cathode, the recovered graphite as the anode, and TEGDME as the electrolyte solvent, with a PP separator, all under balanced mass loading conditions. Comprehensive physical and electrochemical characterizations are conducted on each component individually. The resulting full-cell configuration, C/PP/$Na_3V_2(PO_4)_3$, achieves a maximum energy density of 78 Wh $kg^{-1}$ (based on total active material mass) at room temperature. Further results and detailed insights will be presented during the session.

**Keywords:** Na-ion battery, Graphite anode, Solvent-co-intercalation, Spent Li-ion battery, Recycling



## Magnetic fluid hyperthermia: recent insights from numerical modelling and future challenges

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**Abstract**

Magnetic fluid hyperthermia (MFH) is an emerging and powerful approach in cancer therapeutics. This technique utilizes biocompatible magnetic nanofluids, which are stable colloidal suspensions of superparamagnetic nanoparticles. When injected directly into the cancerous tissue and exposed to a high-frequency alternating magnetic field, these superparamagnetic nanoparticles generate localized heating through Neel-Brown relaxation losses, raising the temperature to the therapeutically relevant levels. The current research activities are intensely focused on tuning the magneto-structural properties of the nanoparticles to maximize the heating performances. However, during practical applications, the heating efficiency is highly influenced by the physiological characteristics of the tumour tissues, such as porosity and thermos-physical properties, as well as the injection strategy. While experimental magneto-calorimetric studies offer valuable insights into the heating behaviour, repeated experiments are often cumbersome and restricted by practical difficulties. Under such a scenario, finite element modelling (FEM) offers a robust computation framework to simulate the spatio-temporal distributions of the thermal profiles during MFH. A few case studies highlighting the importance of numerical modelling will be discussed in this talk. Further, amongst the various injection strategies investigated for loading the magnetic nanoparticles within the cancerous tissues, the four-injection strategy with 90° separation and keeping the overall ferrofluid volume constant, was found to yield the most uniform field-induced temperature rise. The talk will also touch upon the future challenges in the field of magnetic fluid hyperthermia.

**Keywords:** Magnetic nanoparticles, Superparamagnetism, Magnetic fluid hyperthermia, Ferrofluids, Neel-Brown relaxation

## Chemical spray pyrolysis – a versatile technique for semiconductor thin film preparation

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**Abstract**

Chemical Spray Pyrolysis (CSP) has emerged as a versatile and economical thin film deposition technique for producing a wide variety of semiconductor materials with tailored physical and chemical properties. The process involves the atomization of a precursor solution containing suitable metal salts or organometallic compounds, which is then sprayed onto a heated substrate. Upon contact, the solvent evaporates, and the solute undergoes pyrolytic decomposition to form a uniform, adherent, and crystalline thin film. The film characteristics such as thickness, grain size, optical transmittance, and electrical conductivity can be precisely controlled by adjusting the deposition parameters, including solution concentration, spray rate, nozzle–substrate distance, substrate temperature, and carrier gas flow rate. One of the key advantages of CSP lies in its simplicity and scalability. The technique does not require high vacuum or sophisticated equipment, making it suitable for large-area coatings and low-cost fabrication. Moreover, CSP allows for the synthesis of complex and multicomponent materials such as metal oxides, sulfides, and oxysulfides with excellent compositional uniformity. These films have found extensive use in various applications including solar cells, photodetectors, transparent conducting electrodes, gas and humidity sensors, photocatalytic systems, and optoelectronic devices. Recent developments in the field have focused on improving film quality through precursor chemistry optimization, substrate engineering, and post-deposition annealing. The method also offers flexibility for doping and co-doping, enabling tunable band gaps and enhanced functional performance. Binary, ternary and quaternary semiconductor thin films prepared by spray pyrolysis technique for solar cells, gas sensors and photodetector applications.

# Intrinsic Versus Extrinsic Electrocatalyst Activity in Water Splitting

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**Abstract**

Electrochemical water splitting, powered by renewable electricity, represents the most efficient and environmentally sustainable route for producing high-purity hydrogen on a large scale. Rapid advancements in nanomaterials have significantly accelerated interest in improving electrocatalyst performance for the oxygen evolution reaction (OER) at the anode and the hydrogen evolution reaction (HER) at the cathode. However, the surge in research activity has also resulted in frequent misunderstandings and misinterpretations of key performance metrics. Electrocatalytic activity is generally evaluated using two categories of parameters such as extrinsic metrics and intrinsic measures. It I demonstrated that extrinsic parameters are strongly affected by physical factors such as catalyst mass loading and scan rate, which prevents them from accurately representing the catalyst's true molecular-level activity. In contrast, intrinsic descriptors such as turnover frequency (TOF) and Faradaic efficiency (FE) offer deeper insight into the fundamental catalytic processes. Through a detailed experimental and theoretical study, is established that how extrinsic metrics vary with physical testing conditions, and further reveal that even TOF, despite being considered intrinsic, is often influenced by substrate effects, mass loading, and scan rate when calculated using conventional approaches. The findings emphasize the necessity for correct selection and reporting of performance parameters to ensure credible benchmarking and to advance the development of high efficiency electrocatalysts for water splitting and related electrochemical technologies.

**Keywords:** Water splitting, Turnover frequency, Faradaic efficiency, Catalytic activity

# Engineering motion in the solid state: dynamics of smart crystalline materials

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**Abstract**

Smart crystalline materials, a rapidly growing class of solids capable of responding dynamically to external stimuli, are redefining the design philosophy of functional materials[1,2]. These systems exhibit remarkable mechanical responses such as bending, twisting, curling, or jumping upon exposure to heat, light, pressure, or solvent vapors[3-5]. Unlike conventional rigid and brittle crystals, smart crystalline materials integrate the long-range order of crystals with the adaptive behavior of soft materials, creating new opportunities for device-oriented applications. Recent advances in crystal engineering have enabled the rational design of molecular solids that display controlled and reproducible mechanical motion[5-8]. The ability to tune these responses through subtle changes in molecular structure and packing arrangements has opened pathways toward responsive systems that can operate as mechanical actuators, soft robotic components, artificial muscles, and self-actuating devices. Such materials not only demonstrate fascinating physical phenomena but also offer practical value in fields requiring precise, reversible, and energy-efficient motion at the microscale or macroscale[9,10].

This presentation will explore recent developments in the field of smart crystalline materials, emphasizing how their unique mechanical behavior arises from well-defined structure–property correlations. By bridging the gap between crystalline order and mechanical adaptability, these materials represent a promising platform for next-generation functional materials and devices that combine responsiveness, stability, and high performance.

**Keywords:** Smart Crystalline Materials, Solid State, Functional Materials

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# Capacitive In-Memory-Computing: A Device to Systems Level Perspective on the Future of AI Hardware

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**Abstract**

The quest for energy-efficient, scalable neuromorphic computing has elevated compute-in-memory (CIM) architectures to the forefront of hardware innovation. While memristive memories such as resistive random-access memories (RRAMs), phase-change memory (PCM), magneto resistive random-access memory (MRAM), ferroelectric random-access memories (FeRAM) have been extensively explored for synaptic implementation in CIM architectures, their inherent limitations, including static power dissipation, sneak-path currents, and interconnect voltage drops, pose significant challenges for large-scale deployment, particularly at advanced technology nodes. In contrast, capacitive memories offer a compelling alternative by enabling charge-domain computation with virtually zero static power loss, intrinsic immunity to sneak paths, and simplified selector-less crossbar operation, while offering superior compatibility with 3D Back-end-of-Line (BEOL) integration. This talk will highlight the architectural and device-level advantages of emerging non-volatile capacitive synapses, including metal–ferroelectric–metal (MFM), metal–ferroelectric–semiconductor (MFS), ferroelectric field-effect transistors (FeFETs), and hybrid configurations. I will present how material engineering and interface control can modulate synaptic behavior, capacitive memory window (CMW), and multilevel analog storage potential. Furthermore, I will explain critical system-level trade-offs involving device-to-device variation, charge transfer noise, dynamic range, and effective analog resolution bringing to the conclusion that capacitive memories, with custom-built stacks, have the potential to become a foundational technology for the next generation of extremely energy-efficient neuromorphic computing platforms

**Keywords:** Compute-in-memory, Memristor, Capacitive Synapse, FeFET, Ferroelectric, Neuromorphic Computing

# $MoS_2$-graphene interface for molecular sensing and switching

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**Abstract**

This talk encompasses molecular response study of atomically thin heterostructures combining molybdenum disulfide ($MoS_2$), graphene, and hexagonal boron nitride (h-BN). The defect induced interfacial states are created in an atomically thin two-dimensional $MoS_2$ channel by underlying a narrow pattern of a graphene layer in a field-effect transistor. The presence of interfacial states in the channel leads to a conductance fluctuation. Its magnitude is modulated nearly three-order of magnitude at room temperature using the nitrogen dioxide gas molecules in the subthreshold region. The study provides a systematic experimental approach to establish a correlation between modulated conductance fluctuation and the molecular concentration up to parts-perbillion. First-principles density functional theory further explains the role of unique interfacial configuration on conductance fluctuation. The study determines a novel approach to induce charge-state for the modulation of carrier concentration and exploits the role of defect induced interfacial states in atomically thin interfaces for the molecular interaction.

**Keywords:** $MoS_2$,h-BN, Field Effect Transitor, FET, Heterostructure, Interfaces

## Ultra-thin materials for next-generation electronics and optoelectronics technologies

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**Abstract**

Atomically-thin materials possess unique intrinsic properties and are amenable to a range of tuning techniques. We harness these properties underpinned by application demand and work with industry to translate into end-user products.

Firstly, we synthesise a variety of atomically-thin metal oxides, mono/dichalcogenides and elemental 2D materials using solid, liquid and vapour phase techniques guided by application.

Using defect engineering, we have demonstrated neuromorphic vision and processing sensors. We have explored the use of hybrids of dissimilar materials to enhance electronic and optical performance. Ultra-thin layers have been used to develop one of the world's thinnest photodetectors that can sense all shades of light from UV-infrared. We further study strain-tunability in low-dimensional structures via integrating them onto elastomeric platforms.

Recently, we have investigated the influence of defects and strategies for passivation in monolayer transition metal dichalcogenides for applications in optoelectronics and health sensors. Using a cross-disciplinary approach, we deploy multifunctionality of these new material systems into solving technological challenges for industry partners across sectors that require novel materials and functions to be integrated into their products.

**Keywords:** Ultra-thin materials, 2D materials, Defect engineering, Neuromorphic vision, Photodetectors, Optoelectronics, Health sensors

# Oral Presentation

# Plastic waste-derived activated porous carbon through thermochemical conversion: A circular pathway towards sustainable carbon black feedstock

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**Abstract**

Plastics have become indispensable in modern life due to their versatility, adaptability, and low production cost. Plastic waste generation worldwide exceeds 350 million tonnes annually, with only 9% recycled and nearly 50% sent to landfills. Approximately 22% of this waste is mismanaged, adding 8–10 million tonnes to oceans each year. The low recycling rates and use of short-lived packaging emphasize the urgent need for sustainable methods to convert plastic waste into high-value materials to reduce environmental harm. This study explores the conversion of post-consumer plastic waste into high-value carbon materials through pyrolysis and subsequent activation, with the objective of developing an alternative carbon black feedstock (CBFS). Mixed polyolefin plastics (PE and PP) were thermally decomposed at 500–600°C under an inert atmosphere to yield pyrolytic oil and carbonaceous char (pyrochar). The pyrochar underwent chemical activation using potassium hydroxide (KOH) and zinc chloride ($ZnCl_2$) to enhance its porosity, surface area, and adsorption capacity. The effects of activation temperature and chemical ratio were systematically examined to optimize yield and structure. Comprehensive characterization via BET surface area analysis, SEM, and elemental analysis revealed the formation of highly porous, predominantly amorphous carbon with partial graphitic ordering and physicochemical properties comparable to commercial carbon black. The pyrolysis oil fraction was further upgraded through catalytic aromatization to increase aromaticity and viscosity, aligning its composition with that of petroleum-derived CBFS. Comparative assessments showed that the optimized activated carbon achieved a carbon content above 88 wt%, sulfur below 0.5 wt%, and a hierarchical pore structure suitable for reinforcement, adsorption, and conductive applications. Conclusively, the study demonstrates a sustainable and circular approach for transforming plastic waste into activated porous carbon, offering a viable, eco-friendly substitute for conventional carbon black feedstock and reducing dependency on fossil-derived raw materials. The investigation extends to exploring innovative avenues for replacing CBFs with activated pyro-char in industrial applications and conducting its techno-economic assessment.

**Keywords:** Carbon black, Chemical activation, Plastics, Pyrolysis, Sustainable material, Waste-to-Wealth

# SH-Wave propagation in a functionally graded piezoelectric plate clamped between a temperature-dependent layer and a microstructurally coupled substrate

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**Abstract**

The present article investigates horizontally polarized shear wave (SH-wave) into a composite structure comprised of functionally graded piezoelectric material (FGPM) plate clenched between a temperature dependent plate and a microstructural coupled stress half-space subjected to the perfect and imperfect interfaces. A linear temperature variation taken into the uppermost temperature dependent plate, whereas an exponential depth variation considered into the FGPM plate. To analyze the problem, the classical dynamical coupled theory has been adopted. Analytical methods have been employed to compute the displacement and stress components of the each medium. With appropriate boundary conditions, dispersion equations for SH-wave propagation have been developed for both cases: in the absence and in the presence of imperfection interfaces of the structure for electrically short case. Impacts of various involved parameters into the both dispersion equations, on the velocity profile of the SH-wave have been observed by numerical examples and graphical demonstrations. The role of temperature ratio, gradient factor, electric constant, couple tension, imperfection parameter, etc. on the propagation behavior of SH-wave has been extensively investigated in the considered models.

**Keywords:** SH-wave, Dispersion equation, Functionally graded piezoelectric, Phase velocity, Coupled stress, Temperature-dependent, Imperfect interface

# Fabrication and characterization of $Fe_3O_4$ dispersed PEDOT:PSS field effect transistor

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**Abstract**

Nowadays the field of semiconductor electronics is dominated by charge based devices, which have sustained the exponential growth in computational power as described by Moore's Low. Static Magnetic Field Effect Transistor (SMFET) overcomes this limitation by using static magnetic field to modulate carrier transport, reducing leakage and short channel effect without further downsizing. Here carrier concentration is modulated by gate voltage or externally applied static magnetic field. The integration of static magnetic field control enables high precision magnetic sensing, spintronic capabilities and low power multifunctional electronics through SMFET as a promising candidate for advanced nanoscale device applications made through high mobility spin scattering channels.

$Fe_3O_4$ embedded in PEDOT:PSS introduces strong magnetic scattering due to its intrinsic ferromagnetic properties, high spin polarization and carrier mobility modulation under static magnetic field. This property enhances the controlling of channel conductivity[1].It is established as a flexible channel with ionic gating[2] as well as the solid state[3]. PEDOT:PSS offers a high mobility matrix for spin dependent scattering which is attempted in this paper forming a hybrid magnetoelectric FET.

A channel material was formed by curing PDOT:PSS solution with dispersed $Fe_3O_4$ which was further spin coated to form the semiconducting base on an over doped Silicon surface which is P+. The backed semiconducting layer was characterized for its mobility, charge carrier type and charge density. The electrodes were evaporated to form source and drain with bottom gating. The surface morphology was studied with AFM and structural confirmations were done using XRD. Further, the single junction characteristics were studied across source- channel and drain- channel junctions. The junctions were found symmetric and rectifying. The barrier height was computed to be 0.84 eV. Further the transfer characteristic yielded threshold voltage to be 2.36 V at drain voltage of 1 V. The FET was stable over output cycles. The output characteristics were found to be tunable with applied magnetic field. Overall, we demonstrate a spins catering based field effect transistor with on off ratio off the order of $10^5$ which is magnetically as well as electrically tunable.

**Keywords:** Static magnetic FET, Polymer Composite, Bottom gated FET, Electrodoping

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# Quantum conductance in $MoO_3/TiO_2$ heterojunction memristors: crafting controlled analog-to-digital transition for multilevel memory applications

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## Abstract

Future technologies based on quantum phenomena require functional materials that exhibit quantised conductance during resistive switching. The precise control of quantum jumps during conduction is required to achieve such technologies. Here, we report a solution-processed bilayer Au/$MoO_3$/$TiO_2$/FTO resistive switching device showing an excellent memory window and long endurance ($\sim 5000 cycles$). Process-induced oxygen vacancies form the conduction filament, resulting in abrupt jumps in the conductance. By controlling the optimized scan rate, a transition from analog to digital switching is achieved. The SET process can be controlled by means of bias scan range and scan speed, exhibiting quantized conductance levels. Histogram of the quantized conductance over multiple cycles reveals that the SET process proceeds with nG0 jumps ($\sim n = 1 - 6$). Our results show that such bilayer systems can be utilized for next-generation multibit storage devices[1]

**Keywords:** Quantum Conductance, Memristor, Solution-processed, Bilayer Oxide, Heterojunction, Analog-to-Digital Switching, Resistive Switching, RRAM

**References:**

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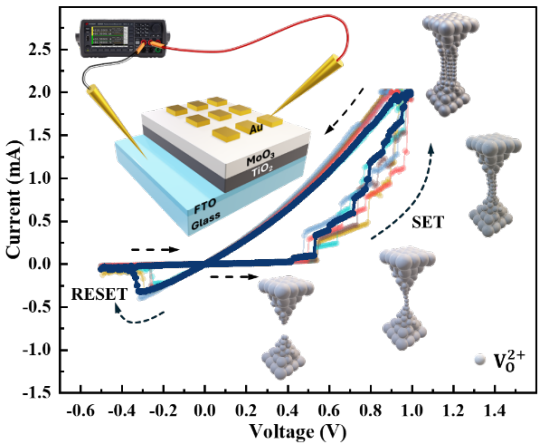


**Figure:** Quantized conductance jumps in $MoO_3/TiO_2$ bilayer-oxide memristor

# Hybrid microwave sintered multifunctional multiferroics as energy harvester and flexible screen printed absorption dominant energy shields: ML driven composition prediction

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**Abstract**

The advancements in energy supply technology for wireless sensor networks within the Internet of Things (IoT) have been significant; however, efforts to implement sustainable and environmentally friendly energy solutions for these sensor networks are still restricted. Additional challenge faced due to implementation of IoT is electromagnetic interference (EMI). Devices that harvest and shield energy through the magnetoelectric coupling effect exhibit significant potential for solving issue of energy supply and EMI. Thus, based on the need we have designed: two possible multiferroics: one for magnetoelectric (ME) energy harvesting using rigid materials, and the other for electromagnetic interference shielding using flexible materials. To start with, the composition of BZT is predicted by modelling Random Forest (RF) algorithm in Machine Learning (ML) keeping $T_c$ and $\epsilon'$as criteria using a data-intensive framework. The study of rigid multiferroics, (($Ba_0.5Zr_0.5T_iO3$ (BZT) + $Y_3Fe_5O_{12}$ (YIG)) (BY)), is being conducted for utilization in ME applications. An optimized microstructure and material composition of a rigid BY composite resulted in an enhanced SME (self-biased ME coupling effect) of 1.74 mV/(cm-Oe). For EMI shielding, we tested PVDF/BY (PBY) flexible films with 10, 20, 30, and 40 wt.% ceramic. With the help of CST Studio Suite Software electromagnetic field simulations for the flexible films is anticipated. A reflection loss of -47.9 dB is observed in experimental research, indicating that the PBY composite with 40 wt% offered outstanding absorption capability.

**Keywords:** Multiferroics, EMI shielding, Machine Learning, Random Forest Algorithm, Energy Harvesting, Screen printing

# Impedance spectroscopic studies of the electric conduction in polycrystalline in Ferrites materials

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**Abstract**

Polycrystalline spinel ferrites have wide applications in various technical fields due to their interesting electrical and magnetic properties. It's well known that the intrinsic properties of ferrites depend on chemical composition, preparation condition and substitution. As they are important materials for applications in various fields like electronic, electrical, engineering, magnetic memories, medicines etc., In the present work polycrystalline sample of $Mg_xCu_{0.5}Zn_{0.5-x}Fe_2O_4$ in which x=(0.0, 0.1, 0.2, 0.3, 0.4 and 0.5) were prepared by double conventional sintering process. The formation of single phase was confirmed by X-ray diffraction. In the present work a systematic study on the AC - DC electrical conductivities of this ferrite were investigated. The measurements were carried out in the temperature range 30°C - 490°C, and in the frequency range from 100 Hz to 1 MHz. Methods for extraction of bulk and grain boundary capacitance from permittivity and electric modulus complex plane plots are discussed. Because it can easily distinguish between bulk and grain boundary effects played an important role in their dielectric behaviour, complex plane impedance and modulus techniques were used to separate out the contribution of grain and grain boundaries A simplified model, consisting of bulk material separated by highly resistance grain boundary layers is proposed when the content of magnesium decreases.

**Keywords:** Ferrites, X-ray diffraction, SEM patterns, Electrical conductivity, Impedance

# Multifunctional polyvinyl alcohol based nanocomposites for water induced shape memory and flexible electronics

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**Abstract**

Shape memory polymers (SMP) are smart materials which can be deformed into a temporary shape and then recover to the original shape upon exposure to an external stimulus. The present investigation water induced SMP was developed by incorporating cellulose nanofibers (CNF) and graphene oxide (GO) to polyvinyl alcohol (PVA). The PVA/CNF-GO hybrid nanocomposite at 1 wt% exhibited synergistic effect with superior water-induced shape memory performance, with 100% shape recovery within 37 sec. Moreover, these hybrid nanocomposite films at 1 wt% demonstrate superior mechanical strength of 77.9 MPa and an improved glass transition temperature ($T_g$) of 61.4°C in dry conditions. PVA based nanocomposites with amine-functionalized multiwalled carbon nanotubes (MWCNTs) were developed for flexible electronics, sensors, and energy storage devices. The electrical percolation threshold was identified at 2 wt% MWCNTs, revealing a remarkable five-order-of-magnitude increase in electrical conductivity of nanocomposites as compared to pure PVA. The mechanical properties demonstrate a critical balance between MWCNTs loading and dispersion, with a peak tensile strength of 50.5 MPa at 3 wt% MWCNTs. Wettability studies demonstrated a reduction in the hydrophilic nature of PVA with MWCNTs, where an increase in the contact angle from 48°for pure PVA to 114°at 5 wt% MWCNTs emphasized the influence of MWCNTs on surface interactions. The investigation summarised the performance benchmarks for PVA nanocomposites for advanced technological applications.

**Keywords:** Polyvinyl alcohol, Cellulose nanofibers, Graphene oxide, Multiwalled carbon nanotubes, Nanocomposite

# PVDF composites: an excellent piezoelectric energy harvesting and storage material for wearable devices

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**Abstract**

Human health and well-being are major focuses of current research worldwide. Self-powered smart wearable technology shows great promise for enhancing human life. However, developing materials with high energy storage capacity for powering sensors, wearables, and portable electronics remains challenging. Accordingly, in this study we fabricated novel PVDF/APTES functionalized-$Ba_{0.7}Sr_{0.3}Zr_{0.02}Ti_{0.98}O_3$(50wt.%)/COOH functionalized-CNT (0, 0.3, 0.5, 0.7 wt.%) composites (PVDF/f-BSZT/ $f_1$-CNT) through solution casting method. Surface modification of fillers contributes to their perfect adhesion with polymer. This contributes to the distribution of applied electric field which improves the breakdown strength and mechanical properties even after a high f-BSZT loading (50 wt.%) along with well-dispersed conductive $f_1$-CNT. The FESEM images displayed aligned PVDF fiber indicating the high $\beta$ phase content of PVDF/f-BSZT/f-CNT. The PVDF/f-BSZT/ $f_1$-CNT (0.5 wt.%) showed outstanding energy storage behavior through representing the highest energy storage density ($U_e$) and energy storage efficiency ($\eta$) of about 14 J/cm$^3$ and 89.6% respectively. Also, PVDF/f-BSZT/ $f_1$-CNT (0.5 wt.%) showed an excellent piezoelectric output voltage of about 25.7V. Accordingly, the PVDF/f-BSZT/$f_1$-CNT (0.5 wt.%) was introduced through various biomechanical movements like finger clapping, tapping and foot stressing to investigate its energy harvesting application A relative comparison of $U_e$, $\eta$, maximum polarization (Pm) along with piezoelectric power density, Voc, and Isc of PVDF/f-BSZT/ $f_1$-CNT (0.5 wt.%) with some recently reported works shows its exceptional energy storage and harvesting properties. Thus, PVDF/f-BSZT/ $f_1$-CNT (0.5 wt.%) is an exciting novel energy material, withholding the possibilities of efficient renewable energy devices.

**Keywords:** PVDF composite, BSZT, Piezoelectric material, Energy storage, Energy harvesting

# Ruthenium nitrosyl complexes based functional soft nanomaterials for cancer therapy

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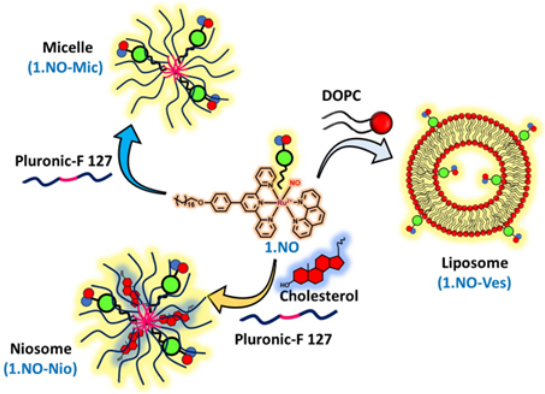
**Abstract**

Nitric oxide (NO), once regarded as an atmospheric pollutant, is now recognized as a key signalling and therapeutic molecule. However, its biomedical use is constrained by its short half-life, poor biocompatibility of existing donors, and lack of spatiotemporal control over release. To address these challenges, we report a newly synthesized amphiphilic ruthenium nitrosyl complex **(1.NO)** as a photoactivatable NO donor and its incorporation into three nanocarrier systems: vesicles **(1.NO-Ves)**, micelles **(1.NO-Mic)**, and, for the first time, niosomes **(1.NO-Nio)**. The NO release behaviour of free and encapsulated **1.NO** was investigated by UV–Vis spectroscopy, Griess assay, and DAF-FM DA fluorescence under 420 nm blue-light irradiation. Free 1.NO liberated up to 11 $\mu$M NO, while nanoencapsulation resulted in more sustained release, for vesicles, micelles, and niosomes, respectively.

In vitro studies against the 4T1 breast cancer cell line revealed potent photo-triggered cytotoxicity for all three nanocarrier formulations, with **1.NO-Ves** exhibiting the highest therapeutic efficacy. These results demonstrate that nanocarrier architecture significantly modulates the release kinetics and biological activity of Ru–NO photo-donors. This work highlights the importance of rational nanocarrier design in advancing controllable NO delivery systems for cancer therapy.

**Keywords:** Ruthenium nitrosyl complex, Nitric oxide delivery, Liposomes, Micelles, Niosomes, Biocompatibility.



# Layer-by-layer deposition of polyurethane/reduced Graphene Oxide/PANI composites for electromagnetic interference shielding application

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**Abstract**
Electromagnetic waves within the microwave frequency spectrum (2–18 GHz) are integral to modern communication and electronic systems. However, their interactions with various materials and living organisms can have significant adverse effects. Electromagnetic interference (EMI) from multiple devices impairs performance and data transfer. Additionally, EMI raises health concerns for individuals subjected to prolonged exposure. Metals, owing to their low skin depth, have traditionally served as effective EMI shielding materials. However, their high density, susceptibility to corrosion, cost, and limited flexibility render them less optimal for contemporary lightweight, portable, and flexible devices. Consequently, there is an increasing interest in developing lightweight, cost-effective, and shape-conforming porous materials as alternatives to EMI shielding. Recently, there have been reports on the use of polyurethane (PU) foams as EMI shields[1-3].
Multiple techniques have been explored for developing flexible materials for EMI shielding applications. Here, we report on the development of an EMI shield utilizing a layer-by-layer (LBL) deposition technique. The LBL technique yields a layer assembly that uses the electrostatic charge distribution of oppositely charged layers to form uniform, thin films. Subsequently, the deposition parameters, including the number of layers, deposition time, and layer composition, play a vital role in the behavior of LBL-deposited samples. The deposition parameters were optimized for porous polyurethane foams using PANI dispersed in DI water and rGO dispersed in DMSO as the precursors. The structural, microstructural, electrical, and EMI shielding efficiency characterization was performed on this system. The formation of layer-by-layer deposited coatings using PU foams has enabled a fourfold enhancement in EMI shielding efficiency in the X–band (8–12 GHz) frequency range. The effect of filler content and conductivity on the EMI shielding efficiency is explored.

**Keywords:** Layer-by-layer deposition, EMI shielding, Polymer composites

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# Engineering ferromagnetism in wide band gap w-AlN for spintronic applications: insights from DFT calculations

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## Abstract

Spintronics, with its promise of enhanced data storage and quantum computing, hinges on the development of practical dilute magnetic semiconductors (DMS)[1]. This presentation details a theoretical investigation into the magnetic properties of Cr, Ru, and Rh-doped w-AlN, using spin-polarized density functional theory (DFT) calculations with supercell models [2]. Analysis of our formation energies of point-defects (Figure 1) reveals that $Cr^{4+}$, $Ru^{4+}$, and $Rh^{3+}$ are the most probable charge states for these dopant atoms substituting Al in w-AlN. Significantly, Cr-doped AlN demonstrates stability in the ferromagnetic state, crucial for spintronic devices, across a range of Cr concentrations (1.85 to 16.67% of Al). Conversely, Ru and Rh-doped AlN, even in their preferred charge state, were found to be unstable in the ferromagnetic configuration.

Further investigation into the electronic density of states (DOS) of ferromagnetic Cr-doped AlN highlights a fascinating evolution: it remains insulating for Cr concentrations below 5.56%, transitions to a half-metal state between 7.40 and 12.96%, and finally becomes a normal metal at 16.67% Cr. This tunable electronic behavior, particularly the half-metallic characteristic, is absent in the energy-favored antiferromagnetic states of Ru and Rh-doped systems[2]. This work provides crucial theoretical insights into engineering ferromagnetic w-AlN, a promising material for future spintronic technologies.

**Keywords:** Ferromagnetic semiconductor, Aluminum nitride (AlN), Charge state of dopants, Spintronics

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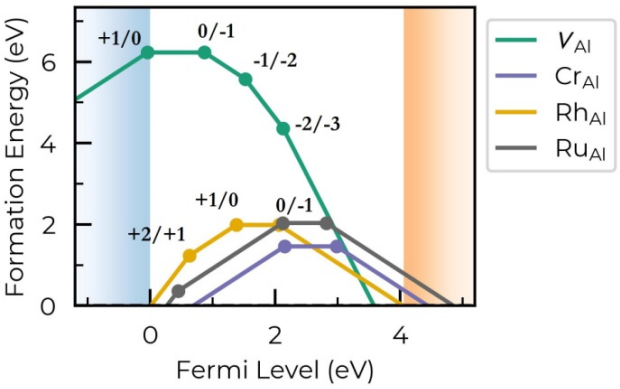


**Figure:** Defect formation energies for point-defects, namely, aluminum vacancy ($V_{Al}$), substitutional chromium ($Cr_{Al}$), substitutional ruthenium (RuAl), and substitutional rhodium ($Rh_{Al}$) in w-AlN as a function of the Fermi level under nitrogen-rich condition

# Investigations of magnetic properties of holmium-doped cobalt–zinc ferrite

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**Abstract**

A vast range of applications of nano cobalt ferrite as a magnetic ceramic in material and biological science and technology suggests a need to optimize its magnetic features. Holmium-doped cobalt–zinc nano sized ferrite with the chemical formula $Co_{0.8}Fe_{2-x}Zn_{0.2}Ho_xO_4$ and with x ranging from 0.00 to 0.03 in step of 0.01 were synthesized by the combustion method and then analyzed to know their magnetic parameters. The magnetic properties of these magnetic materials are manifested in the form of magnetisation, coercivity, squareness ratio of the loop, which can be obtained experimentally through VSM studies. The magnetic energy stored in the material is greatly affected by the thermal energy variations. The order-disorder phase transitions that take place during the studies of variation of magnetisation with temperature is also significant in determining the critical temperature. The domain size, orientation and the exchange interactions between the spin magnetic moments also depend upon the structural parameters. Magnetostriction measurements were measured using strain gauge sensor. It is also envisaged that the magnetic interactions between 3d and 4f subshells of transition and rare earth ions may result in new results. In addition to this, the nano ferrites exhibit superparamagnetic behaviour and may altogether show drastic changes in the above-mentioned magnetic parameters.

**Keywords:** VSM, Magnetization, Coercitivity, Magnetostriction

# Enhancement of the magnetoimpedance ratio of $Co_{77}Si_5Cu_1Nb_2B_{15}$ ribbons with the permalloy coating

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**Abstract**

The Magnetoimpedance (MI) effect refers to the change in the electrical impedance of a soft ferromagnetic conductor under an applied DC magnetic field. This phenomenon can be exploited to develop sensors for detecting weak magnetic fields. The MI effect strongly depends on material properties such as DC electrical conductivity ($\sigma$) and magnetic permeability ($\mu$). For the present study, melt-spun ribbons with composition $Co_{77}Si_5Cu_1Nb_2B_{15}$ were used. The sensitivity of these materials can be further enhanced by magnetic softening, for example, by coating the ribbons with magnetic thin film. Permalloy ($Ni_{80}Fe_{20}$) is well known for its vanishing magnetic anisotropy, high magnetic permeability, and extremely low hysteresis loss compared to other available magnetic materials. Therefore, we coated the $Co_{77}Si_5Cu_1Nb_2B_{15}$ ribbons with permalloy using the electrodeposition technique and conducted MI studies on these coated ribbons. Additionally, DC Joule annealing was performed on the coated ribbons to relieve the induced strains in the deposited films. Interestingly, the MI ratio was found to be significantly higher in the DC Joule-annealed coated ribbons compared to the others. Fig. 1 shows the MI curves of the bare ribbon, coated ribbon, and coated followed by annealed ribbon.

**Keywords:** Magnetoimpedance, Electrodeposition, Sensitivity, Permalloy

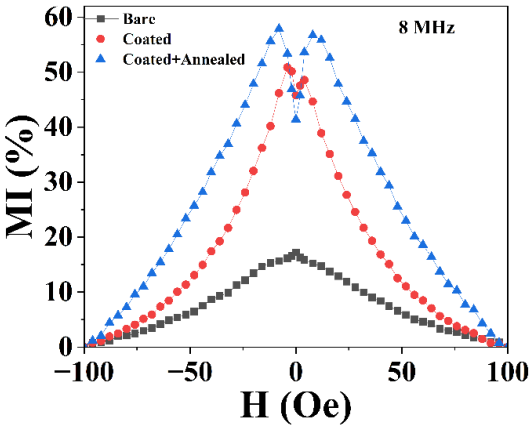


**Figure:** MI ratio of the $Co_{77}Si_5Cu_1Nb_2B_{15}$ ribbons

# Microwave-assisted polyol synthesis of porous $Fe_3O_4$ nanoparticles with tuneable size and enhanced magnetization

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**Abstract**

The rational design of porous magnetic nanostructures remains a critical challenge for multifunctional deployment in catalysis, biomedical delivery, and environmental remediation. Here, we report the microwave-assisted polyol synthesis of porous $Fe_3O_4$ nanoparticles, offering accelerated kinetics, homogeneous nucleation, and process scalability relative to the conventional thermal routes. Systematic modulation of $Fe^{3+}$ precursor concentration (0.1-0.2 mol/L) and digestion time (90-180 mins.) enabled precise control over crystallinity, porosity, and magnetization. Powder X-ray diffraction confirmed phase-pure magnetite with crystallite sizes tunable from ~23 to 42 nm. Transmission electron microscopy studies revealed nanoporous morphologies driven by lattice-oriented attachment and selective dissolution phenomena, further corroborated by compositional mapping. Magnetization measurements confirmed high saturation magnetization values of ~82-84 emu/g, with negligible hysteresis openings resembling near-superparamagnetic responses. Thermogravimetric analyses indicated robust thermal stability, reinforcing the suitability for high-temperature catalytic operations. Collectively, these results establish a direct synthesis-structure-property correlation, positioning the microwave-assisted polyol strategy as a high-throughput, tunable platform for producing porous $Fe_3O_4$ nanostructures. The resulting materials, with their enhanced magnetic response, tunable size, tailored porosity, and thermal resilience, are suitable for various applications such as magnetic separation, drug delivery, and heterogeneous catalysis.

**Keywords:** Porous $Fe_3O_4$ nanostructure, Microwave-assisted synthesis, Polyol synthesis, Tunable porosity

# Fabrication and characterization of benzaldehyde molecular schottky junction with magnetic electrode

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**Abstract**

In this study, we aim to understand the flow of spin in the junction between a metal and a semiconductor by attaching benzaldehyde molecules covalently onto silicon (100) surfaces. This attachment process is facilitated by thermal grafting, which involves the use of silicon-hydrogen (Si-H) groups on the surface. The goal is to create a catalytically active environment, particularly for the ferromagnetic nickel electrode. We investigate how the movement of spin current is influenced in the junction where a ferromagnetic nickel electrode meets a semiconductor (p-Si) by attaching benzaldehyde molecules to the silicon surface. By altering the arrangement of molecules at the junction, we observe changes in the total dipole moment. This change is significant because it affects the magnetoresistance (MR) (the change in electrical resistance under the influence of an external magnetic field) within the junction. We examine the electrical characteristics of the fabricated junction, Ni/$C_7H_6O$/p-Si/Al, by studying both the current-voltage relationship and the capacitance-voltage behavior. This helps us understand how the spin current is affected by the application of a magnetic field. To analyze the electrical properties of the silicon wafer's surface, we employ a modified version of the field emission theory. This theory allows us to effectively track changes in the surface properties of the wafer under the influence of external electrical fields.

**Keywords:** Molecular schottky junction, Benzaldehyde, Barrier height, Ideality factor, Magnetoresistance

# Electrochemical simulation of SnSe coated porous nickel electrodes for supercapacitors

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**Abstract**

The development of high-performance supercapacitors hinges on the design of electrodes with large surface area, excellent conductivity, and stable electrochemical behaviour. In this work, a two dimensional finite element simulation study of porous nickel electrode architecture was conducted to evaluate the electrochemical performance of nickel substrates coated with tin selenide (SnSe) as the active material, immersed in a 6 M KOH electrolyte. A comprehensive literature survey reveals that transition metal dichalcogenides such as SnSe offer pseudocapacitive behaviour with high theoretical capacitance and good structural stability, while porous nickel ensures efficient ion transport and electronic coductivity. The model geometry replicates the interconnected porous network of nickel and physicochemical parameters including electronic conductivity, diffusion coefficients and electric double-layer formation that were extracted from recent experimental studies to ensure realism. Cyclic voltammetry (CV) simulations were performed at scan rates ranging from 5 to 100 mV $s^{-1}$ to characterize redox peak currents and calculate specific capacitance. Galvanostatic charge–discharge (GCD) profiles were generated at current densities of 0.5 to 10 A $g^{-1}$ to determine energy and power densities, while electrochemical impedance spectroscopy (EIS) simulations spanning 10 mHz to 100kHz provided insight into charge-transfer resistance and diffusion-controlled processes. This simulation framework offers a predictive platform for optimizing porous pseudo-capacitor electrodes prior to experimental validation.

**Keywords:** Supercapacitor, Porous nickel, Tin Selenide, Simulation

# Microbial fuel cell from coconut water

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## Abstract

Renewable energy is the future of electricity generation. As the focus shifts from coal and hydrocarbons, many other sources of power are being explored. MFCs hold a great potential in renewable energy. Microbes are present on various solutions, including waste waters, including the rotten or discarded coconut water. The microbes present in the rotten coconut water can be used for our microbial fuel cell. These microbes like *Citrobacter freundii, Klebsiella pneumoniae, Pseudomonas aeruginosa* etc produce chemical energy from organic sources. This chemical energy is converted into electrical energy. The coconut water is kept at the anode side that releases electrons as well as protons. After that, proton moves to the cathode to finish the reaction, and the electrons that remain move through an external circuit to generate electricity. This MFC is cost effective and eco-friendly and helps to generate electricity at cheaper costs with causing less harm to the environment.

**Keywords:** Microbial fuel cell, Spoilt coconut water, Electrode

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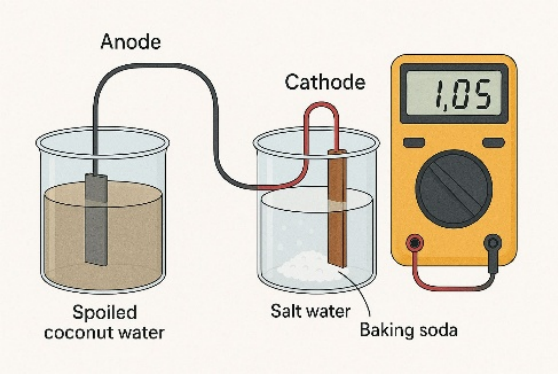


**Figure:** Microbial fuel cell from Coconut water

# Nanostructured $Li_4Ti_5O_{12}$–$TiO_2$ dual-phase electrodes synthesized via sol–gel method for enhanced energy storage applications

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**Abstract**

Nanotechnology facilitates the design of materials at the nanometer scale, providing distinct advantages including elevated surface-to-volume ratios, reduced ion pathways, and adjustable interfaces that improve charge transport, thereby proving to be highly effective for energy storage applications. In this context, dual-phase $Li_4Ti_5O_{12}$–$TiO_2$ nanoparticles (LTO–$TiO_2$) were synthesized using a sol–gel method and characterized through XRD, SEM, TEM, and XPS techniques. The XRD analysis indicated an average crystallite size of approximately 28 nm, and microscopic studies validated a well-defined nanoparticle morphology. This nanoscale architecture, characterized by reduced particle size, increased surface area, and clearly defined phase interfaces, enables swift ion/electron transport and offers numerous active sites for charge storage. Electrochemical evaluations utilizing CV, GCD, and EIS demonstrated a specific capacitance of 350 F $g^{-1}$ at 1 A $g^{-1}$, showcasing remarkable cycling stability with 90% retention after 2000 cycles, along with a coulombic efficiency of 99%. The findings indicate that LTO–$TiO_2$ dual-phase nanoparticles, achieved through advanced nanoscale engineering, serve as highly efficient and durable electrode materials for next-generation electrochemical supercapacitors.

**Keywords:** $Li_4Ti_5O_{12}$, Sol-gel method, Nanoparticles ,Cyclic voltammetry ,Supercapacitor

# First principles investigation of doping induced band gap engineering in $BaZrS_3$ perovskites for solar cell applications

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## Abstract

$BaZrS_3$, a chalcogenide perovskite, has emerged as a promising candidate for photovoltaic (PV) applications due to its direct band gap, high absorption coefficient, and superior thermal and chemical stability[1]. Unlike halide perovskites, $BaZrS_3$ is composed of earth-abundant and non-toxic elements, making it an environmentally sustainable material. However, its relatively wide band gap (~1.7 eV) limits its efficiency in single-junction solar cells, necessitating effective band gap tuning strategies. Doping-based band gap engineering in $BaZrS_3$ can be broadly categorized into two approaches: (i) substitutional cationic doping with elements containing valence d-orbitals, which lower the conduction band edge, and (ii) substitutional anionic doping with elements having valence p-orbitals, which raise the valence band edge. Transition-metal doping at the Zr-site, such as Ti and Sn, has been extensively investigated for band gap reduction. Ti doping effectively narrows the band gap but tends to induce phase segregation and generate defect states at higher concentrations. In contrast, Sn doping provides better phase stability and a substantial band gap reduction, although it requires precise non-equilibrium growth conditions to avoid secondary phase formation. Cation substitution at the Ba site with Ca is structurally favorable compared to Ti or Sn substitution at the Zr site, owing to the structural similarity between $BaZrS_3$ and $CaZrS_3$. Anionic substitution, particularly Se alloying at the S site, also effectively reduces the band gap by raising the valence band maximum while preserving a high absorption coefficient; however, solubility limits and structural stability remain challenging[2]. While previous studies have independently explored the effects of Ti, Sn, Ca, and Se doping or alloying on the band gap tuning of $BaZrS_3$, a comprehensive comparative analysis of these dopants within a unified computational framework remains lacking. This manuscript presents a first-principles investigation using density functional theory with Hubbard corrections (DFT + U) to systematically compare the structural, electronic, and optical effects of Ti, Sn, Ca, Sr, and Se alloying in $BaZrS_3$, focusing on their effectiveness in narrowing the band gap to the optimal range of 1.3-1.5 eV for solar absorption while maintaining structural stability. The optimized structure for various dopants studied (Ti, Sn, Ca, Sr and Se) together with their formation energies are depicted in Fig. 1.

**Keywords:** Perovskites, Ab initio, Solar cell, Band gap

**References:**

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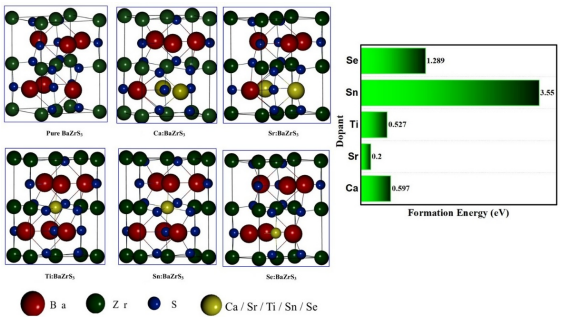


**Figure:** Optimized crystal structure of pure and doped $BaZrS_3$ and corresponding dopant formation energies.

# Doped $WS_2$ and $MoS_2$ semiconductors as ferromagnetic spin catalysts for overall water splitting

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**Abstract**

Ferromagnetic spin catalysts, taking advantage of the spin degree of freedom, are expected to show excellent electrochemical hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) activity due to spin-controlled electrochemical reactions. However, developing low-cost, earth-abundant, and highly efficient spin catalysts remains challenging for overall water-splitting applications. Herein, we demonstrate excellent HER and OER bifunctional activity of Fe-and Co-doped $WS_2$ (Fe-$WS_2$ and Co-$WS_2$) and Ni-doped $MoS_2$ (Ni-$MoS_2$) ferromegnetic spin catalysts in 1M KOH electrolyte. The prepared Fe-$WS_2$, Co-$WS_2$, and Ni-$MoS_2$ exhibit ferromagnetic spin ordering at room temperature with high saturation magnetization. It is noted that Fe-$WS_2$, Co-$WS_2$, and Ni-$MoS_2$ emerge as promising spin catalysts for HER and OER activity, offering long stability, high active sites, and low overpotential operation. The spin-polarized Fe-$WS_2$, Co-$WS_2$, and Ni-$MoS_2$ catalysts deliver a 10 mA $cm^{-2}$ current density at an overpotential of 319, 135, and 175 mV vs. RHE with Tafel slopes of 106, 66, and 70 mV $dec^{-1}$ for HER. On the other side, the same catalyst required 450, 378, and 302 mV vs RHE overpotential to deliver 10 mA $cm^{-2}$ current density with a Tafel slope of 98, 86, and 62 mV $dec^{-1}$ for OER activity. The spin polarized current of magnetic ion-doped $WS_2$ and $MoS_2$ creates spin channels that accelerate charge transfer and the enhance electrochemical activity of catalysts. This work addresses the challenges facing the rational design of efficient and low-cost spin-controlled bifunctional electrocatalysts for electrochemical overall water splitting.

# Cadmium sulfide nanourchins constructed with g-$C_3N_4$ for millimolar photocatalytic $H_2O_2$ production within a few minutes

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**Abstract**

An alternative that has been found to be promising to replace the traditional anthraquinone based industrial process is the artificial production of hydrogen peroxide ($H_2O_2$) with the use of only water, oxygen. Nevertheless, this can only be made possible by the development of cost-efficient, long-lasting, and efficient photocatalysts that do not require the assistance of sacrificial agent. We have successfully synthesized **g-$C_3N_4$-wrapped CdS nanostructures** featuring a **sea urchin-like morphology** and evaluated their performance in **photocatalytic hydrogen peroxide ($H_2O_2$) production**. Under visible light irradiation, the composite achieved a remarkable $H_2O_2$ yield of **1.5 mM within 30 minutes**, which is **15 times** higher than that of pristine CdS. Furthermore, the system exhibited excellent **selectivity**, reaching **92%**, representing an enhancement of **2.3 times** compared to unmodified CdS. The synergistic interaction between g-$C_3N_4$ and CdS, along with the unique structural architecture, contributes to the efficient charge separation, enhanced light absorption, and improved surface reaction kinetics, making this composite a highly promising candidate for sustainable and selective $H_2O_2$ photoproduction.

# Combined optical and electrical control of a low-power consuming (~fJ) two-terminal organic artificial synapse for associative learning and neuromorphic applications

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## Abstract

Optoelectronic synaptic devices outperform electrical synapses in speed, energy efficiency, and integration density. Recent progress in visual sensing and optogenetics has led to the integration of light-sensitive materials in these devices, promising unmatched speed, connectivity, and bandwidth. Here, we present a copper phthalocyanine (CuPc) based optoelectronic synaptic device boasting femto Joule power consumption stable at room temperature. The optoelectronic synapse can be operated with energy consumption as low as 430.4 fJ which is very attractive from the point of view of low-power neuromorphic devices. By modulating light pulses, the neuromorphic behavior can be emulated including excitatory post-synaptic current (EPSC), paired-pulse facilitation (PPF), transitioning from short-term plasticity (STP) to long-term plasticity (LTP), spike-rate dependent plasticity (SRDP) and spike-number dependent plasticity (SNDP), etc. Optical potentiation and electrical depression are observed with combined optical and electrical stimulation, proving the multi-functionality of the synapse. Furthermore, the device demonstrates classical associative learning behaviors like Pavlovian conditioning using optical and electrical stimuli. We have established the pain conditioning processes such as hyperalgesic response and pain extinction effects with varying optical pulse amplitudes. These results render the CuPc-based devices as multifunctional and highly versatile artificial synaptic devices for future computing applications, offering unprecedented efficiency and functionality in neuromorphic systems

**Keywords:** Optoelectronic synapse, Copper phthalocyanine (CuPc), Neuromorphic Computing, Synaptic plasticity

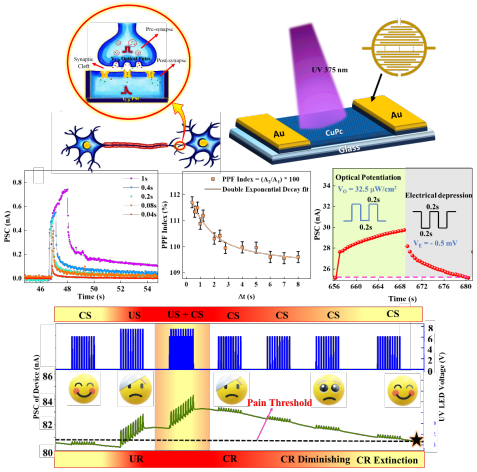


**Figure:** Schematic of biological and artificial synapses with representative optical and electrical synaptic measurements

# Bio-derived neuromorphic device using Aloe vera for energy-efficient computing exhibiting activity dependent synaptic plasticity

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**Abstract**

Neuromorphic computing systems aim to replicate the efficiency and versatility of the human brain by integrating advanced device architectures with bio-inspired elements. The potential of aloe vera, a sustainable, biocompatible, and natural polymer, as an active ingredient in two-terminal devices for neuromorphic applications is investigated in this work. This research reports a cost-effective fabrication method for the efficient fabrication of aloe vera based memristive device for emulating biological synapses. Pencil-on-paper (POP) approach, with multilayer graphene electrodes (MLG) are sketched on paper. The device exhibits excellent synaptic characteristics and can be operated at low energy range (~pJ), which is significant for neuromorphic devices. Activity-dependent measurements indicate that the threshold frequency of pulse trains, at which transition from depression to potentiation, is a function of prior activity. The non-linearity of potentiation-depression curves can be regulated by optimising the pulse parameters. This will help us to design neuromorphic devices with the required synaptic amplification. The pencil-on-paper (PoP) methodology represents an innovative advancement in the electrical domain, potentially leading to the development of flexible, portable, and eco-friendly devices with neuromorphic applications.

**Keywords:** Multilayer Graphene (MLG), Aloe vera, Multilevel memory, Energy consumption

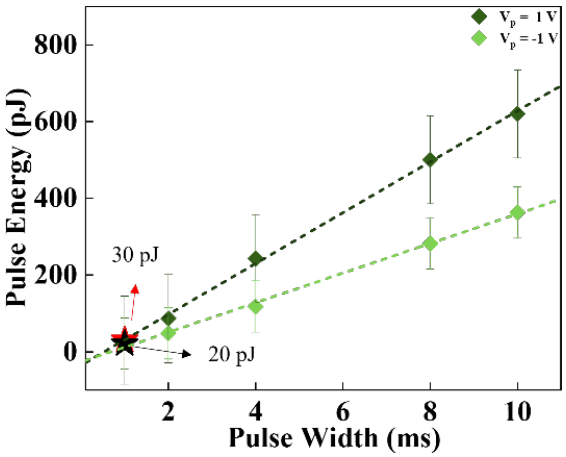


**Figure:** (a) Pulse energy calculated for ±1 V pulse by varying pulse width (Pw). Lowest energies are highlighted using red and black stars for 1 V and -1 V respectively. The read voltage is 0.5 V.

# Electrodeposited copper oxide as potential hole transport material in all perovskites tandem solar cell: numerical simulation-based estimation of power conversion efficiency

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**Abstract**

Thermalization and transmission are two major losses that confine the power conversion efficiency (PCE) of the single-junction solar cell. In this framework, all perovskite tandem solar cell, a combination of a wide bandgap (1.77eV) and a narrow bandgap (1.22eV) is used as a perovskite photoactive layer to study the performance of the device. The electrical and optical simulation was carried out using the solar cell capacitance simulator (SCAPS-1D) and the Transfer matrix method, respectively. Single junction wide-bandgap perovskite was simulated using experimentally prepared $Cu_2O$ and mixed-phase Cu-O($Cu_2O$+CuO) films and proved to be an efficient HTL with an efficiency of 16.18% and 10.59%, respectively. Whereas narrow bandgap solar cell results are in close agreement with the experimental one. Thus, the simulated results of the tandem solar cell pave the development of highly efficient cost-effective solar cells. The narrowband gap ITO/PEDOT: PSS/$FA_{0.7}MA_{0.3}Pb_{0.5}Sn_{0.5}I_3$/$C_{60}$/$SnO_2$/Cu device obtained an efficiency of ~21.85% which is in close agreement with that of the experimental published results with an efficiency of 21.7%. The SCAPS simulation for tandem structured 4-terminal devices, ITO/$Cu_2O$/$FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$/$C_{60}$/$SnO_2$/Au/PEDOT:PSS/$FA_{0.7}MA_{0.3}Pb_{0.5}Sn_{0.5}I_3$/$C_{60}$/$SnO_2$ /Cu and ITO/Cu-O/$FA_{0.8}Cs_{0.2}Pb(I_{0.6}Br_{0.4})_3$/ $C_{60}$/$SnO_2$/Au/PEDOT:PSS/$FA_{0.7}MA_{0.3}Pb_{0.5}Sn_{0.5}I_3$/$C_{60}$/$SnO_2$/Cu has achieved an efficiency of 28.57% and 22.91%, respectively using experimentally obtained value of electron affinity (≈2.84-2.86V). However, the PCE for CuO-HTL 2T PPTSC was 18.54% and that for $Cu_2O$ HTL-based 2T device was 24.15%. When electron affinity of CuO and $Cu_2O$ is increased to 3.80 eV , the corresponding 2T tandem device efficiency was raised up to 24.27% and 24.95% respectively. However, 4T tandem devices exhibit an efficiency >30% for Cu-O based tandem device. Thus, the simulated results of the tandem solar cell pave the development of highly efficient cost-effective solar cells.

**Keywords:** Electrodeposition, $Cu_2O$, SCAPS-1D, Perovskite, Tandem solar Cell

# $V_2O_9Te_2$ nanorods prepared via microwave method for photodetection and NLO applications

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## Abstract

In this work, vanadium oxytelluride (VOT) samples were synthesized successfully through a simple microwave (MW) technique, where the MW power was varied while keeping the irradiation time constant. XRD analysis confirmed the formation of the $V_2O_9Te_2$ phase with an orthorhombic crystal structure belonging to the Fdd2 space group. Raman spectroscopy verified the presence of various vibrational modes corresponding to bonds between the constituent elements, while XPS provided further insights into the chemical states and oxidation levels. Microscopy revealed nanorod-like surface morphologies, and EDX confirmed the elemental composition. Optical characterization showed bandgap energies between 3.63 and 3.69 eV, supporting the semiconducting nature of the samples. Photoluminescence (PL) spectra exhibited emission peaks in the 550–750 nm range, with a noticeable red shift as MW power increased. The photoresponse measurements under dark and illuminated conditions demonstrated appreciable responsivity and detectivity, underscoring the potential of VOT for photodetector applications. Nonlinear optical (NLO) studies using the Z-scan method revealed saturable absorption (SA) behavior and a valley-peak signature consistent with self-focusing, indicating positive $n_2$ values. The observed NLO features arise from a two-photon absorption (2PA) mechanism, while the third-order susceptibility $\chi^{(3)}$ values further establish VOT as a promising material for advanced optoelectronic and nonlinear optical applications.

**Keywords:** Vanadium oxytelluride, Microwave synthesis, Two-Photon absorption, Photodetection

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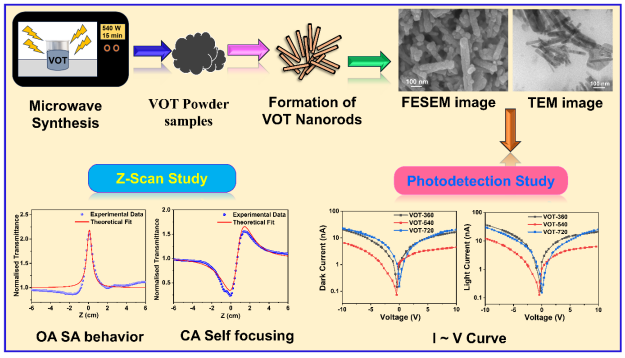

# Probing the relaxation pathways of yellow and narrow red emitting carbon dots by femtosecond transient absorption spectroscopy

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## Abstract

ICarbon dots (C-dots) an excellent luminescent nanomaterial have garnered significant attention due to their tunable optical properties, chemical stability, and low toxicity. Particularly, narrow long wavelength emission such as yellow and red is highly desirable for various applications such as light-emitting diodes, bio-imaging and photonic technologies. It is utmost important to understand the relaxation dynamics at ultrafast scale to enhance the performance of the devices. Herein, we have prepared yellow and red emitting C-dots using same precursor with minor modifications. The structural and functional groups of as prepared (C-dots) were studied using HR-TEM, FTIR and Raman spectroscopy. Steady state absorption band at 410 nm of yellow C-dots gets red shifted due to higher conjugation. The emission at 562 nm (85nm) full width at half maximum (FWHM) of Y-C-dots shifted to 620 nm and FWHM narrowed to (29 nm) implies the conjugation-domination in the surface of red dots. Time resolved photoluminescence measurements (TRPL) showed that increasing in life-time 2 ns of Y-C-dots to 5 ns for R-C-dots which confirm the surface molecular like decay. Ultrafast transient absorption spectroscopy highlights the higher non-relaxation pathways, carrier trapping between yellow and red emitting dots. Our findings unveil the surface chemistry that modulates the excited state relaxation in long wavelength emitting carbon dots which offers applications toward optoelectronic and bioimaging applications.

**Keywords:** Carbon dots, Yellow, Red, Excited-state dynamics, TAS

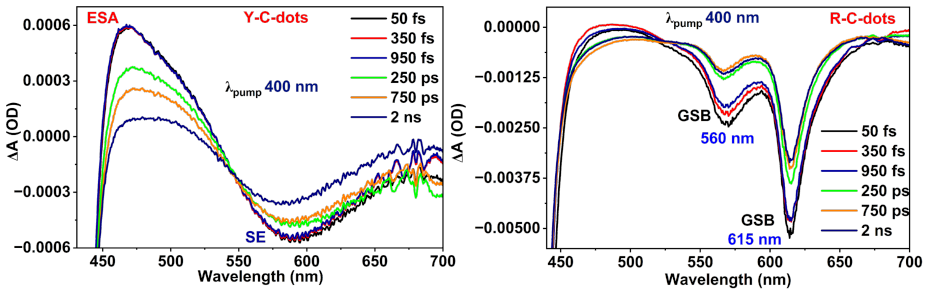


**Figure:** Femtosecond transient absorption spectra of Y and R-C-dots

# Numerical simulation on UV light intensity dependent complex impedance spectroscopy of $SnO_2$ using SCAPD 1D

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## Abstract

Tin oxide ($SnO_2$) is a promising transparent semiconductor that exhibits a direct transition band gap of 3.6 eV with a melting point at 1,630°C and a density 6.95 g/cm$^3$ due to its functional properties it was widely applied for optoelectronic applications[1]. To investigate frequency-dependent electrical conductivity behaviour of $SnO_2$ applied function of frequency, UV monochromatic (300 nm) incident light power and effect of thickness. In the present work, the effect of thickness on the frequency dependent impedance spectroscopy of $SnO_2$ under UV (300 nm) illumination was investigated. Further, activation energy for electrical conduction of different thickness of $SnO_2$ (250, 500, 750, 1000 nm), estimated using Arrhenius plot was found to be (4.42, 3.09, 2.31, 1.82 eV) respectively and a correlation between DC and AC conductivities was also studied by analysing data using BNN relation [3-5].

**Keywords:** Tin Oxide, SCAPS-1D software, Impedance Spectroscopy, Monochromatic light, Arrhenius plot, AC conductivity, Activation energy, BNN relation

**References:**

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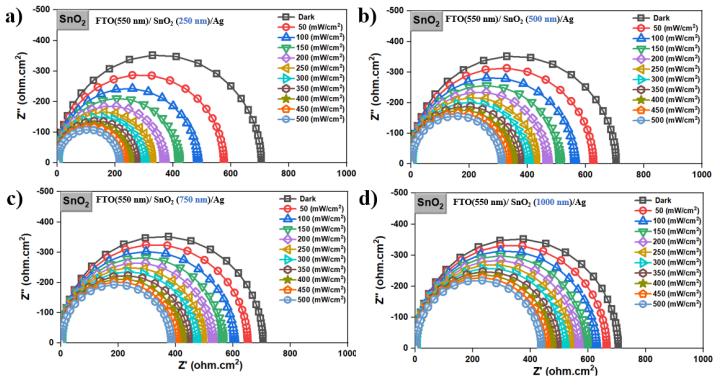


**Figure:** Numerical simulated Cole-Cole plot of FTO/$SnO_2$/Ag for various UV light power (dark to 500 mW/cm$^2$) at different thickness of $SnO_2$ (a) 250 nm (b) 500 nm, (c) 750 nm, and (d) 1000 nm.

# Role of topology in nanopillars and its effects on performance on CdS/CdTe solar cells

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**Abstract**

The increasing global demand for renewable energy sources and miniaturisation of IOT devices for wearable fuelled the path for accelerated research into advanced photovoltaic technologies. CdS/CdTe solar cells have been a strong candidate due to its unique properties and reliability across harsh environments. In this work, the role of nanopillar topology in enhancing the performance of CdS/CdTe nanopillar-based solar cells is systematically investigated by the TCAD simulator SILVACO. Different nanopillar geometries, such as nano-tri-pillars, nano-quad-pillars, nano-penta-pillars, nano-hexa-pillars, and nano-cylindrical pillars, are analysed to evaluate their influence on optical and electrical parameters. Results reveal the potential of each nanostructure and the possibility of improving typical parameters of a solar cell. Behavioural change in the electric field and charge carrier dynamics by the influence of different nanostructures divulge topological impact on optoelectronics devices. This creates a base for future advancements in photovoltaics.

**Keywords:** CdS/CdTe Solar Cells, Topology, Nano-tri-pillars, Nano-quad-pillars, Nano-penta-pillars, Nano-hexa-pillars, Nano-cylindrical pillars, TCAD

# Systematic tuning of optoelectronic properties in lead-free metal halide materials for solar-blind ultraviolet photodetectors

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**Abstract**

Lead-free halide perovskites have emerged as promising alternatives to conventional lead-based counterparts, offering non-toxic compositions with favourable optoelectronic properties. Among these materials, bismuth-based perovskites, such as $A_3Bi_2X_9$, demonstrate significant potential due to their suitable electronic configuration, enhanced stability, and structural versatility, leading to optoelectronic properties that are tunable from the ultraviolet (UV) to the near-infrared (NIR). However, achieving precise compositional control for targeted performance in the UV region has been limited. To address this gap, this study investigates A-site cation engineering as a systematic approach to achieve bandgap control in bismuth halide perovskite thin films for targeted ultraviolet (UV) optoelectronic applications. Thin films were fabricated using a solution-based deposition method, and subsequent characterisation by X-ray diffraction (XRD) confirmed the formation of phase-pure, highly crystalline perovskite structures. The influence of A-site cation substitution was investigated using UV–visible absorption spectroscopy and ultraviolet photoelectron spectroscopy (UPS). This characterization confirmed that strategic cation variation provides direct, systematic control over the material's optical properties, enabling a precise shift of the absorption maxima from 370 nm to 330 nm within the UV spectral region. The absorption characteristics and corresponding bandgap energies exhibited a clear dependence on the ionic radius and electronic properties of the substituted cations. While A-site cation variation alone did not induce large shifts in bandgap energy, subtle structural distortions arising from ionic-size differences enabled fine adjustment of absorption edges. This approach is particularly valuable for applications requiring precise wavelength selectivity. Furthermore, UPS measurements provided critical insights into valence band maximum (VBM) positions and work functions, with observed shifts in energy levels correlating directly with optical trends. The clear correlation between A-site cation properties and band structure modifications establishes a predictive framework for the rational design of these materials. This work confirms that A-site cation engineering is an effective strategy for modulating the electronic and optical properties of lead-free bismuth halide perovskites. By enabling precise, wavelength-specific tuning, this approach offers a strategic pathway for developing environmentally benign materials tailored for next-generation UV photodetectors.

**Keywords:** Lead-free metal halide perovskites, A-site cation engineering, Bandgap tuning, UV photodetectors

# Spectral response of different fluorescent colors under UV excitation

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**Abstract**

Different fluorescent color dyes were painted on paper and illuminated using a UV LED light source[1,2] and their reflectance spectra were recorded as shown in fig.1. Sharp and intense emission peaks were observed, indicating strong fluorescence response from each pigment. These peaks appeared independent of the pigment type and correspond to the excitation wavelength of the UV LED source. In addition to the primary emission peaks, several colors exhibit secondary peaks at shorter wavelengths. These secondary peaks originate from partial reflection or re-emission of the UV excitation light or from overlapping emission bands of the fluorescent dyes. Their relative intensities vary depending on the pigment composition and the degree of UV absorption efficiency of each dye.

The variation in peak positions and intensities among the samples (G, Y, R, and M) indicates that the fluorescence response strongly depends on the pigment composition and its interaction with UV excitation. Dyes emitting in the green-yellow region (515–518 nm) show higher intensity and sharper peaks, suggesting superior optical brightness and efficiency, while those in the red region (584–589 nm) exhibit broader and weaker emissions, indicating reduced fluorescence stability. Overall, these findings demonstrate that the choice of fluorescent pigment plays a crucial role in determining emission color quality and stability, which is essential for applications[3,4] in optical sensing, anti-counterfeiting[5], and photonic materials.

**Keywords:** Ultraviolet, Fluorescence, Spectral power distribution, Emission spectra.

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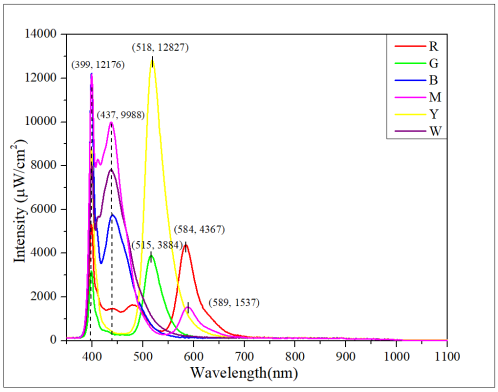


**Figure:** Emission Spectra of different fluorescent color dyes painted on paper. R: Red, G: Green, B: Blue, M: Magenta, Y: Yellow, W: White

# Poster Presentation

# Investigation of the influence of coating cycles and dipping time on ZnS thin films deposited by the SILAR method using an in house developed Arduino Uno-based low-cost coating machine

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**Abstract**

The zinc sulfide (ZnS) thin film is a promising semiconductor material for optical and photovoltaic application. The formation of ZnS thin film is greatly influenced by number of cycle and dipping time in cationic and anionic solution when SILAR method is employed. In this work we have developed an automatic SILAR coating machine based on Aurdino Uno and reciprocating actuator system. This study investigated the influence of coating cycle, dipping time and its effect on grain size, film thickness, shape and energy band gap. The XRD analysis confirmed the formation of film and band gap energy has been obtained in the range from 3.4 to 3.7 eV.

**Keywords:** Thin film, Absorption spectrum fitting, Silar, Band gap, ZnS

# Double-encapsulated red-emitting formamidinium lead halide perovskite nanocrystals for fluorescent sensing and lighting applications

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**Abstract**
In recent years, metal halide perovskite nanocrystals (NCs) have offered several optoelectronic and sensing applications due to their unique photophysical properties. Formamidinium (FA) based perovskite NCs exhibit better thermal and structural stability than the corresponding volatile methylammonium (MA)-based counterpart, which quickly decomposes to release gaseous methylamine. FA-based perovskite NCs also demonstrate more fantastic responses towards different environmental stimuli, which is helpful for different sensing applications. However, $FAPbI_3$ NCs suffer from phase instability and degrade very fast under external stimuli. Here, we synthesized mixed halide $FAPb(Br/I)_3$ NCs by partially replacing I-ions with Br-ions to address the key challenge of phase instability of $FAPbI_3$ NCs. Further, with a surface modification approach like encapsulating the NCs' surface with silica and also double-encapsulated silica-polymethyl methacrylate (PMMA) polymer, we enhanced the stability of the NCs against heat, ion migration, and UV irradiation. Such double-coated red-emitting $FAPb(Br/I)_3$ NCs (emission peak $\sim 642nm$) were tested for temperature sensing, exhibiting a relative sensitivity ($S_r$) of $\sim 12.5\% - K^{-}1$. We also prepared fluorescent humidity sensors that revealed the lowest detection limit of $\sim 5\%RH$. Finally, down-converted WLEDs were fabricated using double-coated green-emitting Cs-doped $FAPbBr_3$ NCs and red-emitting $FAPb(B/I)_3$ NCs in thin-film form and embedded on a blue LED chip. These results will boost the development of high-performance sensors and lighting technologies.

**Keywords:** Metal halide perovskite NC, Temperature sensor, Humidity sensor and WLED

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# Memristor for next-generation surveillance system: A Review

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**Abstract**

A memristor is a two-terminal resistive switching device that can be employed for resistive random access memory applications of Industry 5.O namely artificial intelligence (AI), quantum computing, neuromorphic computing, smart health care services, smart cities, and smart surveillance systems. Memristor can be used for real-time threat prediction, detection, and quick response. It can be harvested as a non-volatile high-speed data storage device for security. Memristor-based sensing devices can detect temperature gradients, suspicious movements, and sounds. Artificial intelligence (AI) supported by memristor plays a big role in the management of smart cities for transportation traffic discipline, disaster management, smart cameras, and video recording. Memristor-supported quantum computing technology finds applications in high-quality signal and image processing, biometric surveillance, global security, and confidential communication. Neuromorphic computing technology uses memristors for artificial synaptic devices. These artificial synaptic devices mimic the neural transmission of the human brain. Therefore, such devices are used in robots to detect suspicious human behaviors, facial and fingerprint recognition in forensic science, autonomous monitoring, and decision-making

**Keywords:** Memristor, Surveillance system, Smart cities, Artificial Intelligence (AI), Quantum Computing, Neuromorphic Computing, Industry 5.O

# Exploring the structural and electrical properties of $Bi^{3+}$ modified $AgNbO_3$ lead-free ceramics

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**Abstract**

The growing demand for high-power density energy storage sources for use in electrical automobiles, compact electronics, and dielectric ceramic capacitor applications. It has prompted investigations into novel dielectric materials for high-efficiency energy storage[1]. Dielectric ceramics are currently acceptable for use in capacitors for high-power energy storage due to their high energy density and high breakdown strength of the materials. Consequently, there is an urgent need to develop environmentally friendly, lead-free materials with excellent energy storage performance[2]. Silver Niobate ($AgNbO_3$) exhibits antiferroelectric and piezoelectric properties at room temperature, making it a fascinating material for prospective applications in energy storage device[3]. In this report, a solid-state method has been proposed for the synthesis of $Bi^{3+}$ modified $AgNbO_3$ ceramics. It is expected that the substitution of Bi3+ions would disturb the antiferroelectric order, leading to enhanced electromechanical properties. X-ray diffraction patterns showed their crystal structure information and are revealed by Rietveld refinement. Furthermore, the prepared samples will be discussed on their P-E loop, Leakage current, temperature-dependent dielectric, and the outcomes will be presented at the conference.

**Keywords:** $AgNbO_3$, Antiferroelectric, energy storage, lead-free

**References:**

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# Structural and magnetoelectric coupling in $Sc^{3+}$, $Sm^{3+}$ co-substituted BFO-BTO ceramics

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**Abstract**

Multiferroic materials are very unique due to the coexistence of both ferroelectricity and ferromagnetism and are being extensively investigated by the researchers worldwide due to their potential applications in novel devices such as sensors, actuators, storage information, spintronics, and microelectronic devices. $BiFeO_3$ (BFO) is one of the most promising single phase multiferroic materials, with high Curie temperature $T_C = 825°C$[1] and great theoretical spontaneous polarization Pr $\sim 90\mu C/cm^2$[2] originating from the hybridization between $Bi^{3+}$ $6s^2$ and $O^{2-}$ 2p orbitals. $BaTiO_3$ (BTO), is a very well-known perovskite material for its large relative dielectric constant. It is a ferroelectric material with impulsive polarization produced commencing the dislocation of $Ti^{4+}$ ions away from the centro–symmetric position within the $TiO_6$ octahedra. The enhancement of multiferroic properties in bismuth ferrite-barium titanate (BFO-BTO) ceramics through doping has attracted significant attention due to their potential in multifunctional device applications.

In this report, a solid state method has been proposed for synthesis of Sc and Sm modified BFO-BTO ceramics. X-ray diffraction analysis indicated co-doped BFO-BTO ceramics have a pure perovskite structure and Rietveld refinement reveals the crystal structure of BFO-BTO ceramics. Further, the ferroelectric and magnetic studies will be measured for the prepared samples. To explore the crystal structure and magnetoelectric coupling of co-doped BFO-BTO ceramics are investigated and will be presented in the conference.

**Keywords:** Multiferroics, $BiFeO_3$ -$BaTiO_3$, Magnetoelectric coupling, Room temperature, crystal structure

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# Structural and electrical properties of metal ions doped $NaNbO_3$ lead free ceramics

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**Abstract**

Lead-free dielectric ceramics have emerged as promising candidates for advanced electronic applications owing to their environmental compatibility, superior power density, rapid charge–discharge characteristics, and reliable performance[1]. They are promising due to the increasing demand for enhanced energy storage density and the ongoing trend toward integration and miniaturization in advanced electronic devices. Sodium niobate ($NaNbO_3$) is a perovskite oxide that hosts two crystallographically distinct Na (Sodium) sites and exhibits a rich sequence of structural phase transitions. At room temperature, it stabilizes in an orthorhombic phase, which evolves through successive symmetry changes associated with octahedral tilting, ultimately reaching a cubic structure near $640°C$[2]. Notably, $NaNbO_3$ undergoes an antiferroelectric transition around $350°C$, highlighting its complex structural dynamics and multifunctional ferroic behaviour[3].

In this report, a conventional solid-state method has been proposed for synthesis of metal ions doped $NaNbO_3$ ceramics. X-ray diffraction analysis indicated pure and metal ions doped $NaNbO_3$ ceramics have perovskite structure and Rietveld refinement reveals that the crystal structure of $NaNbO_3$ ceramics. Further, the ferroelectric and dielectric studies will be measured for the prepared samples. To explore the crystal structure and electrical studies are investigated and these results will be presented in the conference.

**Keywords:** $NaNbO_3$, Pb-free, X-ray diffraction, Ferroelectric, Dielectric, Phase transition

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# Mechanochemical synthesis of complex ceramic oxides: A sustainable route to high-performance functional materials

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**Abstract**

Ceramic materials play a vital role in advanced electronic, optical, and energy applications due to their unique structural and functional properties. We make a review focusing on the mechanochemical synthesis of complex ceramic oxides such as $BaTa_2O_6$, $MgTa_2O_6$, and $BaTiO_3$, highlighting their advantages over conventional high-temperature synthesis methods. Mechanochemistry, particularly through high-energy ball milling, enables the formation of phase-pure, nanostructured ceramics with improved dielectric, piezoelectric, and ferroelectric properties at significantly lower synthesis temperatures. The impact of milling time, annealing conditions, and precursor selection on the microstructure and properties of these ceramics is extensively discussed. Additionally, alternative synthesis routes, including co-precipitation, sol-gel, oxalate decomposition, and hydrothermal methods, are compared with mechanochemical techniques in terms of process simplicity, material homogeneity, and scalability. The review also explores the effects of doping and compositional tailoring on dielectric behaviour, the role of real-time monitoring techniques in understanding mechanistic pathways, and the application potential of these ceramics in sensors, capacitors, actuators, and energy storage systems. Emphasis is placed on the sustainability of mechanochemistry as a green synthesis approach and its capacity to produce defect-engineered, high-density materials with superior performance. This work underscores mechanochemistry as a cornerstone in modern ceramic synthesis, offering versatile, cost-effective, and scalable solutions for next-generation functional materials.

**Keywords:** Synthesis, Comparative study, Performance, Applications

# Growth and complex impedance studies of Ni mixed Co levo tartrate crystals

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**Abstract**
Cobalt tartrate finds several applications[1,2] and to modify its properties the addition of nickel is done. Single diffusion gel growth technique is employed[3]. To grow pure cobalt tartrate $Co(NO^3)^2{\cdot}6H^2O$ supernatant solution is used and 1 molar concentration of $Ni(NO^3)^2{\cdot}6H^2O$ solution is added in $Co(NO^3)^2{\cdot}6H^2O$ solution to grow mixed crystals. The grown crystals are spherulitic and coloration changing from dark reddish to greenish. Powder XRD study suggested orthorhombic structure with slight changes in unit cell parameters on addition of nickel. The nickel content is identified and estimated by using EDAX. The complex impedance plot i.e., Nyquist plot, in frequency range 100 Hz to 1MHz, indicate single semi-circle suggesting the contribution from grain only. Data fitting with software z-view and modelled with parallel resistance and constant phase element (CPE) yield grain resistance, capacitance and relaxation time values and it has been found that the amount of nickel present has pronounced influence on these parameters.

**Keywords:** Cobalt tartrate ($Co(NO^3)^2{\cdot}6H^2O$), Nickel (II) nitrate hexahydrate ($Ni(NO^3)^2{\cdot}6H^2O$), Nyquist plot, Levo Tartrate Crystals

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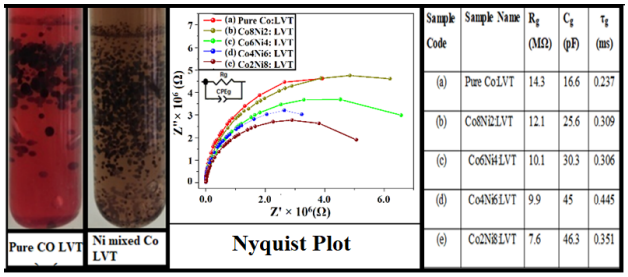


**Figure:** Growth and complex impedance studies of Ni mixed Co levo tartrate crystals

# In-situ Chemically Reduced Graphene Oxide and PANI for Resistive Gas Sensing: Toward FET-Based Sensor Platforms

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## Abstract

The potential of graphene has led to extensive research in various fields, such as gas sensors[1,2], composite materials, supercapacitors, and so on. Graphene oxide reduced through several ways (leading to reduced graphene oxide, rGO) has proven to show enhanced properties similar to pristine graphene. Besides, polyaniline (PANI), a conductive polymer, has also been used for sensing applications[2]. Here, we propose studies on gas sensing using PANI or rGO obtained via an eco-friendly reduction method using L-Ascorbic acid combined with a thermal treatment. In this process, GO is in-situ reduced directly onto the channel (of a field effect transistor (FET)), the reduction extent being controlled by the exposure time to a specific temperature. This method proves not only to be green, non-toxic, and economical but also efficient to attain a better reduction grade that can be easily controlled. PANI is also obtained in-situ directly on the FET by electro-polymerization from its monomer in aqueous solution. Such prepared rGO (and PANI) are well suitable for gas sensing, tested through engineered inter-digitated FETs which were developed via photolithography on flexible polyimide substrates. Performance of our devices with PANI and rGO was tested using FET - I/V characterizations (output and transfer curves), as well as for resistive-gas sensing with a well-established setup having a dedicated chamber and MFCs (mass flow controllers). Reducing gases like Hydrogen ($H_2$) and Methane ($CH_4$) are detected through the electrical characteristics and resistance changes when the gas molecules interact with the sensor surface, as shown in Figure 1. The sample figure shows a response of $0.04 \pm 0.0007$ with a response time of $57 \pm 10s$. The constraints with the selectivity and sensitivity are discussed through selecting suitable composites to make transistors specific for sensing each gas. Meanwhile, characterization like XRD, FTIR, UV, and SEM was performed in order to understand the morphology and structure.
Most such sensors operate at very high temperatures or have dopants aiding in gas molecule adsorption, whereas our proposed idea works at ambient temperature.

**Keywords:** rGO, PANI, chemical reduction, FETs, gas sensing

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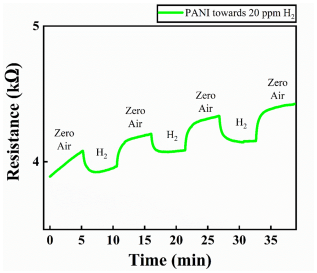


**Figure:** Polyaniline response towards 20 ppm $H_2$

# Numerical estimation of aluminum Gallium Nitride – Gallium Nitride interface Two|Three-Dimensional Electron|Hole Gas (2DEG|3DEG, 2DHG|3DHG) properties

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**Abstract**

Numerical estimates of key electronic|electrical properties (e.g., surface charge density, spontaneous polarization, piezoelectric polarization) of the aluminum gallium nitride – gallium nitride ($Al^xGa^{1-x}NGaN$) interface are presented. In-house developed C computer language programs are used for these computations. The paper includes an exhaustive set of graphs and tables listing these estimated parametersed, along with detailed discussions.

Unique electronic|electrical properties of the $Al^xGa^{1-x}NGaN$ interface are exploited for making both ultra-high frequency (100s of MHz – 10s of GHz e.g., HEMT – High Electron Mobility Transistor), and ultra-high power (10s of Amperes and 100s of Volts) transistors. Some key electronic properties of gallium nitride and its alloy aluminum gallium nitride that make them the ideal choice for such demanding applications include wide band gap (3.5 eV), built-in spontaneous polarization of gallium nitride and interfacial($Al^xGa^{1-x}NGaN$ interface) lattice strain induced piezoelectric polarizationce). Combining spontaneous and piezoelectric polarizations result in two|three dimensional elecron|hole gases (2DEG|3DEG and 2DHG|3DHG). These very interesting points are discussed in detail in the paper.

Numerical estimation of the $Al^xGa^{1-x}NGaN$ interface 2DEG|3DEG and 2DHG|3DHG uses basic material parameters (e.g., aluminum mole fraction in aluminum gallium nitride). The calculations use both deterministic and probabilistic steady state Monte Carlo techniques, as elaborated on in the paper.

**Keywords:** Two|three dimensional electron|hole gas, steady state Monte Carlo, mole fraction, interface properties, High Electron Mobility transistor (HEMT), Spontaneous polarization, Piezoelectric polarization, Band gap, C computer language, Gallium Nitride, Aluminum Gallium Nitride, Polarization doping

# CdSe-Doped Bimetallic ZIF-67-Derived Electrode Materials for High-Performance Supercapacitor

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**Abstract**

Metal-organic frameworks (MOFs), particularly zeolitic imidazolate frameworks like ZIF-67, have garnered attention for energy storage applications due to their high surface area, tunable porosity, and structural versatility. However, their poor intrinsic conductivity caps practical performance. To overcome this, ZIF-67/CdSe nanoparticle composites were synthesized by varying CdSe content while maintaining a constant ZIF-67 ratio via a simple co-precipitation method. The structural and morphological features were confirmed through powder X-ray diffraction (PXRD), Energy-Dispersive X-ray spectroscopy (EDAX), scanning electron microscopy (SEM), and field-emission SEM (FE-SEM). Surface area and porosity were analysed using BET measurements, while X-ray photoelectron spectroscopy (XPS) provided information on elemental states and composition. Electrochemical performance was evaluated in a three-electrode configuration using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). The results indicate that the incorporation of CdSe enhances the capacitive behaviour of ZIF-67, demonstrating its potential as a high-performance material for supercapacitor electrodes. Specifically, CV analysis confirmed excellent reversibility and high charge storage capacity, reinforcing the composite's applicability in energy storage systems.

**Keywords:** Zeolitic Imidazole framework, Energy Storage, Nanoparticle, Composition

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# Flexible electrospun PVDF/BCZT nanofiber composite for efficient piezoelectric energy harvesting

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**Abstract**

In this work, electrospun nanofibers of Barium Calcium Zirconate Titanate (BCZT) – Polyvinylidene fluoride (PVDF) composite were used to fabricate a flexible piezoelectric nanogenerator (PENG). To examine the impact of ceramic loading on the piezoelectric and energy- harvesting performance of the nanofibers, lead-free BCZT nanoparticles were added to the PVDF matrix at different volume ratios 05:95, 10:90, 15:85. The electrospinning procedure improved $\beta - phase$ development in the PVDF matrix by creating homogenous, well aligned fibers with a homogeneous distribution of BCZT nanoparticles. The persistence of the BCZT perovskite phase and the robust interfacial contact between the ceramic and polymer phases were verified by structural and morphological investigations. Higher BCZT concentration increased the nanogenerators output voltage and current because of good dipole arrangement, stronger polarization and more effective stress transmission within the composite network. Superior piezoelectric output was demonstrated by the optimized 15:85 BCZT/PVDF nanogenerator, indicating its potential use in motion sensors, self-powered wearable electronics and flexible energy-harvesting systems.

**Keywords:** Piezoelectric nanogenerator, Polyvinylidene fluoride, Barium Calcium Zirconate Titanate, Perovskite, Energy harvesting

# Impact of electron irradiation on the capacitance and frequency response of GaN MOSFETs at elevated temperatures

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**Abstract**

The study investigates the effects of an elemental particle on semiconductors and their electrical characteristics. High-voltage gallium nitride (GaN) devices are a major player in power electronics, enabling significantly higher efficiency, faster switching speeds, and greater power density with a high voltage rating compared to traditional silicon and even silicon carbide technologies. Here, GaN MOSFET is irradiated with high-energy electron irradiation (6–15 MeV) and its capacitance behaviour is analysed. Commercially available packaged GaN MOSFET samples were subjected to controlled electron irradiation, after which capacitance measurements were systematically performed across Gate-Source ($C_{GS}$) and Drain-Source ($C_{DS}$) terminals. The evaluation was conducted over a broad frequency range from 10 kHz to 10 MHz, enabling detailed analysis of frequency-dependent behaviour. Additionally, the influence of operational temperature was examined from $25°C$ to $125°C$. The results reveal noticeable shifts in both ($C_{GS}$) and ($C_{DS}$) values in pre- and post-irradiation. These findings elucidate the combined impact of electron irradiation and environmental conditions on the capacitance characteristics of GaN MOSFETs, providing valuable insights for the design and deployment of radiation-hardened electronics in harsh environments such as space, nuclear reactors and medical therapy facilities.

**Keywords:** GaN, Power Electronics, Electron irradiation, MOSFET, Frequency response, Temperature dependence

# Impact of antimony substitution on the structural and functional properties of $CuFeS_2$ nanoparticles synthesized by a hydrothermal route

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## Abstract

Pure and antimony (Sb)-substituted $CuFeS_2$ nanoparticles ($CuFe_{1-x}Sb_xS_2$) were synthesized via a hydrothermal method and their physical properties were investigated for potential photocatalytic applications. Structural analysis using powder X-ray diffraction (PXRD) confirmed a tetragonal crystal structure with an average crystallite size of approximately 7.5 nm. Surface morphology and elemental composition were examined using field-emission scanning electron microscopy (FE-SEM) combined with energy-dispersive X-ray spectroscopy (EDS). The FE-SEM images revealed well-defined grains with distinct grain boundaries, while EDS spectra confirmed the presence of host and substituent elements in near-stoichiometric ratios. The average particle size, estimated from FE-SEM micrographs using ImageJ software, was found to be around 271 nm. Optical absorbance was recorded using a UV–Vis–NIR spectrophotometer, and the optical band gap, calculated using Tauc's relation, exhibited a decrease from 1.45 eV to 1.35 eV with increasing Sb substitution. Further the valence states of the host and dopant elements were studied using X-ray photoelectron spectroscopy (XPS). The photoluminescence (PL) properties of $CuFe_{1-x}Sb_xS_2$ nanoparticles were examined using a PL spectrophotometer, revealing a broad emission peak centered around 500 nm. Electrical properties were studied and it shows good conductivity at Sb substituted $CuFeS_2$ nanoparticles. The photocatalytic activity of the $CuFe_{1-x}Sb_xS_2$ nanoparticles was evaluated using Rhodamine B (RhB) and Methylene Blue (MB) dyes under UV light irradiation at various time intervals, and the corresponding absorbance spectra were recorded. The nanoparticles demonstrated a notable photocatalytic response, particularly for Methylene Blue (MB). These results clearly indicate that the photocatalytic efficiency improved with increasing Sb substitution and longer exposure durations.

**Keywords:** Crystal structure, Photoluminescence, Chalcopyrite, Hydrothermal, Photocatalytic

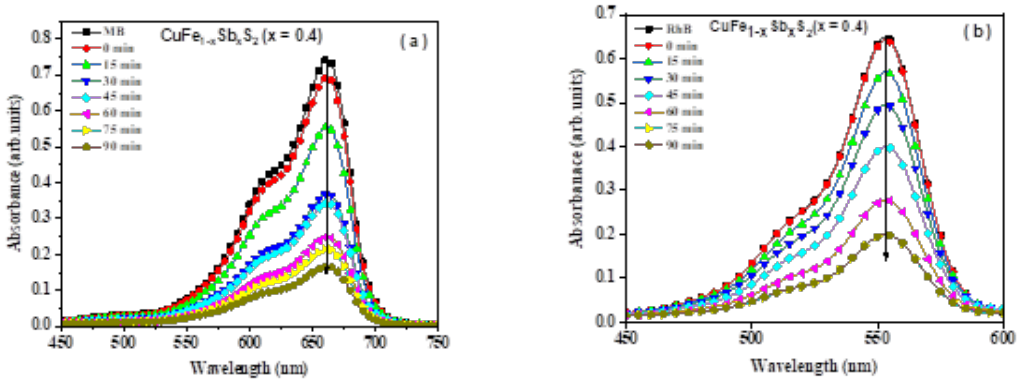


**Figure:** Absorbance spectrum for MB and RhB dyes with $CuFe_{1-x}Sb_xS_2$ nanoparticles as photocatalyst under light irradiation.

# Room temperature photoinduced resistance response of LPCMO thin films

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**Abstract**

Doped manganites are strongly correlated materials with correlation among charge, orbital, spin, and lattice degrees of freedom. This leads to the correlation between their structural, magnetic, and transport properties, resulting in various interesting phenomena, such as colossal magnetoresistance and phase separation, that can be tuned using strain and external perturbation. In the present work, we have synthesized bulk $La_{0.375}Pr_{0.325}Ca_{0.3}MnO_3$ material using solid-state reaction method and confirmed the structure by XRD, and the oxidation state by XPS studies. We have deposited thin films by pulsed laser deposition method on $SrTiO_3(100)$ and $LaAlO_3(100)$ substrates, which gave tensile and compressive strained films respectively. Our study further establishes the effect of photonic perturbation on the films.

**Keywords:** Manganite, Thin film, PLD, Photo-induced

# Optimization of $CsPbBr_3$ perovskite nanocrystals featuring enhanced stability and optical efficiency

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## Abstract

Recent advancements in optoelectronics are focused on replacing traditional silicon-based devices, with perovskite nanomaterials emerging as frontrunners in this paradigm shift. All-inorganic Cesium Lead Halide perovskite $CsPbX_3$ (X = Cl, Br, and I) nanocrystals (PNCs) have been well known in the solution processes nanostructures landscape due to their excellent optical properties, such as defect tolerance, high PL quantum yield, bandgap tunability, high absorption coefficient, power conversion efficiency, and so on, which make them promising candidates in a variety of optoelectronic devices such as solar cells, LEDs, scintillators, photo detectors, etc. However, one key problem these nanocrystals suffer from is their poor stability in air and water, which severely hinders their full-scale industrial use. In this study, we optimize the synthesis of colloidal CsPbBr3 PNCs by systematically altering key parameters like polarity of the solvents, capping functionalities of the nanocrystals and reaction conditions like reaction temperature and reaction time, to enhance efficiency and improve stability. For particles prepared via Ligand Assisted Reprecipitation (LARP), we found that tweaking reaction time and temperature enables precise control over crystal sizes and the crystal purity respectively. More importantly, changing the polarity of the nanocrystal environment was found to directly influence the particle size of the synthesized PNCs. PNCs synthesized using a high polarity environment induced by Ethyl Acetate resulted in smaller particles compared to when toluene (comparatively lower polarity). This is of great significance, as it introduces a new dimension to tune the optical properties of these samples. Furthermore, we also explore the role of different passivating agents rich in amines and oxides with the aim of enhancing stability and making the PNCs compatible for sensing applications. PNCs synthesized using toluene present high PL quantum yield with narrow emission while the ones made using ethyl acetate exhibit multi-fold longer stability. The proposed approach is a viable trade-off strategy to improve the efficiency and stability of PNCs, further solidifying their potential in the field of optoelectronics.

**Keywords:** Perovskites, Colloidal nanocrystals, Optoelectronics, Stability

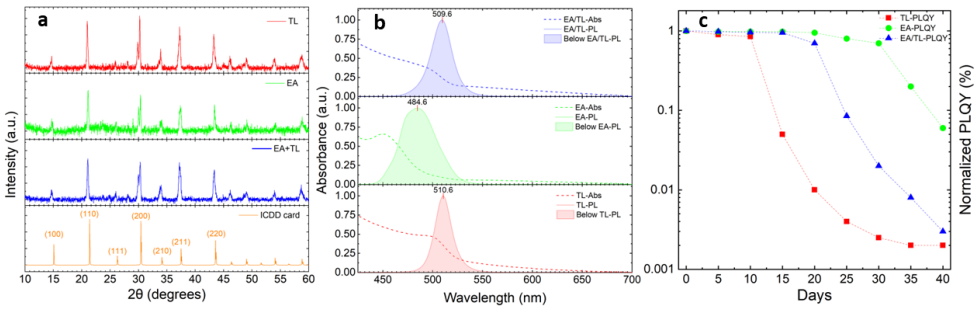


**Figure:** (a) X-Ray diffraction pattern of the synthesized PNCs under different polar environments showing a consistent cubic structure. (b) UV-visible absorption spectra and respective PL curves excited at 400 nm at 300 K. (c) Stability studies portraying rate of decrease in the PL quantum yield of the PNC under different environments.

# Emulating Ebbinghaus forgetting curve via characterization of excitatory synaptic transmission in a ZnO-based optoelectronic synapse with ultra-low power consumption

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**Abstract**

Optical synapses provide high bandwidth operation with low power consumption for neuromorphic computing. ZnO is established as a potential semiconductor for optoelectronic synapses with its high photosensitivity in the ultraviolet (UV) region. In this work, we focus on emulating Ebbinghaus forgetting curves via conductance decay and memory retention in a lateral synaptic device based on ZnO nanoparticles. Under UV light stimulation, the memory retention can be seen up to 2500 sec showing long-term potentiation which is useful for memory and learning. Long-duration memory retention using optical spiking is achieved and the decay characteristics of the memory are studied. A transition from short-term plasticity (STP) to long-term plasticity (LTP) can be induced by tuning the optical pulse width. The conductance decay follows the Ebbinghaus forgetting curve. We have demonstrated the effect of various measurement parameters such as pulse width, pulse frequency, and pulse amplitude on memory decay. The synaptic device can be operated with energy consumption as low as 1 fJ which paves the way for very low energy-consuming synaptic devices for neuromorphic applications.

**Keywords:** Optoelectronic synapse, UV stimulation, ZnO, Low power consumption, Ebbinghaus forgetting curve

# Agro-industry waste derived akermanite a photo catalyst for industrial wastewater purification

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**Abstract**
Water pollution has become one major environmental issue due to the rapid growth of industrial sector as they dispose the waste water directly to the water bodies. The waste water contains various heavy metal ions and organic dyes which need to be treated before exposing to the environment. The present study reports the facile synthesis of akermanite nanoparticles from agro-industry waste rice husk ash and ground granulated blast furnace slag by hydrothermal method. The prepared product was investigated by X- ray diffractometry, field emission scanning electron microscopy, UV-visible and fourier transform infrared spectroscopy characterization techniques. XRD and FTIR revealed the prepared powder is akermanite and the standard crystallite size was determined. FESEM demonstrates the morphology of the material and bandgap was analysed using diffuse reflectance spectroscopy. The photocatalytic activity of akermanite nanoparticles was studied using standard mythelene blue dye. The effect of initial dye concentrations, catalyst dosage on the degradation of methylene blue were studied under visible light irradiation.

**Keywords:** Photo catalyst, Wastewater purification, Akermanite nanoparticles, Mythelene blue dye

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# Tuning ZIF-8 with different electrolyte concentrations for enhanced supercapacitor performance at multiple potential windows

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**Abstract**

An essential component of any nation's economic growth and human development index (HDI) is energy. Clean energy production from renewable energy sources is given significant attention in order to attain sustainable energy production, given the magnitude and complexity of the world's current energy dilemma. Zeolitic Imidazolate Frame- works (ZIFs) are a subclass of metal-organic frameworks composed of metal ions (typically $Zn^{2+}$ or $Co^{2+}$) bridged by imidazolate linkers, exhibiting zeolite-like structures with high thermal and chemical stability.The ZIF-8 combines the structural precision of MOFs with the robustness of zeolites, making it highly versatile for applications in gas sep- aration, catalysis, sensors, and energy storage. In this study, ZIF-8 was synthesized by chemical co-precipitation and optimized using various electrolyte concentrations (1 to 6 M KOH) to explore its electrochemical performance across different potential windows (0.8V, 1V, 1.2V) following basic characterization, for use in supercapacitors. Asymmetric two-electrode configurations were analyzed using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The optimized system demonstrated that electrolyte tuning plays a crucial role in achieving superior supercapacitor performance.Overall, it reveal that 1 M KOH delivers the most favorable electrochemical performance in the three-electrode setup, while operating the device within a 1 V potential window ensures enhanced stability and energy storage efficiency. This work highlights the individual potential of ZIF-8 material for next-generation energy storage devices.

**Keywords:** ZIF-8, Supercapacitor, Electrolyte concentration, MOFs, Energy storage

# Investigation of structural and optical properties of unique MOF-5 synthesized via facile chemical precipitation method

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**Abstract**

MOF-5 nanoparticles, a porous and highly tunable metal–organic framework, were synthesized via a solution-based route and characterized for their structural, morphological, and optical properties, followed by an investigation of their photocatalytic performance. Structural analysis using X-ray diffraction (XRD) confirmed the formation of the cubic phase of MOF-5, while Raman spectroscopy validated the structural quality of the framework. High-resolution transmission electron microscopy (HR-TEM) provided insights into the morphological features of the nanoparticles. Optical analysis using UV–Vis DRS and PL spectroscopy confirmed the material's promising optical and photocatalytic properties. The optical bandgap, estimated as 3.66 eV using the Kubelka–Munk model, suggests its suitability for light-driven processes. Photoluminescence analysis also elucidated the recombination dynamics of photo-generated charge carriers. The photocatalytic efficiency of MOF-5 was evaluated through the degradation of organic dyes, achieving maximum degradation rates of 59.7% for Rhodamine B, 69.8% for Eriochrome Black, 72.0% for Alizarin Red, and 77.1% for Malachite Green, demonstrating its significant potential in environmental remediation. Furthermore, adsorption isotherm and kinetic studies supported the efficacy of MOF-5 nanoparticles as a promising photocatalyst for the degradation of organic pollutants. Scavenging studies were conducted to identify the predominant reactive species driving the dye degradation process, elucidating the underlying photocatalytic mechanism. Overall, this work shows that the solution-synthesized MOF-5, with its controlled nanoscale structure and improved optical properties, is an efficient and stable photocatalyst suitable for various environmental applications.

**Keywords:** Adsorption isotherm, Environmental remediation, MOF-5, Metal Organic Framework, Photocatalysis

# Metal oxide based ferroelectric random access memory (FeRAM) for neuromorphic computing applications

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**Abstract**

The exponential growth of data in this digital era, requires advancement in both storage and processing technologies as classical von Neumann architecture-based computing systems have a few shortcomings due to the von Neumann bottleneck. It can be resolved by neuromorphic computing systems, which mimic the function of the human brain. The neuromorphic computing systems are made up of artificial spiking neurons and synaptic devices. Non-volatile Ferroelectric Random-Access memory (FeRAM) can mimic biological neurons and synapses by using the properties of ferroelectric material. The 1T-1C structure of FeRAM features a metal-ferroelectric-metal (MFM) structure, and each memory cell consists of one access transistor and one ferroelectric capacitor. The access transistor is a Metal Oxide Semiconductor Field Effect Transistor (MOSFET). FeRAM stores information in ferroelectric capacitor in the form of ferroelectric dipole orientation which can be switched by applying external electric field. Due to compatibility with CMOS, scalability to sub-10 nm thicknesses, fluorite-structured $HfO_2$-based ferroelectric materials are a good choice for FeRAM. The orthorhombic phase of $HfO_2$-based thin films shows the ferroelectric property. The MFM structure and back gated FeRAM structure can be fabricated by Pulsed Laser Deposition (PLD) technique. The MFM structure has been used to study the device characteristics.

**Keywords:** Ferroelectric thin films, Ferroelectric Random Access Memory, $HfO_2$, Pulsed Laser Deposition.

# Synthesis and characterization of semi organic single crystal DL-Malic Acid Strontium Nitrate (DLMSN)

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**Abstract**

The growth of high–quality nonlinear optical (NLO) materials remains a challenging endeavor for material science. Crystals of large size and with structural perfection are required for fundamental research and practical implementation in photonic and optoelectronic technology. This research aims to look into the synthesis, growth, and properties of Semi organic crystals of DL-Malic acid and strontium nitrate. Single crystals of semi organic material Dl-Malic Acid Strontium Nitrate (DLMSN) have been grown by the slow evaporation of an aqueous solution of distilled water. The grown crystals were characterized by XRD, FTIR, UV- Vis NIR, and TG-DSC. The lattice parameter values of DLMSN crystal are identified using XRD analysis. The presence of functional groups and the protonation of ions were confirmed by Fourier transform infrared transmission (FTIR). Optical transmittance of the grown crystals have been studied by UV-vis NIR spectrum. Optical studies show that the crystal has wide transmission range with UV cut off. Thermal stability of the crystal was investigated using Thermogravimetric and Differential Scanning Calorimetry. Optically good quality single crystals of semi organic DLMSN have been grown using slow evaporation solution growth technique. The grown crystals are observed to be transparent and colorless with well-defined edges. The grown DLMSN crystal is having a high transparency in the visible region and it can be used for optical application in the visible region.

**Keywords:** Single Crystal, NLO, Strontium nitrate, Dl-malic acid

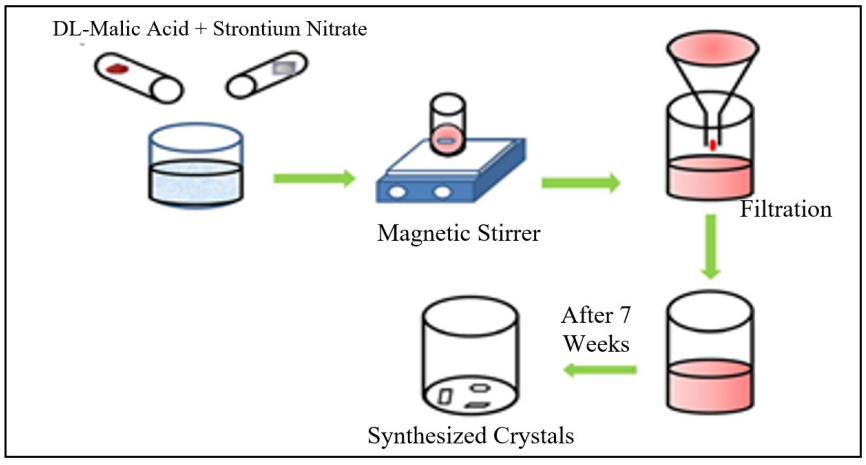


**Figure:** Synthesis of Semi Organic Single Crystal DL-Malic Acid Strontium Nitrate

# Self-rectifying second-order memristive behavior in PLD deposited tungsten oxide thin films

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## Abstract

Resistive Switching devices are highly suitable candidate for memory and neuromorphic computing applications owing to their conductance change similar to that of synaptic weight. The crossbar array fabrication of the devices allows sneak path current, which disturbs the activity of the nearby device. To rectify this issue, in this study, we fabricated a Pt/$WO_3$/FTO device structure using the Pulsed Laser Deposition (PLD) technique. The fabricated devices exhibit Self-Rectifying Memristive (SRM) behaviour, which allows current to flow in one direction, thus preventing the crosstalk between the devices. The fabricated device shows a rectifying ratio exceeding 10. However, next-generation computing devices require higher levels of complexity. In this context, the $WO_3$-based device exhibits second-order memristor actions, indicating that the synaptic weight is influenced not only by the present applied voltage but also by the device's operational frequency history. The potentiation and depression measurements were also performed, which indicate that non-linearity can be controlled by changing the pulsing sequence. The fabricated neuromorphic memory devices demonstrate excellent capabilities as a memory storage unit, with a retention time of approximately $10^3$ seconds and endurance of up to $2.5 \times 10^3$ cycles.

**Keywords:** Memristor, Self-rectifying Memristor, Resistive Switching, Second-order Memristor, Neuromorphic Computing

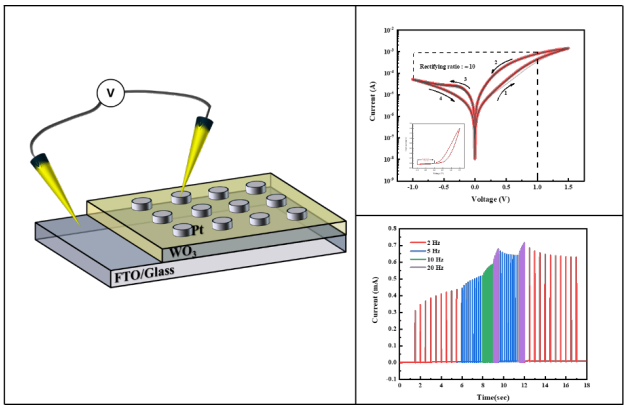


**Figure:** Self-rectifying second-order memristive behavior in PLD deposited tungsten oxide thin films

# Enhanced crystallization behavior in GaSb/$Sb_2Te_3$ heterojunction phase change materials

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**Abstract**

Antimonide-based phase change materials (PCMs) are promising candidates for next-generation non-volatile memory devices due to their fast crystallization kinetics and structural simplicity. The explosive crystallization behavior of antimony (Sb) enables rapid switching between two distinct stable states, making it suitable for data storage. However, conventional chalcogenide PCMs such as GeTe–$Sb_2Te_3$ suffer from phase segregation, resistance drift, and high-power consumption. Gallium antimonide (GaSb), a III–V compound, exhibits a smaller density change upon phase transition and lower resistance drift, offering improved reliability. This study explores the design of GaSb/$Sb_2Te_3$ heterojunction PCMs, where the $Sb_2Te_3$ confinement layer promotes enhanced crystallinity and controlled crystallization temperature. The bilayer structure remains thermally stable without intermixing, demonstrating strong potential for developing energy-efficient and high-performance PCM devices.

**Keywords:** Phase change materials (PCMs), Non-volatile memory, Gallium antimonide (GaSb), Heterojunction

# Vanadium oxide thin films for neuromorphic memory and computing applications

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**Abstract**

Current era of growing artificial intelligence and Internet of things (IoT) which requires and generates enormous amount of data for training and inferences. But the systems which we use are made of traditional Von Neumann architecture where memory and processor are separated.To process the information each time shuttling of data takes place as it should pass through RAM, then through cache memory, and finally to CPU registers for processing, where results in reduction of speed which will be a bottle neck and the challenges will be huge energy consumption, requirement of large memory storge to get faster computing speed with considering this physical and architectural limitations. The inspiration from brain can be the solution to this problem which is neuromorphic computing where mimicking of biological neurons and synapse can be done. Mott insulators are a unique class of materials which show Insulator to Metal Transition (IMT) due to strong electron-electron correlations, which is controlled by varying pressure, temperature and voltage. This enables reversible switching between insulating and conducting states, similar to resistive switching. Owing to these characteristics, the Mott insulators have excellent potential in resistive Random-Access Memory (RRAM) and neuromorphic memory and computing. Among the Mott insulators, $VO_2$, due to its near room temperature Insulator to Metal transition, has been studied for various applications. This work will explore the voltage driven mott transition in $VO_2$ thin films grown using Pulsed Laser Deposition technique for neuromorphic memory.

**Keywords:** Neuromorphic memory and computing, Resistive Random Access Memory (RRAM), Mott Insulators, Insulator to Metal transition (IMT), Pulsed Laser Deposition (PLD).

# Effect of titanium doping on the physical properties of nickel oxide thin films for electrochromic smart windows applications

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**Abstract**

With the rapid development of economy, energy crisis and environmental pollution have become the focus of whole society. Developing new kinds of materials with dual or multi functions may be the key to resolving the conflict. As a capacitor and an anodic electrochromic material, NiO has been proved to be a promising bifunctional material for integrated devices such as electrochromic capacitors and energy storage smart windows. However, there are still great challenges in engineering between energy storage and electrochromic devices. Herein, we fabricated pristine and titanium (Ti)-doped nickel oxide (NiO) thin films to study the influence of Ti doping on their structural, optical, morphological, and electrochemical properties. X-ray diffraction confirmed the formation of polycrystalline cubic NiO with a preferential (111) orientation, and Ti doping induced slight lattice strain without altering the primary phase. Optical analysis revealed enhanced transmittance and a minor reduction in band gap from 3.92 to 3.84 eV upon Ti doping, indicating improved crystallinity and modified electronic structure. Photoluminescence spectra showed near-band-edge and defect-related emissions, with Ti doping suppressing radiative recombination and improving charge separation. Surface morphology of the materials were evaluated in Scanning Electron Microscopy (SEM). Cyclic voltammetry indicated quasi-reversible redox behavior associated with $Ni^{2+}/Ni^{3+}$ transitions, with Ti-doped films exhibiting larger voltammogram areas, signifying enhanced ion diffusion and charge-transfer kinetics. Overall, Ti doping effectively improved the optical transparency, structural stability, and electrochemical performance of NiO thin films, highlighting their potential for electrochromic smart windows applications.

**Keywords:** Metal oxide thin films, Electrochromic devices, Energy Efficient Smart Windows, Sustainable energy Goals

# Tuning blue hue of $V_2O_5/MoO_3/V_2O_5$ electrochromic trilayer film prepared by thermal evaporation

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**Abstract**

Heterostructure metal oxide thin films have emerged as promising materials for smart windows because of multicolor options, efficient intercalation and enhanced stability. Optimal electrochromic performance of displays relies on precise tuning of primary colours. Our work improves optical modulation of blue-hue and enhances cyclic stability through a $V_2O_5/MoO_3/V_2O_5$ triple-layer heterostructure. The XRD, Raman and XPS analyses confirm the structural purity and oxidation states of the material. Cyclic voltammetry and EIS results demonstrate its electrochromic capability and ion intercalation governed by diffusion-driven processes. Chronoamperometric studies reveal the kinetics of the heterostructure film, exhibiting high optical modulation and enhanced stability over 500 on–off cycles without compromising the change in transmittance ($\Delta T$). A power-efficient electrochromic performance is demonstrated in a proposed heterostructure highlighting its potential for pixelated displays.

**Keywords:** Heterostructure, Metal oxide thin films, Electrochromic

# Atomically dispersed iron catalyst-based catalase nanozyme for distinctive determination of hydrogen peroxide

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**Abstract**

Nanozymes are trending in today's world owing to their ability to mimic naturally existing enzymes with enormous advantageous features such as robustness, ease of synthesis, cost-effectiveness, and reproducibility. However, few of the reported nanozymes lack selectivity, and this drawback could be overcome by tuning the structure of the nanozymes. Of late, single atom nanozymes are being investigated because of the ability to mimic the active metal centre of the natural enzyme and additionally afford enhanced activity owing to the uniformly dispersed active sites. Ever since the discovery of iron-based single atoms (FeSA), it has been exploited world-wide for various applications such as catalysis, energy and sensing. Howbeit, very little attention has been given to FeSA in the field of electrochemical sensors. Though several reports are available on the peroxidase-mimicking activity of FeSA, the catalase-like activity of FeSA has been rarely investigated. This inspired us to probe the catalase-mimicking activity of the well-known FeSA, and to employ it towards the electrochemical sensing of hydrogen peroxide ($H_2O_2$) at neutral pH. The Michaelis-Menten parameters, $K_m$ and $v_max$ of FeSA were calculated to be $233.3\mu M$ and $333.3\mu A$, respectively, which evidences the enhanced enzyme-substrate affinity compared to the natural catalase enzyme. Notably, the developed sensor was inspiringly capable of detecting $H_2O_2$ at zero applied potential and portrayed two linear ranges from 5˘$75\mu M$ and $75\mu M$ – 1.4 mM with a very low detection limit of $1.22\mu M$.

**Keywords:** Enzyme-mimetic, Single atom nanozymes, Catalase

# Enhancing GaN HEMT performance through AlGaN barrier thickness and aluminum composition engineering

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**Abstract**

This paper explores how changing the thickness of the AlGaN barrier layer and the amount of aluminum in it affects the performance of GaN-based HEMT devices using TCAD Silvaco simulations. When the AlGaN thickness was adjusted between 15nm and 30nm at a drain voltage of 4V, an interesting peak in current flow was observed at 25nm, caused by an increase in polarization-induced charges at the interface. Additionally, varying the aluminum content from 5% to 35% led to a noticeable shift in the device's threshold voltage toward more negative values. When the aluminum composition exceeded 25%, even small voltage changes caused significant shifts in current. These effects, driven by increased polarization charges and threshold voltage shifts, ultimately help improve device performance.

**Keywords:** AlGaN barrier thickness, Aluminum mole fraction, GaN-based HEMT, Polarization-induced charges, Threshold voltage shift, TCAD Silvaco simulation

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# Ferrocene-anisole-appended centrosymmetric push-pull barbiturate and thiobarbiturate dyes for non-linear optics

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## Abstract

Anisole-substituted ferrocenyl (thio)barbiturate dyes FcABA, FcATBA, FcADMBA, and FcADMTBA were synthesized and structurally characterized using $^{1}$H, $^{13}$C-NMR, ESI-Mass, and single crystal X-ray diffraction analysis. FcADMBA and FcADMTBA dyes (N-methylated dyes) were crystallized in centrosymmetric triclinic system while the non-methylated dyes were more amorphous. Also, absorption and emission solvatochromism were done to examine the Intramolecular Charge Transfer (ICT) process, one of the key factors to obtain Second Harmonic Generation (SHG). Absorption solvatochromism of all the dyes showed that the hydrogen bond donor solvents and chlorinated solvents showed a bathochromic shift in all the dyes which shows that they could be good NLOphores in those solvents. Thermogravimetric analysis (TGA) showed that the barbiturate dyes are more stable than the corresponding thiobarbiturate dyes. The cyclic voltammetry analysis revealed that FcABA, FcADMBA, and FcADMTBA are almost reversible systems with a current ratio of 0.94, 0.97, and 0.99, respectively. In addition, the theoretical calculations were done to correlate the experimental results using various functionals like B3LYP, CAM-B3LYP, M06, and LC-BLYP with the 6-31G(d,p) basis set and the outcomes were summarized and presented.

**Keywords:** Donor-$\pi$-Acceptor, Thio-barbiturate dyes, SHG, NLO, DFT studies

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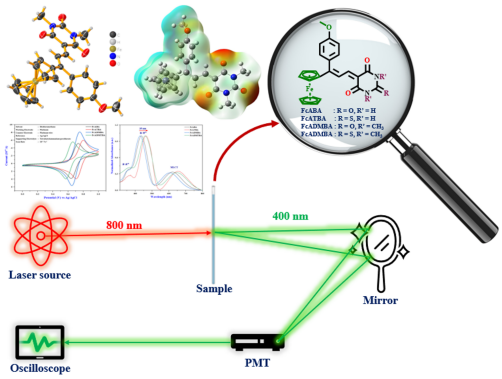


**Figure:** Ferrocene-anisole-appended centrosymmetric push-pull barbiturate and thiobarbiturate dyes for non-linear optics

# Ferrocenecarboxylates and nitro phenanthroline-based monomeric and dimeric Zn (II) and Cd (II) complexes: Structural, electrochemical, luminescence and nonlinear optical properties

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**Abstract**

A new series of Ferrocene-based metal complexes [Zn(FcCOO)$_2$(N-Phen)] (1), [Cd(FcCOO)$_2$(N-Phen)] (2), [Zn(FcCH=CHCOO)$_2$(N-Phen)] (3), [Cd(FcCH=CHCOO)$_2$(N-Phen)] (4), [Zn$_2$(Fc(COO)$_2$)(N-Phen)H$_2$O]$_2$ (5) [Cd$_2$(Fc(COO)$_2$)(N-Phen)H$_2$O]$_2$ (6) ), which FcCOO = ferrocene carboxylic acid, N-Phen = 5-nitro-1,10-phenanthroline have been synthesized and characterized by using analytical and spectroscopic methods. The crystal structure of [Zn$_2$(Fc(COO)$_2$)(N-Phen)H$_2$O]$_2$ (5) has been determined by single-crystal X-ray diffraction and zinc complex (5) is a centrosymmetric dimer crystallizing in the Monoclinic system with P21/c space group. The results were revealed that the Zn(II) ion is a distorted octahedral environment with two nitrogen atoms from ligand and four oxygen atoms from two Fc(COO)$_2$. The crystal packing was further stabilized with the aid of $C\breve{}O\cdots H$, and $\pi\cdots\pi$ intermolecular hydrogen bonding and $\pi\breve{}\pi$ interaction between cyclopentadienyl ring of ferrocene and 5-nitro-1,10-phenanthroline. The photophysical properties were performed by UV-visible and fluorescence spectroscopic methods and the complexes (1-6) exhibits broad emission band, indicating ligand-to-metal charger transfer (LMCT) or metal-to-ligand charger transfer (MLCT) nature. The redox wave of the complexes (1-6) was determined by cyclic voltammetry, revealed that one electron transfer ability of the ferrocene to ferrocenium ion ($Fe^{II} \leftrightarrow Fe^{III}$) moiety. In addition, density functional theory calculations have been employed to optimize the geometry of the molecules, followed by HOMO and LUMO values are good agreement with the theoretical calculation by B3LYP method using 6-31+G** as basis set and frontier molecular orbital levels for understanding the charge transfer, electrochemical and non-linear optical properties. The third-order nonlinear optical (NLO) properties were determined by the Z-scan technique and the effective third-order NLO susceptibilities $\chi^(3)$ obtained are 8.50 (1), 8.79 (2), 4.60 (3), 4.14 (4), 7.82 (5), and 6.01 (6) $\times 10^-6$ esu respectively. The SHG efficiency of the centrosymmetric 5-nitro-1,10-phenanthroline and ferrocene-carboxylate ligands mainly arises from the distorted atom and non-covalent interactions which preclude the dipoles in the antiparallel arrangement in crystal packing.

**Keywords:** Ferrocene; Photophysical properties; electrochemical studies; DFT calculations; non-linear optics

# The effect of aluminium doping in magnetite spinel on the catalytic wet peroxide oxidation of antibiotics in batch and continuous reactors

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**Abstract**

The presence of persistent antibiotics in wastewater is a concerning issue that we must address. These substances are not easily degradable and they can remain in the environment for a long time. This not only poses risks to our ecosystems but also raises serious concerns about the potential for promoting antibiotic resistance. Fenton oxidation is a powerful advanced oxidation process, renowned for its ability to generate highly reactive hydroxyl radicals ($\bullet OH$) with a remarkable redox potential of 2.8 V. This capability makes it an incredibly effective solution for the degradation of a diverse array of contaminants. In this study, we successfully synthesized Al-doped magnetite spinel nanoparticles encapsulated in a carbon matrix ($Fe(FeAl)_2O_4$@C), using a straightforward co-precipitation method. The catalytic activity of the $Fe(FeAl)_2O_4$@C was examined towards the degradation of antibiotic pollutants such as 20 ppm ciprofloxacin (CIP) and 10 ppm Sulfamethoxazole (SMX) in batch reactor. Under the optimized conditions, 0.5gL-1 of $Fe(FeAl)_2O_4$@C in batch reactor mineralized 51% of CIP within 180 min at 50°$C$ and pH 3 by utilizing 1.2mM or 4S $H_2O_2$ (S = stoichiometry; 47 mol $H_2O_2$:1 mol CIP) which is significantly less concentration compare to other heterogeneous Fenton catalysts. The same catalyst demonstrated 60% mineralization of SMX under the optimized reaction conditions. Impressive long-lasting catalytic activity was exhibited by the Fe(FeAl)2O4@C catalyst in the up-flow fixed bed reactor for 110 hours with 44% TOC removal and less than 1 ppm Fe leaching in the effluent water. Kinetic studies on the rate of decomposition of $H_2O_2$ revealed that $Fe(FeAl)_2O_4$@C effectively decomposed the $H_2O_2$ like the homogeneous Fenton catalyst. The XPS results indicate a significant shift toward higher binding energy for $Fe^{3+}$, confirming the effect of aluminum on the iron ions within the magnetite spinel structure. This change introduces a more electropositive character to $Fe^{3+(\delta+)}$, which accelerates the otherwise slow reduction reaction of $Fe^{3+}$ with $H_2O_2$ to produce the $HOO\bullet$

**Keywords:** Al-doped Magnetite; Spinel nanoparticles; Advanced oxidation process; Antibiotic degradation; Fixed-bed reactor

# Effect of Ni-doping on $SnO_2$ nanoparticles for the scrutinization of physico-chemical properties for gas sensing applications

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**Abstract**

In real-world scenarios, the demand for gas sensors is steadily increasing due to their indispensable ability to detect a wide range of volatile organic compounds (VOCs) as well as toxic, flammable, and non-flammable gases. Metal oxide-based gas sensors are extensively employed in diverse fields such as healthcare, food processing, air quality monitoring, explosive detection, industrial safety, environmental pollution control, and agriculture. In this work, nickel-doped tin oxide (Ni–$SnO_2$) nanoparticles with varying Ni concentrations (2–8%) were successfully synthesized via a simple chemical co-precipitation method and investigated for VOC detection at room temperature. Structural analysis confirmed the formation of a rutile-type tetragonal $SnO_2$ phase without any secondary phases, indicating the successful substitution of Ni ions into the $SnO_2$ lattice. TEM analysis revealed the polycrystalline nature of $SnO_2$, exhibiting spherical nanoparticles for both pure and Ni-doped samples. The incorporation of Ni induced a slight lattice distortion, enhanced defect density, and increased oxygen vacancies, as evidenced by optical and surface characterization. A gradual reduction in the optical band gap from 3.53 eV to 3.40 eV with increasing Ni content indicates the formation of defect states and oxygen vacancies within the $SnO_2$ lattice. These defects serve as active sites for gas adsorption, while the reduction in crystallite size enhances the effective surface area. Electron paramagnetic resonance (EPR) analysis showed an increased signal intensity with a main peak at g = 2.01, confirming the presence of paramagnetic unpaired electrons associated with oxygen vacancies in Ni-doped $SnO_2$. The 2% Ni-doped $SnO_2$ sample exhibited an improved BET surface area of 27 $m^2/g$ with a mesoporous structure. I–V measurements performed under both low and high bias voltages revealed a linear (ohmic) response for Ni-doped $SnO_2$, contrasting with the rectifying behavior observed for pure $SnO_2$. This linearity suggests that Ni incorporation enhances donor-like defect density and free-carrier concentration, narrowing the interfacial depletion width and reducing grain-boundary barriers. Consequently, charge injection becomes more efficient and bulk conduction dominates within the measured bias range. Furthermore, X-ray photoelectron spectroscopy (XPS) and EPR analyses confirmed the presence of abundant oxygen vacancies and chemisorbed oxygen species, with the characteristic spin-orbit splitting of 8.4 eV verifying the formation of $SnO_2$. Overall, Ni-doped $SnO_2$ nanoparticles demonstrate excellent potential as an efficient sensing material for VOC detection due to their enhanced surface reactivity and superior physico-chemical properties, making them a promising candidate for next-generation gas sensor applications.

**Keywords:** Co-precipitation Method, VOC detection, Surface Area, Healthcare, Donor-defects, Oxygen vacancies

# Biosensing structure-based design of metal–carbamate complexes as cholinesterase inhibitors for alzheimer's disease

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**Abstract**

The rational design of biofunctional metal complexes is essential for advancing biosensing and therapeutic strategies targeting neurodegenerative disorders such as Alzheimer's disease. In this study, phenyl and hetero-alkyl carbamate derivatives derived from Rivastigmine were synthesized and coordinated with transition metals to evaluate their potential as cholinesterase inhibitors. Molecular docking studies using AutoDock Vina were employed to predict the binding affinities and interaction profiles of the complexes toward acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), the key enzymes implicated in Alzheimer's pathology. The docking analyses revealed that metal coordination substantially enhanced enzyme–ligand interactions through $\pi^{\smile}\pi$ stacking, hydrogen bonding, and metal-assisted stabilization within the catalytic gorge. The optimized metal–carbamate complexes exhibited higher binding energies compared to their corresponding free ligands, indicating improved inhibitory potential. These results highlight the dual applicability of the designed complexes as biofunctional materials for cholinesterase biosensing and as promising therapeutic scaffolds for cholinesterase-associated neurological disorders. Based on the combined in silico and experimental evaluations, carbamate derivatives 1 and 7 demonstrated strong and selective BChE inhibition, suggesting their potential as lead candidates for further neurotherapeutic development.

**Keywords:** Biosensing, Molecular Docking, metal complex, In silico, Cholinesterase

# Environmentally friendly hydrometallurgical approach for sequential precipitation of critical metals from spent LIBs

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**Abstract**

Recycling of spent lithium-ion batteries (LIBs) is crucial for ensuring safety disposal as well as addressing the growing demand of critical metals such as lithium (Li), manganese (Mn), nickel (Ni), and cobalt (Co). This work describes a simple and effective hydrometallurgical approach of leaching and recovering of critical metals from spent LIB using organic acid as leaching agents. The cathode materials were separated from the aluminium current collectors after safe discharge of spent LIBs collected from discarded laptops. Structural and compositional analyses of spent cathode material using XRD and ICP-MS revealed that the cathode materials was of NCM type consisted of Lithium, Nickel, Cobalt and Manganese. The spent cathode was thoroughly washed with dimethyl carbonate (DMC), heated at 450°*C* for 4 hours to remove binder residues followed by leaching using oxalic acid. The metals were sequentially recovered through a controlled precipitation process from the leachate. Mn was selectively precipitated as $Mn(OH)_2$ using ammonium hydroxide, Li as $Li_2CO_3$ by sodium carbonate treatment, Ni as $[Ni(DMG)_2]$ complex through dimethylglyoxime reaction, and finally Co was recovered as cobalt(II) oxalate using oxalic acid by tuning pH. The structure and composition of the recovered products were confirmed by XRD, FTIR, EDX and ICP-MS analyses. The efficiency of the recovery of the metals were 88% (Li), 89% (Mn), 98% (Co), and 94% (Ni). Thus, the hydrometallurgical process developed demonstrates sustainable and scalable recycling of NCM-based lithium-ion battery (LIB) cathodes.

**Keywords:** Spent lithium-ion batteries, NCM cathode material, Hydrometallurgy, Sequential precipitation, Metal recovery

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# Understanding the impact of activation methods on biomass-based hard carbon anodes in sodium-ion batteries

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**Abstract**

Hard carbon (HC) has emerged as an efficient anode material for sodium-ion batteries (SIBs) owing to its low cost, abundance, and excellent electrical conductivity. This study adopts a sustainable "waste-to-wealth" approach to synthesize HC from Sterculia foetida fruit shells, a renewable biomass resource. The preparation involved fragmentation, pre-carbonization, high-temperature carbonization ($\geq 800°C$), impurity removal, and subsequent activation. To enhance porosity and surface properties, chemical activation using KOH and physical activation via hydrothermal treatment at 150, 180, and $200°C$ for 24 hours were implemented. Structural and morphological characteristics were analysed through SEM, Raman spectroscopy, XRD, and BET surface area measurements. SEM images showed a hierarchical porous structure, while Raman spectra confirmed the presence of disordered carbon domains typical of non-graphitizable HC. XRD results displayed broadened (002) and (100) peaks, indicating low crystallinity. BET analysis revealed type IV isotherms, confirming hierarchical porosity and increased surface area in activated samples. Electrochemical evaluations using EIS, CV, and GCD in sodium half-cells demonstrated that physically activated HC exhibited enhanced specific capacity, lower resistance, and improved cycling stability. The study underscores the effectiveness of physical activation in tuning microstructure and electrochemical behaviour, providing a sustainable route for producing high-performance HC anodes from biomass waste for SIBs.

**Keywords:** Sodium -Ion Batteries, Hard Carbon, Activated Carbon, Sterculia foetida, biomass

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# CuFeZnO trimetallic nanoparticles decorated on reduced graphene oxide: A multifaceted nanocomposite for sustainable environmental and healthcare applications

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**Abstract**

Solar-driven photocatalytic methods for the elimination of organic contaminants from wastewater and other aqueous solutions are attracting interest due to their sustainability and environmental advantages. This study generated Copper-Iron-Zinc trimetal decorated rGO nanocomposite (CuFeZnO/rGO) via a low-temperature chemical co-precipitation approach and utilized them as catalysts for the breakdown of Phenol red (PR) and Acridine orange (AO) dye under UV radiation. Photocatalytic tests were performed two nanocomposite CuFeZnO and CuFeZnO/rGO nanocomposite, revealing that CuFeZnO/rGO nanocomposite efficiently destroyed Phenol red (84.57%) and Acridine orange (83.01%) dye under UV irradiation. The total deterioration efficiency was associated with reduction in the band gap energy of CuFeZnO/rGO (2.32 eV) nanocomposite, which were formed during nanoparticle synthesis and facilitated absorption in the UV spectrum. Recycling studies conducted over five consecutive runs validated the reusability of CuFeZnO and CuFeZnO/rGO nanocomposite, demonstrating their practical applicability for various uses. With the antibacterial results demonstrating significant efficacy against gram-positive (S. aureus) and gram-negative (E. coli) microbiological infections. The studies demonstrated the environmental remediation capabilities of CuFeZnO/rGO nanocomposite.

**Keywords:** Antibacterial activity, Electron–hole recombination, Nanocomposite, Dye degradation, ROS generation

# Synthesis and characterisation $Zn_{1-x}Fe_xTiO_3$ (x=0.2,0.4,0.6,0.8) by sol-gel method for energy storage application

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**Abstract**

Fe doped $ZnTiO_3$(ZFT) nanoparticles were prepared using sol–gel method.This materials is good in magnetic as well as electric nature, which will have potentially dielectric properties.It exhibits the good value of permeability, permittivity, resistivity, and other beneficial properties that make them promise candidates for applications in photocatalytic and magnetic properties. XRD shows that three phase structure, Hexagonal and Rhombohedral & Cubic structure. FTIR tetrahedral coordination of Fe-O, Zn - O and Ti - O shows the band at $553cm^{-1}$ to $612cm^{-1}$.Absorption edge is found in the 200 to 300 nm from the UV-Vis analysis.VSM confirm paramagnetic in nature.

**Keywords:** Sol-Gel, Dielectric properties, Perovskite, Permeability, Electrical properties

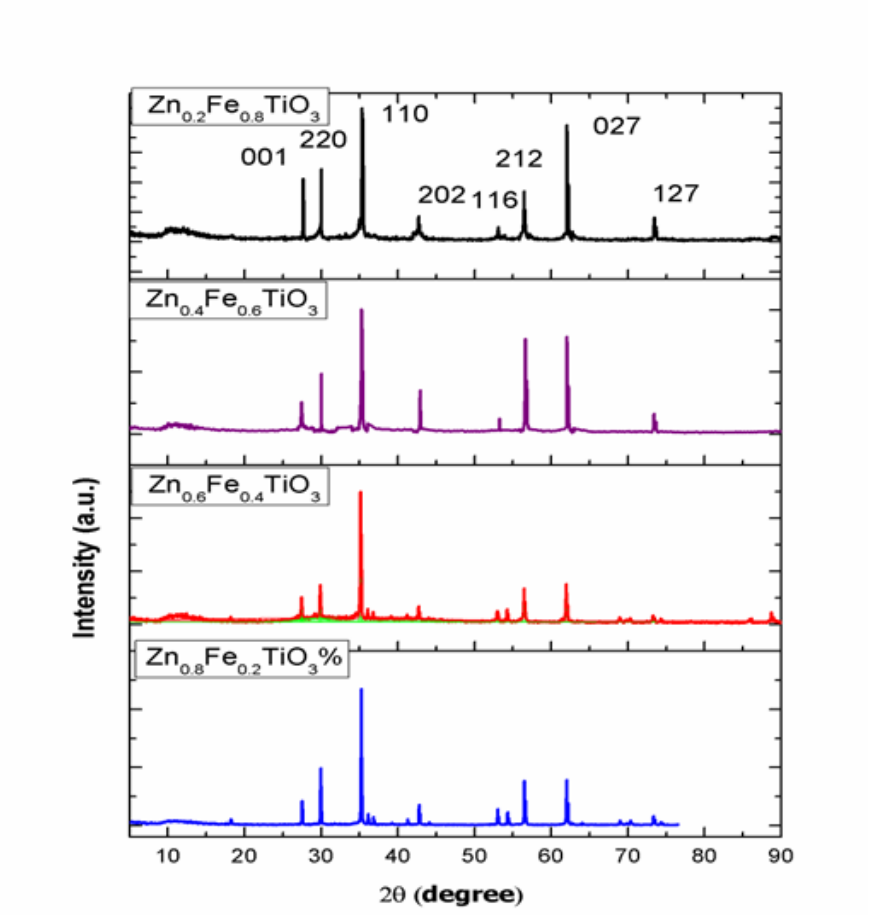


**Figure:** XRD pattern of ZFT

# Photophysical Properties of Aurone Derivatives: Solid-State Fluorescence and Solvatochromic Effects

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## Abstract

Aurones are natural or synthetic pigments that belong to the flavonoid family. Aurones are structurally defined by a benzofuranone heterocyclic configuration and are distinguished by the presence of a phenyl group connected via a carbon–carbon exocyclic double bond.[1] Importantly, the aurone structure is highly regarded in medicinal chemistry due to its architectural significance. [2] Along with this biological activity, aurones exhibit fluorescence properties due to their denominated hemi-indigo structure, absorbing light at longer wavelengths.[3,4] In this work, we introduce the solid-state fluorescence of aurone derivatives along with their solvatochromism. In the solid-state emission, the aurones showed Stokes shift values ranging from 150 nm to 80 nm. While studying the solvatochromism of the aurones, the methoxy-substituted aurones showed a blue shift.

**Keywords:** Aurones, Solid state fluorescence, Solvatochromism, Stokes shift, Blue shift

**References:**

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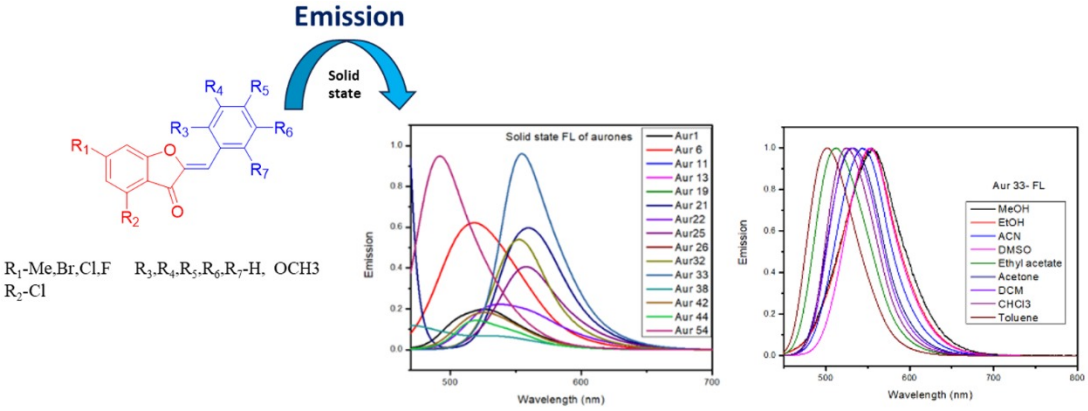


**Figure:** Solid state fluorescence of Aurones.

# Expression, purification and biophysical Characterization of the Conopeptide Mo1692 from *Conus monile*

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**Abstract**

Conotoxins are short peptides derived from the venom of marine cone snails. This venom comprises a diverse array of bioactive peptides that selectively target ion channels and receptors. These toxins have garnered significant scientific interest due to their remarkable specificity—not only for distinct ion channels but also for particular receptor subtypes [1]. The unique conformations adopted by conopeptides are crucial for their high-affinity and highly selective interactions with target proteins [2]. Investigating the structural conformations of these peptides, especially in complex with receptor fragments, holds promise for the development of novel pharmacological agents. In this context, the current study focuses on the biophysical characterization of Mo1692, a linear 15-residue peptide isolated from the venom of *Conus monile*

**Keywords:** Conus monile, Conopeptides, Biophysical characterization

**References:**

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# Fabrication and comparison of flexible electromagnetic interference shields with simulation and experimentation: screen printed bulk metallic glass verses nanocrystalline ferrite for electromagnetic interference shielding

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**Abstract**

With the proliferation of electronics and wireless communication, there has been a great focus on the potential consequences of electromagnetic radiation (EMR). The use of crystalline and amorphous fillers in polymer matrices for electromagnetic interference (EMI) shielding is a new and exciting breakthrough in this field. The design of tunable screen-printed polymer composite films with different fillers provides several avenues for producing magnetic and electrical properties that may be fine-tuned, which are necessary material features for effective EMI shielding. With its huge specific surface area, high porosity, and structural flexibility, crystalline and amorphous fillers-based polymer composites are promising candidates to block electromagnetic radiation on various scales. In this study, the critical function of structural design, specifically using crystalline and amorphous fillers in polymers, is examined in relation to their shielding performance. The screen-printing technique utilized to prepare the current EMI shields is described in detail, along with a thorough simulation using the CST Studio Suite Software to visualize the electric and magnetic field propagation. Experimentally, the shielding performance of the polymer-based crystalline and amorphous filler films is evaluated, and the shielding mechanisms are explained in terms of their structural characteristics. Furthermore, the absorption-dominance of the EMI shields formed from polymer-based crystalline and amorphous fillers is investigated.

**Keywords:** EMI Shielding, Screen printing, Polymer composite

# Synthesis and characterization of barium nickel titanium oxide by sol-gel method

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**Abstract**

A good quality nonlinear optically single crystal of 2-amino-5-chloropyridinium 4-hydroxybenzoate (ACH) was cultivated successfully by adopting slow evaporation technique. The unit cell parameters and the centro symmetric nature of the crystal were verified by single crystal XRD. From the vibrational modes, structural confirmation was done using FTIR studies. UV–Vis–NIR spectral analysis reveals that the optical transparency of ACH is more than 89 % in the entire Vis–NIR region, which confirms its colourless nature and suitable candidate for applications in optoelectronic devices. Z-Scan technique was adopted to find the third order susceptibility of the grown crystal.

**Keywords:** ACH, XRD, FT-IR, Single Crystal, Z-Scan

# Synthesis and characterization of barium nickel titanium oxide by sol-gel method

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## Abstract

Barium nickel titanium oxide particles ($Ba_2NiTi_5O_13$) were synthesized by sol-gel method followed by calcination and sintering. Of all the piezoelectric ceramics, barium nickel titanium oxide ($Ba_2NiTi_5O_13$) has an important place as an electromechanical transducer. In the present article $Ba_2NiTi_5O_13$ synthesized by sol–gel technique and microwave processed is presented. The sintered $Ba_2NiTi_5O_13$ is found to be of high density. The sintered $Ba_2NiTi_5O_13$ crystal structure and crystallinity confirmed by powder X-ray diffraction monoclinic crystal structure. Prepared $Ba_2NiTi_5O_13$ functional groups confirmed by FT-IR spectrum. Sample spherical morphology confirmed by high-resolution scanning electron microscopy (HRSEM). The particle size found to be 47 nm from HRSEM. The variation of dielectric constant and ac conductivity with temperature and frequency of $Ba_2NiTi_5O_13$ are investigated.

**Keywords:** $Ba_2NiTi_5O_{13}$, XRD, Dielectric Studies, HRSEM, AC conductivity

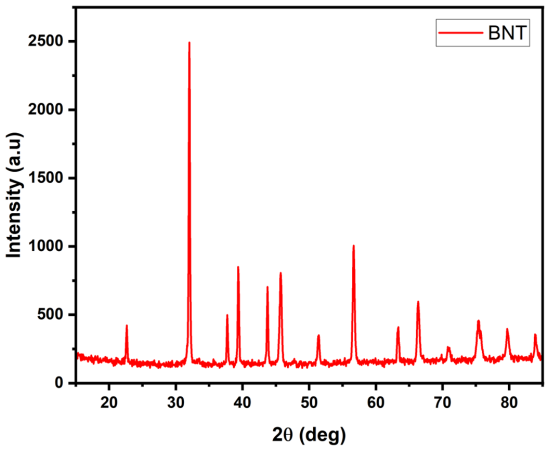


**Figure:** XRD pattern of $Ba_2NiTi_5O_{13}$

# $Co_3O_4/Ti_3C_2T_x$ MXene composite as catalase mimetic nanozyme towards selective electrochemical detection of $H_2O_2$

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**Abstract**

Hydrogen peroxide ($H_2O_2$) is an essential reactive oxygen species that is significantly involved in several applications in the fields of biological, chemical and environmental processes. However, excessive concentration of $H_2O_2$ can cause oxidative damage, cardiovascular problems, cancer and neurological diseases. Therefore, development of highly sensitive non-enzymatic electrochemical sensor for the detection of $H_2O_2$ is vital for food safety and biomedical diagnosis. In this context, the judicious design of metal-organic frameworks (MOF) derived $Co_3O_4$ nanoparticle (NPs) with natural enzyme activity have gained significant interest due to their distinct characteristics like high active sites, unique porous structures and tunable morphology. In this work, we have designed and developed a novel $Co_3O_4/Ti_3C_2T_x$ MXene nanocomposite as an effective catalase-mimetic nanozyme and checked their efficacy towards the electrochemical reduction of $H_2O_2$. The 2D $Ti_3C_2T_x$ MXene offers high surface and conductivity to uniformly anchor $Co_3O_4$ NPs. Further, the modified electrode was prepared by immobilizing the synthesized nanocomposite over glassy carbon electrode and employed it for the electrochemical detection of $H_2O_2$ in neutral pH. The fabricated sensor exhibits wide linear range, low detection limit and remarkable selectivity, which could be due to catalase enzyme like activity of $Co_3O_4$ and synergistic interaction between $Co_3O_4$ and $Ti_3C_2T_x$. Additionally, the developed non-enzymatic sensor displayed excellent operational stability and reproducibility. This superior electrocatalytic activity of the constructed sensor demonstrates that the nanocomposite $Co_3O_4/Ti_3C_2T_x$ MXene has potential applicability to selective detection of $H_2O_2$ in real samples.

**Keywords:** MXene, Catalase mimicking, Nanozyme, Electrochemical sensor, $H_2O_2$ detection

# Fabrication and study of PVA–PEG blend nanocomposite solid polymer electrolytes incorporating ZnO nanofillers

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**Abstract**

Solid polymer electrolytes (SPEs) have attracted significant attention due to their potential applications in electrochemical energy storage and conversion devices. In this work, nanocomposite solid polymer electrolyte (SPE) membranes based on a poly (vinyl alcohol) (PVA)–poly(ethylene glycol) (PEG) blend complexed with zinc-based salts such as zinc sulfate ($ZnSO_4$) and zinc triflate ($Zn(CF_3SO_3)_2$) were successfully prepared using the solution casting technique. To enhance the ionic conductivity and mechanical stability, Zinc oxide (ZnO) nanoparticles were incorporated as nanofillers at various weight percentages. The structural, morphological, and electrochemical characteristics of the prepared membranes were systematically investigated using standard characterization techniques. The results revealed that the incorporation of ZnO nanoparticles improved the dispersion of the polymer–salt matrix, leading to enhanced amorphous nature and favourable ion transport pathways. The developed PVA–PEG–ZnO nanocomposite electrolytes exhibit good mechanical flexibility, improved ionic conductivity, and interfacial stability, demonstrating their potential suitability for solid-state electrochemical applications such as batteries and supercapacitors.

**Keywords:** Solid polymer electrolyte, PVA–PEG blend, Zinc triflate, Zinc sulfate, ZnO nanofiller, Solution casting, Ionic conductivity

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# Tunable polyaniline–polyvinyl pyrrolidone composite for flexible and biodegradable acetone vapor sensing application

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## Abstract

Polyaniline–polyvinyl pyrrolidone (PPVP) composite has been prepared by physical blending of in-situ polymerized polyaniline (PANI) and polyvinyl pyrrolidone (PVP). The composite, applied as ink on cellulose substrate, has been developed as a porous, flexible electronic system. The employed computational study used density functional theory (DFT) to analyze the optical band gap, electrostatic potential surface, and chemical descriptors like chemical hardness, electrophilicity index. The morphological analyses of PANI and PPVP confirmed the reduction in surface roughness and an increase in agglomeration index (A. I.) from 4.313 to 75.253. X-ray diffractograms revealed the structural properties with the presence of compressive micro-strain within the range of 0.3017% to 0.3385%. DFT study revealed variation in optimized geometrical parameters, interaction energy, and the energy gap between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), on addition of PVP in the polymer matrix and further on introduction of acetone vapor into the system. The electrical properties are evaluated, and the variation at low concentrations of acetone vapor has been observed. The composite with 33.33% of PVP demonstrates the highest sensitivity, achieving a 52% current sensitivity at approx. 7% (v/v) acetone vapor concentration, while any further increase in PVP content reduced the performance. The sensing response is driven by physisorption of vapor-phase acetone onto the polymer matrix. This results in enhanced charge carrier mobility, leading to increased electrical conductivity under vapor exposure. The conductivity, sensitivity, and mechanical flexibility of the PPVP composites are subject to the variation of PVP content in the composite. Thus, in this work, a low-concentration acetone vapor sensor has been prepared whose performance can be tuned by optimization of the polymer ratio. DFT studies are carried out to analyze the properties of the developed system. The tunable PPVP system demonstrates its potential for practical sensor applications as a low-cost, flexible, and biodegradable chemical vapor sensitive material.

**Keywords:** Polymer, Polyvinyl pyrrolidone, Flexible electronic material, Density functional theory, Sensor

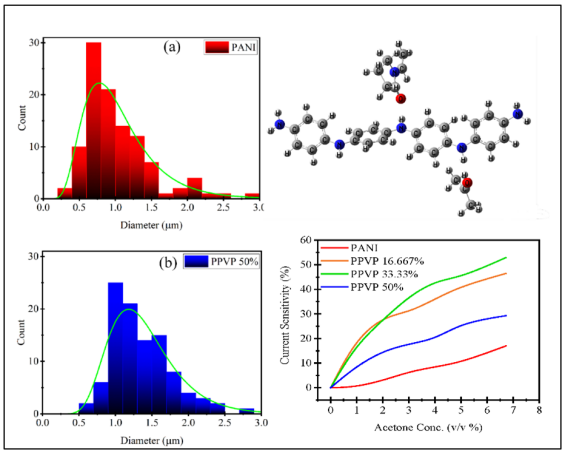


**Figure:** Graphical abstract of polyaniline-polyvinyl pyrrolidone ink as flexible acetone sensor

# 2D FEM-based study on the performance of XLPE insulation material in submarine power cable systems

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**Abstract**

This study presents a two-dimensional finite element method (2D FEM)-based investigation into the performance of cross-linked polyethylene (XLPE) insulation in submarine multi-core power cable systems. In such installations, induced circulating currents lead to inevitable power losses and heating effects, particularly in the presence of metallic components such as lead sheaths and steel gland plates. The analysis focuses on a medium-voltage XLPE-insulated cable system commonly used in harsh environments, such as oil refineries, where cables are buried underground or submerged. A magnetic–thermal coupled analysis is performed using ANSYS Multiphysics to evaluate the electromagnetic fields and calculate Joule heat losses generated within copper conductors and surrounding metallic components. These losses serve as heat sources in a steady-state thermal analysis to determine temperature distribution throughout the cable system. The study reveals that thermal performance, current-carrying capacity, and eddy current behavior are significantly influenced by the material properties of the XLPE insulation, the geometry of the cable system, and the thermal conductivity of the surrounding environment, including soil and gland plate regions. The results provide key insights into how XLPE insulation behaves under coupled electromagnetic and thermal stress, offering guidance for the improved design and deployment of submarine power cables to ensure reliability and efficiency in energy transmission.

**Keywords:** Underground power cable (UGC), Finite element analysis (FEA), Power loss calculation, Magnetic characteristics, Thermal estimation

**References:**

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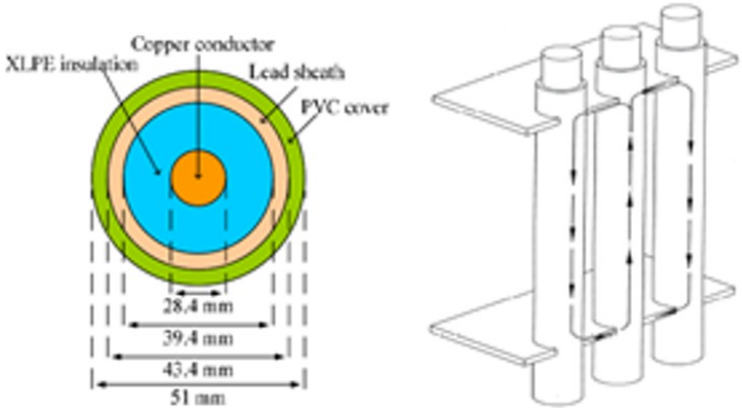


**Figure:** Cable with metal gland plate.

# Ionic transport and structural analysis of zinc chloride doped ι-Carrageenan solid polymer electrolytes for energy storage devices

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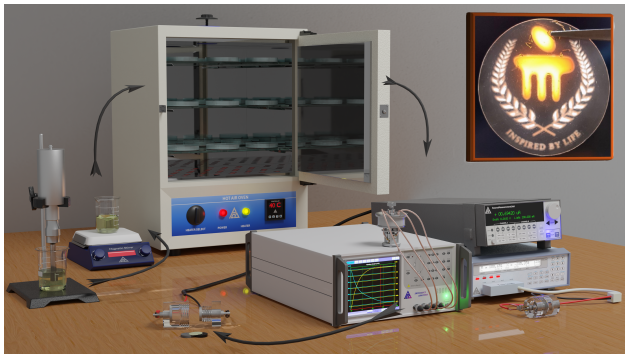
**Abstract**

Liquid electrolyte, mostly volatile organic liquids, usage has posed risks of leakage; enclosed packs puff up from their decomposition and even risk explosion in cases of fully charged cells. These risks are attempted to be mitigated using solid electrolytes, but they lack sufficient conductivity. Gel electrolytes were later introduced to improve the conductivity, although they suffer from weak mechanical strength. Solid electrolytes could be enhanced further by dissociating appropriate salts into their matrix, which aids in their ionic conductivity.[1] The selection of the polymer and the salt play a vital role in its performance, but one must also be conscious of the end-of-life of the cells in which it is used. This work thus aims to prepare a solid polymer electrolyte (SPE) with high ionic conductivity using biopolymers to be applied in zinc-ion cells. The SPEs are prepared from a facile solution-casting technique involving ι-Carrageenan[2] and zinc chloride using de-ionised water as a common solvent. FTIR studies are carried out to understand the interaction between the polymer chain and the ions, while XRD patterns are analysed to calculate their crystallinity and to verify the dissociation of the salts. Ionic conductivity is calculated from Impedance spectroscopy, scanned from 100 Hz to 1 MHz, using a custom holder and yielded a maximum conductivity of $(2.2\pm0.2)\times10^{-4}$ S $cm^{-1}$. The contribution of the cations to this conduction is calculated from the Bruce-Vincent[3] method, achieved with a custom LabVIEW program on a Sourcemeter and an LCR meter. A primary cell was fabricated and characterised to evaluate the feasibility of the SPE in a cell, and it was concluded that, with a few minor improvements, this is a viable SPE for zinc-ion cells

**Keywords:** Solid polymer electrolyte, Zinc cell, Impedance spectroscopy, Cation transference number, Iota@ι-Carrageenan



# Hybrid approach to enhancing PMMA radiation shielding using $WO_3$ and BaO modifiers

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**Abstract**

The escalating utilization of ionizing radiation across diverse scientific disciplines necessitates advanced strategies to mitigate associated health risks, thereby emphasizing the critical importance of effective radiation shielding materials. The development of lightweight, efficient, and non-toxic radiation shielding materials has become a crucial research focus as alternatives to traditional lead-based shields. In this study, polymethyl methacrylate (PMMA) was employed as a polymer host matrix due to its transparency, structural stability, and ease of fabrication. To enhance its radiation shielding efficiency, PMMA was reinforced with high-Z fillers tungsten trioxide ($WO_3$) and barium oxide (BaO)—via the solution casting technique. Composite samples were prepared with varying $WO_3$ concentrations (5–25 wt%) combined with a constant 10 wt% BaO, alongside pure PMMA as a reference material.

The shielding properties of the prepared composites were systematically evaluated against gamma radiation using a sodium iodide [NaI(Tl)] detector. Standard gamma-ray sources included Cs-137 (0.662 MeV) and Co-60 (1.173 MeV and 1.333 MeV). Experimental values of linear attenuation coefficient (LAC) and mass attenuation coefficient (MAC) were obtained and validated against theoretical predictions from Phy-X/PSD software and the XCOM photon cross-section database. Secondary shielding parameters including half-value layer (HVL), effective atomic number ($Z_{eff}$), effective electron density ($N_{eff}$), build-up factors, effective conductivity, and fast neutron removal cross section (FNRC) were also evaluated to provide a comprehensive characterization of the composites.

Morphological characterization using Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Analysis (EDAX) confirmed the homogeneous distribution of $WO_3$ and BaO fillers within the PMMA matrix, with EDAX spectra verifying elemental composition. While minor particle agglomeration was observed at higher loadings, the overall dispersion remained suitable for effective radiation attenuation.

The results indicated a significant enhancement in shielding efficiency with the progressive addition of $WO_3$. Both LAC and MAC values increased consistently with filler concentration, demonstrating the superior role of tungsten oxide in gamma-ray interaction. Correspondingly, HVL values decreased with rising $WO_3$ content, reflecting improved attenuation capacity. The calculated $Z_{eff}$ and $N_{eff}$ values further supported the enhanced photon interaction probability of the composites compared to pure PMMA. The build-up factor analysis confirmed reduced secondary photon contribution in the composites, while improved effective conductivity and FNRC values highlighted the potential of these materials not only for gamma shielding but also for neutron protection. Comparative analysis between experimental and theoretical attenuation parameters revealed close agreement, validating the reliability of both experimental techniques and computational models. The hybrid incorporation of $WO_3$ and BaO successfully produced a composite that combines structural versatility, reduced toxicity, and superior shielding performance. In particular, the PMMA sample with 25 wt% $WO_3$ and 10 wt% BaO exhibited the highest shielding effectiveness, marking it as a potential candidate for practical applications.

In conclusion, the incorporation of high-Z fillers such as $WO_3$ and BaO significantly enhances the radiation protection capabilities of PMMA-based composites. The improvement in LAC, MAC, $Z_{eff}$, $N_{eff}$, build-up factors, HVL reduction, electrical conductivity, and FNRC demonstrates the multi-faceted shielding potential of these materials. These findings suggest that PMMA/$WO_3$–BaO composites can serve as promising alternatives to conventional lead-based shielding materials in medical, nuclear, and industrial applications, offering a lightweight, environmentally safer, and efficient solution for radiation protection.

**Keywords:** Gamma-ray attenuation, Polymethyl methacrylate, Shielding, Tungsten Oxide

# Quercetin-loaded chitosan microneedle patches for efficient wound management – preparation, characterization, and in vivo evaluation

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**Abstract**

Microneedles are micron-sized needles that are used for delivering drugs precisely into skin. When compared with the conventional hypodermic needles, microneedles are regarded as minimally invasive and caused less pain. They have gained significant attention in the field of dermatology. In the present study, quercetin-loaded microneedles were prepared using PDMS micromolds. The microneedles were characterized using scanning electron microscope, fourier infrared spectroscopy and UV-visible spectroscopy. MTT and scratch wound assays were carried out to determine the cytocompatibility and in vitro wound healing activity of the microneedles. In vivo experiments were carried out using the rat excisional wound model to evaluate the wound healing efficacy of the microneedles. Scanning electron microscopic analysis revealed sharp-edged quercetin-loaded microneedles that were arranged in an orderly manner. Fourier infrared spectroscopic analysis showed peaks at 1641 $cm^{-1}$, 1418 $cm^{-1}$, and 2925 $cm^{-1}$ respectively. UV-visible spectroscopic analysis of microneedles showed maximum absorption at 262 nm and 373 nm. The microneedles showed good antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*. In vitro experiments carried out using microneedles treated NIH 3T3 fibroblasts showed enhanced wound closure than the untreated control cells. In vivo experiments showed complete closure of wounds within 16 days of treatment with the microneedles. Histological analysis showed the formation of granulation tissues and collagen deposition in rats treated with quercetin-loaded microneedles. The prepared quercetin-loaded microneedles can be used for transdermal drug delivery applications.

**Keywords:** Microneedles, Chitosan, Wound, Rats

# Performance analysis and comparative study of additively manufactured scintillators with BC408 for cosmic ray detection

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**Abstract**

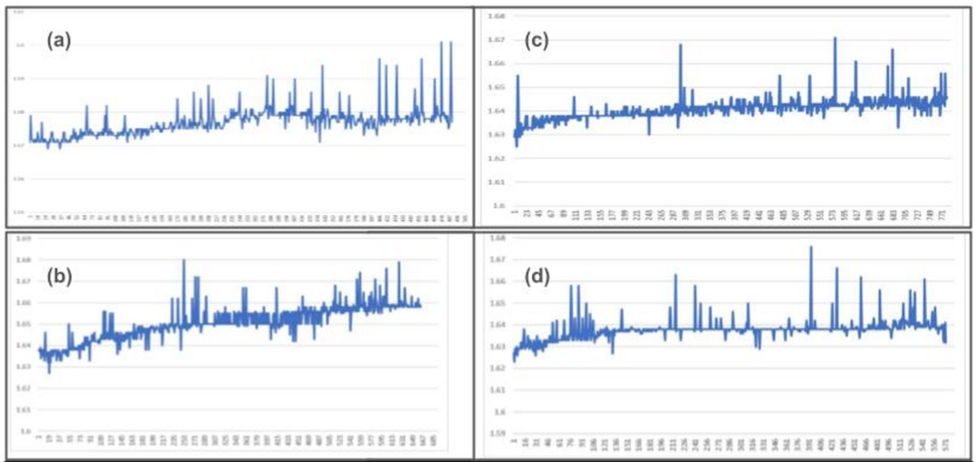
Scintillators are functional materials that convert ionizing radiation into visible light through scintillation. When high-energy particles pass through the material, it absorbs their energy and re-emits it as photons. These photons are subsequently detected by reliable photodetectors. Based on material type, scintillators are broadly classified into organic and inorganic. Various manufacturing methods are employed for their production: polymerization and single-crystal growth for organic scintillators, while techniques such as the Bridgman–Stockbarger and Czochralski methods are commonly used for inorganic scintillators.

Recent research and advances in additive manufacturing (AM) of scintillators have opened up possibilities that extend beyond the limitations of conventional fabrication methods. AM enables the design of lightweight, complex, and application-specific architectures suitable for medical probes, particle physics experiments, and space payloads. It also facilitates rapid prototyping and significantly reduces the manufacturing time required by traditional methods.

This study investigates the performance of additively manufactured organic scintillators for cosmic-ray detection, with a focus on muons, and compares it with a commercial BC408 scintillator. The additively manufactured scintillators were prepared at the Radiation Detectors and Spectroscopy Laboratory-IIT Roorkee.The experiments employ the MIT-CosmicWatch approach, using SiPMs as photodetectors and analog readout electronics to evaluate the performance of both the additively manufactured and commercial scintillators.

The initial results show promising results enabling AM scintillators to perform just as equally or better than commercial scintillators therefore demonstrating functional detection capability. This highlights the promise of additive manufactured scintillators in design possibilities, especially where complex geometries or application-specific configurations are required.

**Keywords:** Scintillator, Additive manufacturing, Radiation detection, Particle physics




Plot of voltage(readout from sipm) against time(s): (a)Additive-manufactured scintillator with a thickness of 3.9mm (b)Additive-manufactured scintillator with a thickness of 6.2mm (c)Commercial BC-408 scintillator with 10mm thickness (d)Additive-manufactured scintillator with a width of 8.2mm

# Performance analysis and comparative study of additively manufactured scintillators with BC408 for cosmic ray detection

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**Abstract**

The C–C coupling reactions by palladium (Pd)-based catalysts are very well known; however, the serious problem that remains is Pd leaching, and this leads to the limiting practical applications due to the toxicity of residual palladium species in organic products. To address this, we have prepared novel polyurethane foams, namely loaded with Pd(II), which were further reduced to the Pd(0) species (PUCS-Pd, PUCS-CA-Pd, PUCS-TA-Pd, and PUCS-GA-Pd (PU = polyurethane; CS = chitosan; CA = citric acid; TA = tartaric acid; GA = gallic acid)). These heterogeneous catalysts were employed in C–C coupling reactions. These materials demonstrated excellent catalytic activity with yields of 80–98% at room temperature and negligible leaching of Pd during the catalytic transformations. All the catalysts and organic products were structurally characterized by various analytical and spectroscopic techniques. Notably, PUCS-CA-Pd exhibited outstanding performance even at low Pd loading, maintaining high activity for more than 10 consecutive reaction cycles.

**Keywords:** Palladium catalysts, Polyurethane foam, C–C coupling reactions, Recyclable catalyst, Heterogeneous catalysts

# Sodium ion conducting biopolymer electrolyte from eucalyptus gum and chitosan blended polymer electrolyte for solid state energy device

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## Abstract

The growing interest of cost-effective and sustainable energy source solutions has driven the development of sodium-based batteries as viable alternatives to lithium-ion technologies. Mostly, organic liquid electrolyte used in commercial sodium-ion batteries are highly flammable susceptible to leakage, posing significant environmental hazards. To address this challenge, our focuses is primarily on polymer electrolytes owing to their flexibility, processability, and intrinsic safety. In this work, we used the solution casting technique to fabricate solid blend biopolymer electrolytes comprising of eucalyptus gum and chitosan, with varying weight fractions of sodium triflate. XRD analysis of the synthesised biopolymer membrane confirms its amorphous nature, while FTIR results verify the successful incorporation of sodium triflate into the polymer matrix. The electrical characteristics of the membrane were examined using electrochemical impedance spectroscopy which revealed that the film containing 30% salt has highest ionic conductivity of $1.53\times10^{-4}$ S/cm at room temperature. Transference number measurement confirms the ions are predominantly in the conduction of electrolyte. The highest conducting polymer electrolyte can be used to fabricate cost effective electrochemical device

**Keywords:** Solid state device, Transference number, Sodium triflate

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# Self-assembled NDI amphiphiles as esterase mimics in aqueous media

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**Abstract**

Enzymes achieve remarkable catalytic efficiency in water through precise self-assembly and structural organization. Inspired by this principle, the development of biomimetic catalysts has gained significant attention for replicating enzymatic efficiency using synthetic systems[1]. Among these, organocatalysts offer a simple yet powerful means to mimic enzyme catalysis. However, most organocatalysts operate in non-aqueous environments, which is far from natural conditions[2]. To overcome this limitation, we will discuss an imidazole-based naphthalenediimide (NDI) amphiphile that spontaneously self-assembles in water via $\pi - \pi$ stacking and hydrogen-bonding interactions[3]. The resulting supramolecular nanostructures exhibit a layered morphology, forming hydrophobic pockets and spatially ordered catalytic sites analogous to natural enzyme active centers. These assemblies demonstrate efficient hydrolysis of *p*-nitrophenyl esters and aspirin under aqueous buffer conditions, revealing pronounced esterase-like activity. This work bridges the gap between natural enzymatic systems and synthetic organocatalysts, highlighting the potential of self-assembled amphiphilic systems as robust, water-compatible enzyme mimics for green catalysis and environmental remediation

**Keywords:** Organocatalysis, Self-assembly, Naphthalenediimide, Enzyme mimic

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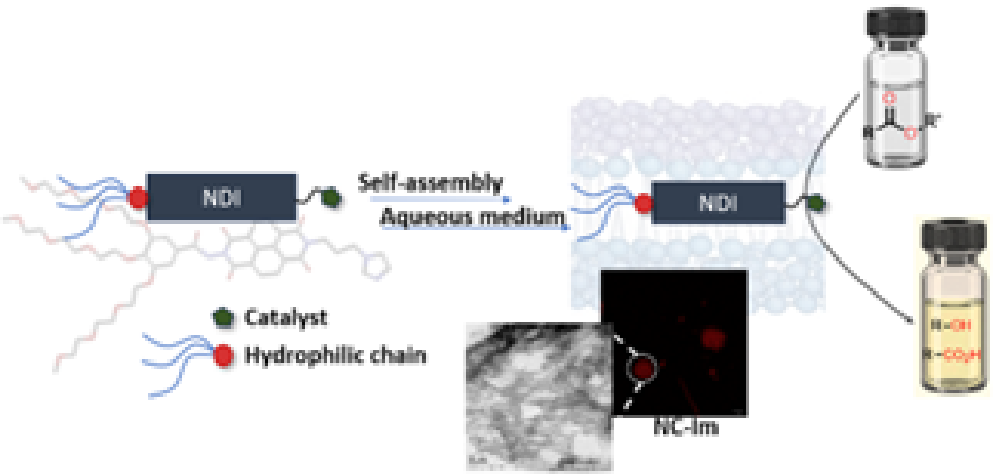

# Investigations on plasticized solid biopolymer electrolytes developed for sustainable Na-ion capacitor

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**Abstract**

Biopolymer electrolytes have emerged as promising alternatives to conventional liquid electrolytes owing to their low cost, non-toxicity, and environmental sustainability. In this study, the impact of addition of glycerol as plasticiser on the electrochemical performance of solid biopolymer electrolytes (SBPEs) composed of carboxymethyl cellulose (CMC) and polyvinyl alcohol (PVA) poly blend and sodium acetate was investigated. Polymer blending and plasticisation were employed to enhance ionic conductivity and mechanical strength of solid biopolymer electrolytes (SBPEs). Glycerol is a commonly used plasticizer which has potential to enhance ionic conductivity by weakening the polymer chain interactions, promoting amorphous ion-conductive phase because of its hydrophilic nature, and high dielectric constant. The free-standing films were systematically characterised using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), AC impedance spectroscopy, galvanostatic charge–discharge testing, cyclic voltammetry (CV), and thermal analysis. The optimised SBPE composition exhibited a three-order-of-magnitude improvement in ionic conductivity, increasing from $10^{-7}$ to $10^{-4}$ S $cm^{-1}$ at room temperature. Thermal analysis revealed the stability of SPE up to around 240 0C, ensuring safety at higher temperature. Furthermore, CV analysis in an electric double-layer capacitor (EDLC) and Na-ion capacitor configuration demonstrated the suitability of the developed SBPEs for efficient and eco-friendly sodium-based energy storage applications.

**Keywords:** Solid polymer electrolytes, Polymer blending, Plasticiser, Biopolymer electrolytes, Na-ion capacitor

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# Green synthesis of Mg-Zn nanoferrites using lemon extract; modification in dielectric and magnetic properties by Co-substitution

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**Abstract**

Cobalt-substituted Mg-Zn ferrites were prepared by the green synthesis technique using lemon extract as the fuel.X-ray diffraction patterns confirm the spinel structure for all samples, showing no traces of secondary phases. The experimental results show a strong correlation between the structural, mechanical, and magnetic properties. The lattice parameter values obtained are in satisfactory agreement with their theoretical values. The crystallite size calculated by using the Debye-Scherer formula and also by the Williamson-Hall plot was in the range of 21 nm to 54 nm, which confirms the nanocrystalline nature of the ferrites. The morphological investigations with FE-SEM exhibited that the particles are agglomerated in shape. Stoichiometric analysis of the samples was carried out by using energy-dispersive X-ray spectra. The presence of specific absorption bands in the FTIR spectrograph cross-verified the formation of spinel ferrites. The Mg-Zn ferrite with the cobalt composition x=0.42 exhibited the highest saturation magnetization of 7.67 emu/g and exceptional mechanical flexibility. The coercivity study demonstrated an increasing trend with cobalt substitution, and the highest is 538.26 Oe at x=0.56, attributed to the strong magnetic anisotropy of $Co^{2+}$ ions at B sites. The dielectric study was carried out for the prepared ferrite samples, revealing a lower concentration of space charge polarization at low frequencies. With increasing cobalt concentration, a rhombohedral grain structure appeared; due to this alteration, a decline in the dielectric constant was observed.

**Keywords:** Green synthesis, Nanoferrite, Structural properties, Magnetic properties, Dielectric properties

# One-pot hydrothermal synthesis and characterization of silver nanoferrites ($AgFe_2O_4$)

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**Abstract**

NanoFerrites have distinct electric, dielectric and magnetic characteristics which makes the materials with potential applications in technology. One of the most intriguing material groups for researchers is **Silver Nanoferrites** ($AgFe_2O_4$). The Silver Nanoferrites has been notable, reflecting its increasing significance in various fields. The hydrothermal synthesis method is a most powerful technique to tune the morphology of a prepared sample by altering the synthesis conditions. The technique was carried out with extremely high ferrite purity, and the result was well-structured nanoferrite. This method is used to fabrication of Silver Nanoferrites. This study reports the successful and simple synthesis of **Silver Nanoferrites** ($AgFe_2O_4$) via a cost-effective, **one-pot hydrothermal method**. Stoichiometric metal salts of silver and iron were reacted in an alkaline medium within a sealed autoclave at a controlled temperature and pressure. The synthesized powder was subjected to a comprehensive suite of characterization techniques to confirm its phase purity, structure, morphology, chemical composition, and magnetic properties. **X-ray Diffraction (XRD)** analysis confirmed the formation of a single-phase $AgFe_2O_4$ and allowed for the calculation of the average crystallite size using the Scherrer formula. To investigate the inherent strain and average crystalline size using XRD peak broadening examinations, W-H plot techniques were applied. The crystallographic formula exhibits crystal properties, which confirm that the material has a Hexagonal structure. **Fourier-Transform Infrared (FTIR) Spectroscopy** provides the evidence for the presence of Functional groups in the sample by stretching vibrations. **UV-Visible Spectroscopy (UV-Vis)** was used to investigate the optical properties, yielding the direct and indirect band gap energies, which are crucial for photocatalytic and semiconductor applications. **Scanning Electron Microscopy (SEM)** confirmed the uniform, nanostructured morphology. Finally, **Vibrating Sample Magnetometry (VSM)** at room temperature confirmed the **Magnetic behaviour** of the $AgFe_2O_4$ nanoparticles, revealing a measurable Saturation Magnetization (Ms), Retentivity (Mr), and Coercivity (Hc). The facile hydrothermal synthesis and the resulting material's desirable structural, optical, and magnetic properties makes Silver Nanoferrites highly promising for diverse applications, including Magnetic materials and spintronics.

**Keywords:** One-pot hydrothermal method, Silver nanoferrites, Spintronics

# Tailoring Mn substitution in $SmCo_5$ for enhanced $(BH)_{max}$ using mechanical milling

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## Abstract

The $SmCo_5$ magnet is a first-generation permanent magnet (PM) featuring a noticeable Curie temperature of 750°C and exceptionally high uniaxial magnetocrystalline anisotropy $K_u \sim 1.7 \times 10^8$ erg/cm$^3$ [1]. Hence, it still dominates the high-temperature applications even today. However, the performance factor $(BH)_{max}$ is limited by the low $M_s$ in the $SmCo_5$. Therefore, the concept of a composite magnet consisting of a hard and soft phase suitably dispersed and mutually exchange-coupled, offering both coercivity ($H_c$) and magnetization ($M_s$) was discovered. The recent work by Zhang et al. [2] reported that the substitution of non-ferromagnetic Mn with Co at the site results in local ferromagnetic coupling. Mn having twice the magnetic moment of Co enhances the $M_s$ in the system. However, the impact on $H_c$ and $(BH)_{max}$ has not been investigated in detail. Therefore, in this work, we report the optimization of Mn content and milling conditions that result in an enhanced (BH)max with both $H_c$ and $M_s$ from the parent. It is to be noted that $SmCo_5$ crystallizes in the $CaCu_5$ type hexagonal structure with atomic sites Sm (1a), Co1(2c), and Co2(3g). Figure 1(a) depicts the room temperature XRD patterns of the as-casted $Sm(CoMn)_5$ alloys. It is observed that the alloy with x = 0.1 exhibits a purely 1:5 phase, while for x = 0.2 and 0.3, a 2:7 phase with poor intensity is present. Figure 1(b) displays the shift in the position of the (111) peak of the 1:5 phase. It is observed that the peak is displaced to the lower angle side for x = 0.1, 0.3, and higher angles for x = 0.2. The lower angle shifting signifies that Mn substitutes the Co sites ($r_{Mn} > r_{Co}$) majorly, while the higher angle explains Mn replaces the Sm sites ($r_{Mn} < r_{Sm}$). This behavior is also consistent in magnetic properties. Figure 1(c) illustrates the *M-H* loop of 0.5 hrs milled alloys. It can be seen that the $M_s$ is increased for x = 0.1 and 0.3 from the parent shows the ferromagnetic coupling Co-Mn-Co, while for x = 0.2 the $M_s$ is decreased indicating the weak ferromagnetic interaction Co-(Sm-Mn)-Co. Figure 1(d) shows all extracted properties from the *M-H* loop. It is observed that the x = 0.1 alloy exhibits increased $H_c$, $M_s$, $M_r/M_s$ from the parent leading to 17% enhanced in $(BH)_{max}$ from the parent.

**Keywords:** Ferromagnetic, Permanent magnet, Saturation magnetization, Energy product

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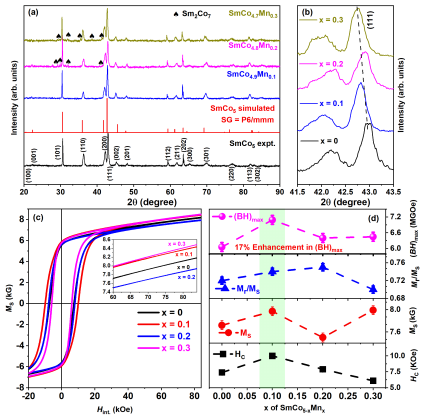


**Figure:** (a) Room temperature XRD patterns of as-casted, (b) enlarged view of shifting of (111) peak, (c) *M-H* loops for samples milled for 0.5 hrs, and (d) extracted magnetic properties for $SmCo_{5-x}Mn_x$ alloys.

# Electronic, magnetic and spin orbit coupling properties of antisite defect induced monolayer 2H-$MoS_2$ for spintronics applications

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**Abstract**

The discovery of materials exhibiting high spin polarization and efficient spin transmission is crucial for the advancement of spintronics. Two-dimensional (2D) materials, with their tunable electronic structures, have emerged as promising candidates for next-generation spintronic, opto-electronic, and nano-electronic devices. In this study, we systematically investigated the electronic, magnetic properties of the pristine and defect-engineered monolayer hexagonal molybdenum disulfide (2H-$MoS_2$) using spin-polarized density functional theory (DFT). The introduction of antisite defects transformed the nonmagnetic pristine $MoS_2$ into robust magnetic systems, attributed to the presence of unpaired d-electrons in substituted molybdenum atoms. The defected systems exhibited magnetic moments of 1.78, 3.47, and 5.15 $\mu$B/cell, respectively, whereas the pristine monolayer remained nonmagnetic. Incorporation of spin–orbit coupling (SOC) revealed distinct band splitting and band-gap modulation in the defected structures. Ab-initio molecular dynamics (AIMD) simulations confirmed the thermal stability of the defect-induced $MoS_2$ systems at room temperature. Furthermore, spin-resolved quantum transport calculations demonstrated a high spin-filtering efficiency (SFE) of up to 99.9%, indicating nearly perfect spin selectivity. These results highlight that antisite defect engineering in 2H-$MoS_2$ provides an effective route toward achieving stable, highly spin-polarized 2D materials suitable for spintronic device applications.

**Keywords:** 2D materials, Antisite defects, Spin-orbit coupling, Spin polarization, Spin transmission, Spin filtering efficiency

# Structural, microstructural, and magnetic properties of melt spun ribbons of $LaFe_{13-x}Si_x$ alloys

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## Abstract

In this study, the effect of annealing time on magnetocaloric properties of melt-spun $LaFe_{13-x}Si_x$ (x=1.2, 1.4, 1.6, and 1.8) ribbons was investigated by X-ray diffractometry (XRD), Scanning Electron Microscopy (SEM) and Vibrating Sample Microscopy (VSM) measurements. The ribbons were prepared at a wheel speed of 34 m/s in a single roller melt spinner and subsequently annealed at 1323 K for 2h in vacuum ($10^{-5}$mbar) followed by air quenching. The XRD and SEM results show melt-spun ribbons have 1:13, 1:1:1, and $\alpha$-Fe phases in the as melt spun condition and annealing helps to increase the volume fraction of the 1:13 phase at the expense of 1:1:1 and $\alpha$-Fe phases. In addition, annealing also brings the Curie temperature towards room temperature which will prove advantageous as far as application in refrigeration is concerned. Annealing of melt-spun ribbons also shows improvement in magneto-caloric properties.

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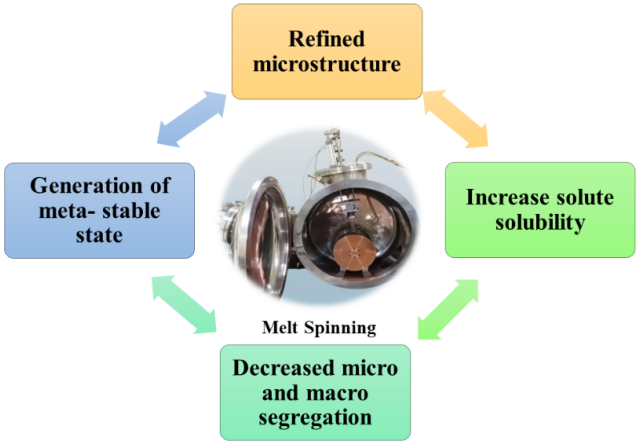


**Figure:** (a) Properties of Melt spun materials

# Microwave-assisted synthesis of cobalt ferrite: a fast and efficient route to tailor magnetic and dielectric properties

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**Abstract**

Here we demonstrated an efficient, cost-effective route for fabricating high-quality cobalt ferrite with significantly reduced synthesis time using microwave reaction and compared with the routine solid state reaction method. The structure and phase purity is confirmed by Rietveld refinement of the X-ray diffraction (XRD) patterns. The results are further supported by X-ray photoelectron spectroscopy (XPS). Deconvolution of the high-resolution Co 2p and Fe 2p spectra revealed the distribution of cations across the tetrahedral and octahedral sites. The samples prepared via microwave-assisted and conventional solid-state reaction routes exhibited average grain sizes of approximately 368 nm and 771 nm, respectively. The high heating rate during microwave sintering favored the formation of particles with well-defined octahedral morphology. Magnetic measurements showed variations in saturation magnetization and coercivity, primarily attributed to differences in cation distribution, while size effects were negligible due to the relatively large particle dimensions. The dielectric behavior of both samples followed Koop's theory. The solid-state-synthesized $CoFe_2O_4$ with the high dielectric constant, moderate saturation magnetization, and low dielectric loss can be suitable for high-frequency device applications. While, the microwave-sintered $CoFe_2O_4$, exhibiting a high squareness ratio, moderate saturation magnetization, and low coercivity, can be promising for magnetic recording and microwave absorption applications.

**Keywords:** Cobalt ferrite, Solid-state reaction, Microwave assisted solid-state reaction, Dielectric properties, Magnetic properties

# Studies on the influence of neodymium-doped strontium hexaferrite/cobalt-zinc ferrite nanocomposites for microwave absorption properties in the X-band region.

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**Abstract**

The growing number of electronic devices and wireless systems has increased the demand for efficient microwave absorption materials to reduce electromagnetic interference and ensure device dependability. Ferrite-based materials, with their distinct magnetic and dielectric characteristics, are attractive prospects for high-performance microwave absorbers. In this work, Nd-doped strontium hexaferrite ($SrFe_{12}O_{19}$) was combined with cobalt-zinc ferrite ($Co_{0.7}Zn_{0.3}Fe_2O_4$) and mixed in various ratios (0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.3, & 1) to develop nanocomposites using the sol-gel auto-combustion method. Further, the prepared material was annealed at a temperature of 1100 °C for 4 hrs to achieve the phase formation of the nanocomposites. The synthesized composites were characterized and analysed utilizing a variety of techniques. XRD analysis confirms the phase formation and coexistence of SNFO and CZFO phases in the synthesized nanocomposite. VSM was used to examine the magnetic properties of the samples, including saturation magnetization, coercivity, and remanence. High saturation magnetization allows the material to maintain its magnetic properties over a broad frequency range. The microwave absorption performance of the composites was evaluated using a Vector Network Analyzer (VNA). The combination of hard and soft ferrite phases increases magnetic and dielectric losses, which leads the material to absorb microwaves more effectively. This work highlights the promise of rare-earth-doped ferrite composites as efficient, lightweight, and versatile microwave absorbers

**Keywords:** Hard-Soft ferrite nanocomposites, Sol-gel auto combustion technique, Reflection loss, Exchange coupling interaction, Microwave absorption behaviour

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# Structural and magnetocaloric investigation of $L2_1$-Ordered $Co_2MnAl$ exhibiting Griffiths Singularity

Aiswarya R Prasad[1], Shilpa Mariam Mathew[1], Sanjay Ravichandran[1], Senthur Pandi Rajasabai[1,*]

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## Abstract

The search for advanced magnetic materials with tunable transitions and novel disorder-driven phenomena is integral to modern functional materials science. In this context, we present a comprehensive study of the structural, magnetic, and magnetocaloric properties of $L2_1$-Ordered $Co_2MnAl$ Heusler alloy, synthesized via vacuum arc melting. X-ray diffraction confirmed the formation of a cubic $L2_1$ phase, which aligns with standard JCPDS 57618 data, underscoring the structural integrity of the sample.

Magnetic characterization revealed a Curie temperature ($T_c$) of 694 K, indicating robust ferromagnetism well above room temperature-an attractive attribute for magnetocaloric applications. Detailed temperature- and field-dependent magnetization measurements, analyzed with local magnetic models and the modified Bloch law, establish long-range ferromagnetic ordering below $T_c$. Notably, the investigation uncovers the onset of Griffiths singularity above $T_c$, evidenced by deviations from Curie-Weiss behavior and supported by non-unity exponents ($\lambda$) in susceptibility analysis. This peculiarity highlights the coexistence of short-range magnetic clusters within the paramagnetic matrix, a fingerprint of the Griffiths phase as observed in related Heusler and transition metal alloys.

The role of disorder and its modulation by the external magnetic field were elucidated: increasing the strength of the applied field was found to promote uniform magnetization and systematically suppress the Griffiths phase, as indicated by the reduction of $\lambda$. The magnetocaloric response, inferred from field-induced entropy change and spin-wave-driven enhancement in long-range correlations, substantiates the potential of $Co_2MnAl$ for efficient magnetic refrigeration near ambient temperatures. Our investigation provides compelling experimental evidence for intrinsic Griffiths singularity in this system.

**Keywords:** $L2_1$ – Structure, Modified Bloch law, Griffith phase, Curie temperature

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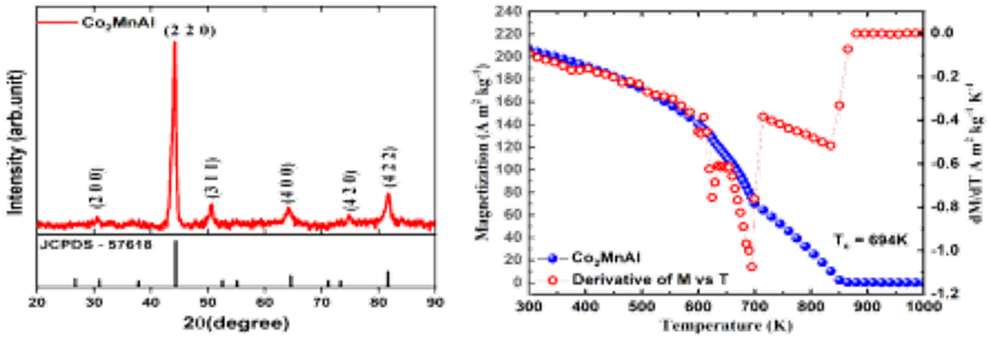


**Figure:** X-ray Diffraction and M vs T analysis of the L21 structured Co2MnAl

# Griffiths Singularities and long-range ferromagnetic ordering in half-Heusler CoMnAl Alloy

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## Abstract

Half-Heusler alloys have emerged as promising candidates for spintronic and magnetocaloric applications due to their unique electronic structure and tunable magnetic properties. In this study, we present a comprehensive investigation of the structural, magnetic, and thermodynamic properties of CoMnAl half-Heusler alloy, synthesized via vacuum arc melting, with particular emphasis on the observation of Griffiths singularity-a rare magnetic phenomenon that bridges ferromagnetic ordering and paramagnetic behavior. X-ray diffraction analysis confirmed the formation of a cubic $Cl_b$-type structure consistent with standard JCPDS data (57-618), establishing the structural integrity of the synthesized alloy. Comprehensive thermomagnetic measurements revealed a Curie temperature ($T_c$) of 624 K, indicating robust room-temperature ferromagnetism essential for practical applications. Critical magnetic behavior analysis employing local magnetic models and temperature dependent saturation magnetization demonstrated excellent agreement with the modified Bloch's law (with exponent $\lambda$), confirming long-range ferromagnetic ordering below $T_c$.

Most significantly, our investigation reveals compelling evidence for Griffiths singularity in the paramagnetic region above $T_c$, characterized by deviations from classical Curie-Weiss behavior and manifested through non-unity $\lambda$ values in magnetic susceptibility analysis. Systematic field-dependent studies (0.5 T) demonstrated that the external magnetic field effectively suppresses magnetic disorder by promoting uniform magnetization, as evidenced by the reduction in the Griffiths phase exponent. The linear relationship between $1/\chi$ and ($T–T_c$) confirms the Griffiths-like phase, while the sub-unity value of $\lambda$ quantitatively establishes the degree of magnetic inhomogeneity. The spin-wave contribution extracted from Bloch's law fitting provides quantitative characterization of magnetic disorder, revealing the microscopic origin of the observed phenomena. These findings establish CoMnAl as a model system for understanding disorder-driven magnetic transitions in half-Heusler compounds and highlight its potential for applications in magnetic refrigeration and spintronics, where controlled magnetic inhomogeneity can be advantageous. Our results contribute fundamental insights into the interplay between structural order and magnetic behavior in half-Heusler alloys, opening new avenues for designing materials with tailored magnetic properties through controlled disorder engineering.

**Keywords:** Half Heusler, $Cl_b$ – structure, Bloch law, Griffith phase

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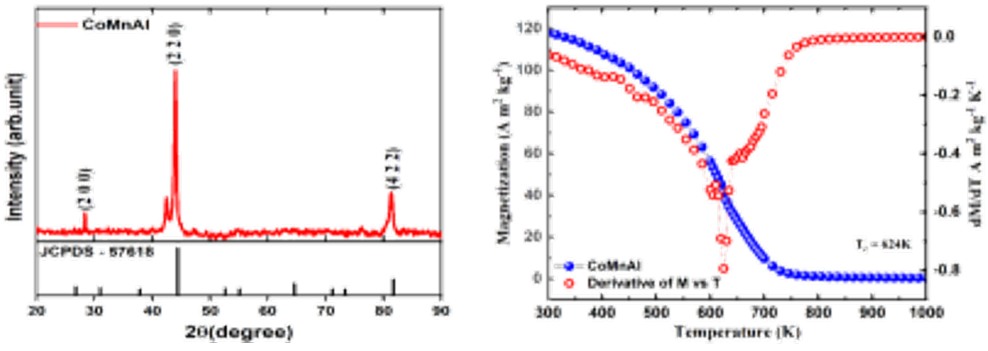


**Figure:** X-ray Diffraction and M vs T analysis of the L21 structured Co2MnAl

# Hydrothermally synthesized cobalt-doped $VS_2$ for Supercapacitor application

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**Abstract**

The rapid growth in population and industrialization has led to a significant increase in global energy consumption. The depletion of fossil fuels and the associated energy crisis have intensified the search for renewable and efficient energy storage solutions. Efficient storage of energy derived from renewable sources demands advanced and sophisticated storage systems. Two-dimensional (2D) transition metal dichalcogenides (TMDs) [1], such as $VS_2$, have attracted considerable attention due to their structural similarity to graphene and their unique chemical and physical properties. In this context, hydrothermally synthesized cobalt-doped $VS_2$ has demonstrated promising supercapacitive performance. X-ray diffraction (XRD) analysis confirms the formation of a hexagonal crystal phase, while field emission scanning electron microscopy (FESEM) images reveal a nanosheet-like morphology (Fig. a). The electrochemical performance was evaluated using a three-electrode setup, where the sample with the lowest cobalt doping exhibited the best supercapacitive behavior (Fig. b)

**Keywords:** $VS_2$, Hydrothermal method, Supercapacitor

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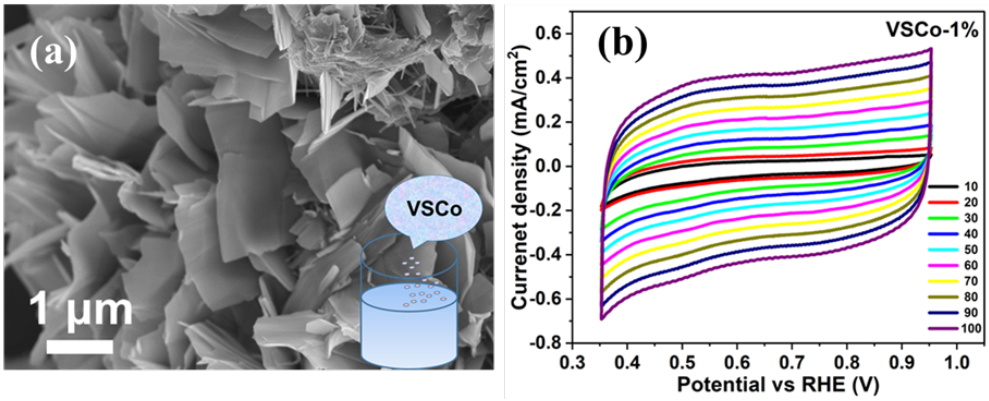


**Figure:** Supercapacitor application

# Hybridizing NiFe-LDH and MXene nanosheets for high performance energy storage application

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**Abstract**

The exceptional energy storage properties of supercapacitors make them a compelling candidate for clean energy application. Layered double hydroxides (LDH) have emerged as intriguing candidates for energy storage materials due to tunable compositions exceptional theoretical capacities; however, their practical implication is limited by inherent drawback such as easy tendency to agglomerate and poor electrical conductivity. To address these obstacles, an in-situ hydrothermal method was used to synthesize NiFe-LDH/MXene maocomposites, which produced a 3D architecture. The strong interfacial interaction and efficient electronic coupling between the NiFe-LDH aggregated nanosheets and $Ti_3C_2T_X$ MXene layered nanosheets enhance the electrolyte accessibility, structural stability and electrical conductivity. NiFe-LDH/5 mg MX nanocomposite is a promising electrode material for a high performance battery-type supercapcitor due to the specific capacitance of LDH and the remarkable electrical conductivity of MXene. Current density of 2 A/g, the NiFe-LDH/5mg MX electrode validated a remarkable specific capacitance of 1135 F/g. An asymmetric device was built using VC as the negative electrode and NiFe-LDH/5 mg MX as the positive electrode. Device produced an exceptional power density of 7617.6 W/Kg at an energy density of 58.19 Wh/Kg, and it revealed exceptional cyclic stability by holding onto 71% of its initial capacitance even after 3500 cycles at 8 A/g.

**Keywords:** Energy Storage, MXene nanosheets, Supercapacitor

# Unravelling the effect of addition of inorganic electroactive additives to triazolium ionic liquid- making them into ternary and quaternary ions electrolytes for EDLC applications

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**Abstract**

Research on enhancing the performance of supercapacitor devices is inevitable, yet the scope for improvement remains restricted to modifications in the electrode or electrolyte materials. On the electrolyte side, two major categories exist: aqueous and organoelectrolytes. While aqueous electrolytes are limited by the 1.23 V water-splitting potential, organoelectrolytes overcome this barrier and thereby enable a wider potential window. Among them, ionic liquids (ILs) have gained prominence due to their superior electrochemical characteristics.

A recent strategy to further improve performance involves incorporating electroactive additives into the electrolyte. These can be classified as neutral (e.g., hydroquinone, anthraquinone), which offer only a few options, or ionic, which provide virtually unlimited possibilities from both inorganic and organic systems. The incorporation of such electroactive additives transforms the system into a ternary or quaternary ion electrolyte, depending on the cation–anion combinations involved.

In this study, we investigate 1,2,4-triazolium-based ionic liquid as organoelectrolytes for EDLC-type supercapacitors. These ILs exhibits promising electrochemical properties. To investigate their potential, we employed a small-sized cationic IL and examined its behaviour with KI (as a quaternary ion system) and $KPF_6$ (as a ternary ion system), thereby assessing their impact on EDLC performance.

**Keywords:** Supercapacitors, Organoelectrolytes, Ionic Liquids, Electroactive additives

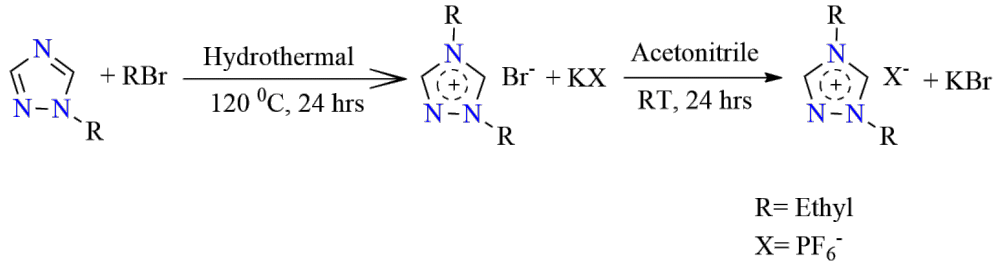


**Figure:** Synthesis Scheme of Ionic liquid: 1,4-diethyl-1,2,4-triazolium hexafluorophosphate

# Hydrothermal synthesis of $CoMn_2O_4$ nanostructures as efficient electrode materials for next-generation supercapacitors

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**Abstract**

The increasing worldwide demand for sustainable and environmentally friendly energy solutions has heightened research into sophisticated energy storage devices. Electrochemical energy storage devices, particularly supercapacitors, have become highly appealing options due to their swift charge-discharge capabilities, extended cycle life, and environmental compliance in comparison to traditional batteries. Spinel-structured transition metal oxides have garnered significant interest as electrode materials due to their extensive redox activity, structural stability, and availability. Cobalt–manganese oxide ($CoMn_2O_4$, CMO) provides superior electrochemical performance due to the synergistic effects of Co and Mn ions.$CoMn_2O_4$ (CMO) nanostructures were effectively produced via a hydrothermal method employing urea as a structure-directing agent, utilizing varying urea concentrations (CMO-3.5, CMO-4, and CMO-4.5) to modulate the material characteristics. X-ray diffraction verified the tetragonal phase of $CoMn_2O_4$ (JCPDS Card Number. 04-018-1864) with space group I41/amd crystalline phase, with an average crystallite size of around 36 nm. Microscopic examinations utilizing FE-SEM combined with EDAX, alongside TEM, demonstrated a consistent nano particles morphology, with TEM analysis corroborating the structural and morphological findings from XRD and SEM. The electrochemical assessment conducted using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS) revealed that the optimized electrode provided a specific capacitance of 230 F $g^{-1}$ at a current density of 1 A $g^{-1}$. The electrode demonstrated an impressive coulombic efficiency of 99% and notable cycling stability, maintaining 80% of its initial capacitance after 1000 cycles. The findings indicate that urea-mediated synthesis provides an efficient method for customizing $CoMn_2O_4$ nanostructures, rendering them suitable candidates for high-performance supercapacitor electrodes.

**Keywords:** $CoMn_2O_4$ Hydrothermal method , Nanostructures, Cyclic voltammetry Supercapacitor

# Exploring the amino acid–ionic liquid systems through machine learning approaches

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**Abstract**
Ionic liquids are considered promising electrolytes for supercapacitors due to their high energy density, high capacitance, high thermal stability and wide electrochemical window. There are various types of ionic liquids that are serving as the electrolytes, one among them is the amino acid – ionic liquid. Amino acid-ionic liquids are composed of a cation and an amino acid anion and are found to exhibit better capacitive performances than other regular combinations of ionic liquids. Thus, it becomes vital to understand the structure and interaction of these amino acid-ionic liquids. In this work we have explored the characteristics [EMIM][GLY] using Density Functional Theory (DFT) and compared with the results obtained from DPPF (Deep Learning Force Field) using DeePMD kit, which has high accuracy and low computational cost would be a better replacement for the traditional methods. This work would subsequently pave the way for implementing more ML-based approaches to discover such novel electrolytes.

**Keywords:** Amino acid-Ionic liquid, DFT, DPPF

**References:**

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# Hydrogen storage capacity of $BaCdH_3$ perovskite hydride: theoretical analysis

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**Abstract**

The ever-growing need for energy has intensified the search for efficient hydrogen storage compounds. Perovskite hydrides are attracting attention as potential compounds for solid-state hydrogen storage due to their high volumetric capacity and strong hydrogen affinity. In this research, $BaCdH_3$-based perovskite hydrides were investigated using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method implemented in WIEN2k. Structural stability was assessed through energy-volume optimization and formation energy calculations. Mechanical properties, evaluated via elastic constants ($C_{11}$, $C_{12}$, $C_{44}$), indicate that $BaCdH_3$ is mechanically stable, exhibits anisotropic behavior, and can display either brittle or ductile characteristics. Electronic structure analysis reveals metallic behavior, supporting reversible hydrogenation and dehydrogenation processes. Thermodynamic properties, including specific heat capacity, free energy, entropy and enthalpy, were studied across a range of temperatures. Hydrogen storage performance was quantified, yielding a gravimetric density of 1.196 wt% and a volumetric density of 64.76g $H_2$/L. These results demonstrate that BaCdH3 is an effective hydrogen storage medium and provide a theoretical foundation for future experimental studies aimed at clean and sustainable energy applications.

**Keywords:** Solid-state Hydrogen storage, Perovskite hydrides, Gravimetric, Volumetric density

**References:**

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2. Nanlin Xu et al., "International Journal of Hydrogen Energy" 50, (2024), 114-122.

# Influence of protonation states on the excited-state dynamics of Chlorophyll-A

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**Abstract**

Chlorophyll-a (Chl-a), the primary pigment in photosynthesis, functions as a photosensitizer and undergoes distinct structural modifications under varying protonation states, particularly under high-light conditions. In this study, we explore the non-radiative decay pathways of Chl-a across different pH environments, where protonation-induced changes occur while the chlorin ring remains intact. These structural variations were characterized using steady-state absorption and photoluminescence spectroscopy. Circular dichroism measurements revealed a bisignate geometry at neutral pH, which transforms under acidic conditions and vanishes at basic pH. Transient absorption spectroscopy (TAS) further uncovered pronounced pH-dependent differences in excited-state dynamics: non-radiative decay dominates under both acidic and alkaline conditions, whereas a more balanced relaxation pathway is maintained at neutral pH.

**Keywords:** Chlorophyll-A, protonation states, photosynthesis

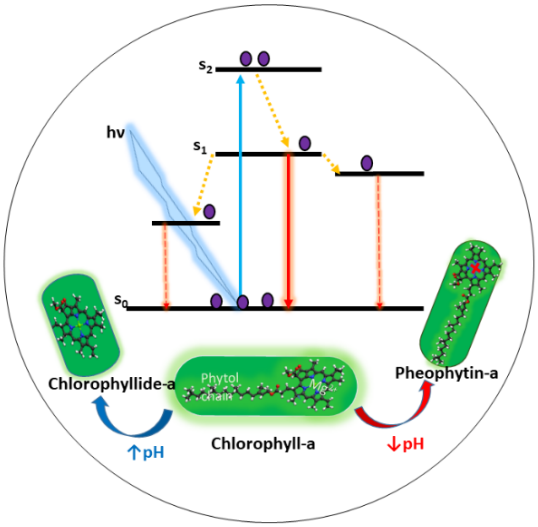


**Figure:** Influence of protonation states on the excited-state dynamics of Chlorophyll-A

# Synthesis of 211 MAX phases by a probe sonication approach

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## Abstract

MAX phases are layered hexagonal transition metal carbides, nitrides, and carbonitrides – a main precursor for the synthesis of MXenes nanosheets. MAX phases exhibit large thermal conductivity and electrical conductivity due to their unique combination of ceramic and metallic properties [1]. In general, MAX phases are synthesized by mixing elemental precursors at an appropriate stoichiometric ratio, followed by sintering them at high temperature [2]. Most of the MAX phase synthesis involves homogeneous mixing of elemental precursors by a ball milling unit. Herein, we report on the synthesis of MAX phases such as $Ti_2AlC$ and $Cr_2AlC$ by a probe sonication-assisted approach for mixing the precursor powders [3] at different time intervals (1hr, 2hr ,3hr, and 4hr) followed by pressureless sintering at 1400$^{\circ}C$ under inert atmosphere. The structural analysis of the synthesized MAX phases is confirmed through XRD analysis. We successfully obtained $Ti_2AlC$ in 2hr and $Cr_2AlC$ at 4hr mixing of elemental precursors followed by high temperature sintering.

**Keywords:** MAX phase, Mixing, Probe sonication, Pressureless sintering

**References:**

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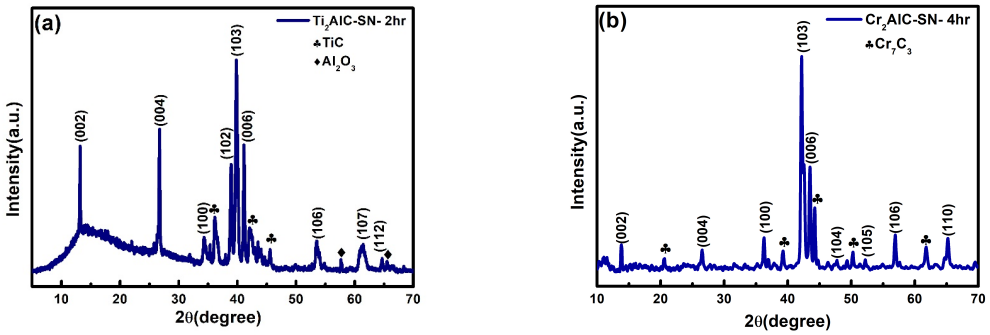


**Figure:** XRD Pattern of a) $Ti_2AlC$ with the sonication time of 2 hr and b) $Cr_2AlC$ MAX phase with the sonication time of 4 hr

# Fabrication of an exfoliated h-BN-$Bi_2S_3$ hybrid supercapacitor device for superior electrochemical performance

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**Abstract**

Supercapacitors and batteries are foremost in energy storage technology and thus applicable in many electronic applications and electric vehicles. A higher power density of supercapacitors has a great advantage as opposed to batteries, yet its lower energy density reduces its practical application field. However, in the present study, the energy density can be improved by the constructed hybrid supercapacitor device of exfoliated h-BN-$Bi_2S_3$//AC. Though its vibration, structural, and morphological properties have been confirmed from Raman, XRD, XPS, and HRTEM. A constructed device has been tested in a two-electrode system for a practical utilization test, and also its primary electrochemical characterization of cyclic voltammetry and galvanostatic charge and discharge was studied, which resulted in superior electrochemical performance. An exfoliated h-BN-$Bi_2S_3$ was synthesized by the less costly method of the ultrasonic approach assisted with hydrothermal technique.

**Keywords:** Liquid phase exfoliation, Hydrothermal Method, Specific Capacity, Electrochemistry, Pseudocapacitor

**References:**

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# Electrical properties of sodium ion conducting boro tellurite glasses: Materials for battery applications

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## Abstract

The solid electrolytes with high ionic conductivity are fascinating area of research due to its better performance in optical devices, sensors and batteries. These solid electrolytes are most suitable materials to compensate for the limitations of liquid electrolytes for specific applications, which is the topic of most intense and emerging area of research across the world. In the present study, the $Pr^{3+}$ ion doped sodium boro-tellurite glasses of the composition $30Na_2O–60B^2O^3–10TeO^2–(10–x)Pr^2O^3$ (where x = 0, 0.1, 0.5, 1.0 and 1.5 mol%) were synthesized by melt quenching technique. The frequency dependent real and imaginary parts of the impedance (Z', Z"), ac electrical conductivity $\sigma_a c$ complex-dielectric constant ($\varepsilon$', $\varepsilon$") and electric-modulus (M', M") were investigated in the frequency of 100 Hz to 5 MHz and from the temperature range of 443 K to 563 K. The analysis of the conductivity data gives a clear insight of the compositional and temperature dependence of glass structure with its electrical properties. The dc conductivity found to increase with temperature clearly depicts that the electrical conductivity in the glass is thermally activated process. The frequency dependent conductivity has been fitted to an Almond–West type of expression using a single power law exponent S and is found to be independent of temperature. The frequency dependent electric modulus shows well-defined peaks and the frequency, $f_0$ shifts towards the higher frequency side. The dielectric data has been analyzed using modulus formalism, the stretched exponent $\beta$ values have been calculated from the dielectric relaxation peaks and is found to be independent of temperature. The incorporation of modifier oxide in the borate glass modifies the glass structure by reconverting the four-coordinated tetrahedral boron ($BO_4$) to three-coordinate trigonal boron ($BO_3$) by creating a non-bridging oxygen atoms (NBOs). The creation of NBO atoms in the glass network decreases the connectivity and dimensionality of the borate glass network. The formation of NBO in the glass network creates more ionic bonds thereby impeding the motion of alkali cation such as $Na^+$, enhancing the ionic conductivity. The electrical conductivity and di-electric relaxation mechanism of the obtained results are discussed in view of its structure-property relations.

**Keywords:** Electrical properties, Cole-Cole model, Dielectric relaxation, Glasses

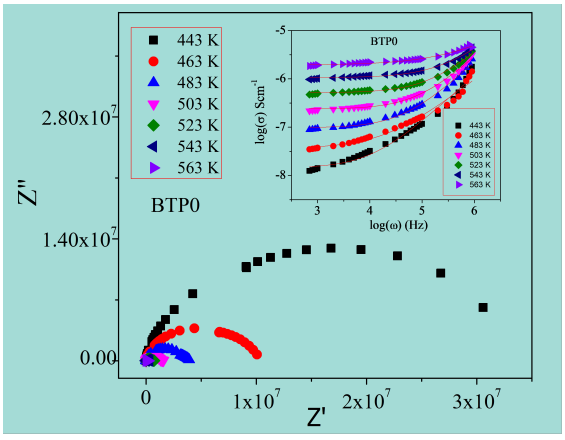


**Figure:** Variation of impedance plot. (Inset: Typical plot of ac conductivity versus frequency)

# Formability-microstructure-performance linkages in lightweight alloys for energy-efficient transportation: A materials-centric review of hydroforming as a validation platform

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**Abstract**

Lightweight alloys are essential for extending electric-vehicle range, yet their widespread use is hindered by limited ductility at ambient temperatures and unpredictable weld-zone behaviour under complex forming. This review presents hydroforming not merely as a shaping technique but as a materials validation platform for advanced Al-5xxx/6xxx, Mg AZ31/ZE10, and AHSS DP600/DP800 alloys. Through a microstructure–formability–performance perspective, we highlight three core advances: (1) warm-forming regimes that activate additional slip systems to expand Al/Mg forming-limit envelopes by 40–60%; (2) anisotropic yield formulations that predict ERW weld-zone bursting with better than 95% accuracy; and (3) adaptive pressure–feed strategies that maintain wrinkle indices within safe thresholds under multi axial loading. We then connect these developments to key functional metrics—enhanced specific strength and crash energy absorption, superior stiffness-to-weight ratios in closed-section rails, and reliable performance of hydro formed battery enclosures under combined mechanical and thermal loads. Finally, we propose a decision framework that links alloy class, forming temperature, and control methodology to anticipated formability improvements and structural outcomes, offering a clear roadmap for alloy selection and accelerated design iteration. Collectively, these materials-focused innovations establish hydroforming as a robust pathway for scaling lightweight functional materials in energy-efficient transportation.

**Keywords:** Lightweight alloys, Hydroforming, Warm forming, Forming limit diagrams, Anisotropy, Energy absorption, Battery enclosures, Electric vehicles

# Impact of electrolyte concentration on electrochemical performance of lanthanum ferrite ($LaFeO_3$) perovskites for aqueous based supercapacitors

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**Abstract**

Supercapacitors are becoming a major focus of current research in energy storage technologies. Electrode and Electrolyte are the key components of a supercapacitor device. Electrochemically active and thermally stable nanostructured anode electrodes are required for developing high-performance and long-lasting storage devices. The electrolyte functions as a lane for ion migration between the electrodes, and the choice of a suitable electrolyte with optimal concentration is vital to achieve high ionic conductivity and efficient charge transfer at the interface. Recently researchers showed much attention to Lanthanum ferrites as electrode material due to their interesting physiochemical properties. Lanthanum Ferrite ($LaFeO_3$) material has interesting electrochemical properties because Fe undergo multiple oxidation states $Fe^{3+}$ during the electrochemical reactions. In this work $LaFeO_3$ anode electrode were synthesized by wet - chemical Sol-gel technique and attain its pure phase formation at $600°C$. The X-Ray diffraction indicates that $LaFeO_3$ exhibits orthorhombic structure with an average crystalline size of 22.6nm. TEM and FESEM micrographs exhibit spherical shaped morphology. EDX spectrum confirms the presence of desired elements. BET analysis shows the Mesoporosity with specific surface area of $70.86m_2/g$. Half-cell electrochemical measurements were performed in alkaline KOH electrolyte at various concentration ranges from 0.5M to 3M. CV and GCD measurements show reversible redox Pseudocapacitance behaviour for all the electrolyte concentrations but the discharge time is higher in 1M concentrations. The specific capacitance calculated from CV and GCD exhibits 87.5F/g and 82.16F/g at 5mV/s and 0.5A/g in optimal concentration of 1M KOH.

**Keywords:** Perovskites Lanthanum ferrites, Sol-gel, Optimal electrolyte concentration, Redox pseudocapacitance

# Sustainable Intelligence: A survey on ultra-low-power embedded systems and their enabling technologies

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**Abstract**

The emergence of energy-autonomous systems in areas like the Internet of Things (IoT), edge artificial intelligence (AI), and biomedical instrumentation is increasingly made possible by ultra-low-power (ULP) embedded systems. Driven by the requirement for long-term operation under severe power restrictions, dramatic advances in ULP design have been made. In this article, a systematic and in-depth overview of the enabling technologies is provided, comprising novel non-volatile memory technology like resistive RAM (ReRAM) and magnetic RAM (MRAM) devices, hardware/software co-design methodologies, and energy-conscious architectures optimized for edge intelligence. Principal challenges encompassing power management, security delivery, and decentralized coordination in embedded networks are analyzed. Based on the latest research findings, basic design paradigms and design guidelines are established to facilitate the realization of scalable, secure, and sustainable ULP embedded systems that can satisfy the energy as well as the performance needs of next-generation intelligent and connected environments.

**Keywords:** Ultra-Low-Power (ULP) Embedded Systems, Edge AI, Energy Harvesting, ReRAM, MRAM, TinyML, Hardware-Software Co-design

# Development of direct current (DC) biomechanical energy harvesters using p-ZnO:N nanowires / organic polymer bilayers

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**Abstract**

The present research work reports on the development of direct current (DC) piezovoltage-based biomechanical energy harvesters (BEH). Nitrogen-doped p-ZnO nanowires with randomly aligned morphology were grown on a flexible aluminium (Al) foil substrate. The structural and morphological analyses confirmed the formation of randomly aligned p-ZnO:N nanowires. To evaluate the biomechanical energy harvesting performance, the p-ZnO nanowires were subjected to periodic biomechanical stimulation, generating a DC output voltage of 1.9 V upon human finger press/release and 4.3 V upon human finger tapping tests. It was proposed that the presence of the buckling effect in the role of randomly aligned p-ZnO:N nanowires contributes towards the generation of DC output voltage. Moreover, recombination of free electrons with the NO–$V_{Zn}$ acceptor complex suppresses the screening effect, thereby enhancing piezoelectric potential. To improve the device performance, the p-ZnO:N nanowires were integrated with PVDF organic polymer layers, which yielded an increased DC voltage of 4.5 V under finger press/release and 7.18 V under finger tapping, corresponding to a power density of 6.398 nW/cm$^2$. The impact of triboelectric effect-assisted testing on the enhancement of output piezovoltage in the fabricated biomechanical energy harvesters (BEH) was investigated.

**Keywords:** Biomechanical energy harvester, ZnO nanowires, PVDF polymer, Screening effect

**References:**

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# Efficiency enhancement of chalcogenide based thin film solar cells

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## Abstract

Humanity always depended on conventional energy sources like fossil fuels, coal, and natural gas for a wide period. But this usage has led to significant environmental degradation, pollution, melting ice glaciers and damaging the ecosystem. This brings us to a need for a new type of energy source – Solar Energy which is not only non-renewable but also can prevent environmental damage at a higher rate than conventional energy resources[1].

Chalcogenide thin film solar cells are known to have excellent optoelectronic properties and hence can become a promising technology for solar energy conversion. Also, research in chalcogenide PV's focuses on improving the performance and cost effectiveness by optimizing the material characteristics[2,3,4].

In this work, we're going to focus on increasing the Power Conversion Efficiency (PCE) by varying significant parameters of different layers of a solar cell such as Thickness of Absorber layer, defect density, band gap, electron affinity and interface defects by using the simulation software SCAPS 1D (Solar Cell CAPacitance Simulator). The material chosen for absorber layer is Tin Monoselenide (SnSe) and the other layers are preferably chalcogenides. The reason for the choice in SnSe as the absorber layer is mainly because of its high absorption coefficient ($<10^5$), material abundance, low toxicity and ideal band gap (1.2eV). By changing parameters such as the band gap and the thickness, the property of the overall solar cell with multiple layers changes such as electron-hole recombination and generation which in turn improves the solar cell's efficiency.

**Keywords:** Chalcogenides, Absorber layer, Tin Monoselenide (SnSe), SCAPS 1D

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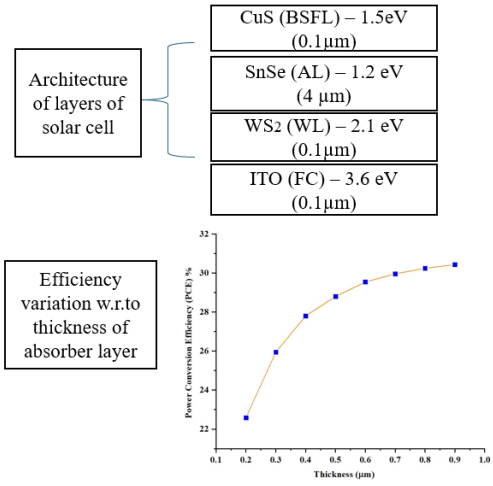


**Figure:** Efficiency enhancement of chalcogenide based thin film solar cells

# An extensive investigation on the structural, morphological, dielectric and ferroelectric properties of Nd doped $BiFeO_3$-$BaTiO_3$ solid solutions

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**Abstract**

Recently the need for cost effective, ecofriendly, energy storage device that can store electrical energy has been peaked. Among the commercially available systems the dielectric capacitors are employed in a variety of applications ranging from modern consumer electronics to various pulsed power applications due to its high charging and discharging speeds. Dielectric materials serve as fundamental elements in dielectric capacitors, directly influencing their operational efficacy.In this work Nd doped $BiFeO_3$ - $BaTiO_3$ (BFO-BTO) solid solutions are prepared by cost effective conventional solid state reaction method. X-ray diffraction analysis reveals a single-phase distorted perovskite structure with rhombohedral symmetry.The Scanning Electron Microscopy results indicate that the incorporation of Nd has a significant impact on the grain size of BFO-BTO. The dielectric permittivity, dielectric loss, and Curie temperature of the samples are analysed using an LCR meter operating within the frequency range of 1 Hz to 1 MHz. The well defined polarization–electric field hysteresis loop of the samples at room temperature suggest that Nd substitution at the Bismuth site of the solid solution strongly affects remnant and saturated polarization of the materials. These findings highlight the potential of Nd-doped BFO-BTO solid solutions for advanced energy storage applications.

**Keywords:** Dielectric capacitors, Energy storage, Multiferroic Ceramics, Polarization

# Effect of $ZnSO_4$ and $Zn(CF_3SO_3)_2$ on dendrite formation in aqueous zinc ion batteries

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**Abstract**

In recent years, there has been a significant surge in global energy use. The primary energy source now utilized is fossil fuels, which is on the verge of depletion within the next several years. These contributed to the demand for clean and renewable energy sources, as well as efficient and cost-effective energy storage technologies. At present, lithium-ion batteries are the dominant energy storage technology in the market because of their superior energy density. However, the reliability of lithium-ion batteries is being questioned due to the limited availability of lithium and safety concerns associated with organic electrolytes. Substituting organic electrolyte with aqueous electrolyte is viewed as a viable method for addressing the safety issues associated with LIBs. Additionally, the ability to manufacture under normal conditions enables cost reduction. Aqueous zinc-ion batteries (AZIBs) are regarded as extremely promising electrochemical energy storage devices because of their cost-effectiveness, inherent safety, abundant zinc supplies, and optimum specific capacity. The major issue faced by AZIBs is the dendrite formation over cycling which can lead to short circuit and cell failure. In this study the effect of $ZnSO_4$ and $Zn(CF_3SO_3)_2$ electrolyte with various molar concentration on the formation of dendrite by analysing various factors such as ionic conductivity, electrolyte affinity towards zinc, hydrogen evolution, corrosion etc will be studied. Further the effect of electrolyte on electrochemical performance (columbic efficiency, charge stability, discharge capacity, EIS studies) in full cell configuration is studied by taking $\alpha - MnO_2$ as cathode.

**Keywords:** Batteries, Electrolyte, Electrochemical energy storage devices

# Sustainable and low-cost catalytic conversion of carbon dioxide and hydrogen into formic acid using a copper complex as a green catalyst

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**Abstract**

The increasing concentration of atmospheric carbon dioxide ($CO_2$) has prompted growing interest in its sustainable conversion into value-added chemicals and fuels. In this study, a low-cost and greener catalytic approach has been developed for the efficient hydrogenation of $CO_2$to formic acid using a copper complex as a catalyst. The copper complex, synthesized under mild and environmentally benign conditions, exhibited excellent catalytic activity and selectivity toward formic acid formation. Under optimized reaction conditions (temperature: $160°C$, pressure: 20 bar, reaction time: 5 hrs), a $CO_2$ conversion efficiency of 65% and a formic acid selectivity of 88% were achieved. These results surpass those of conventional Cu/ZnO and Ru-based catalytic systems, which typically yield around 50–55% conversion under similar conditions. The reaction proceeds without the use of toxic solvents or precious metals, thereby reducing both cost and environmental impact. Spectroscopic and thermal analyses confirmed the structural integrity of the catalyst, which retained over 90% of its initial activity after five successive reaction cycles, demonstrating excellent stability and recyclability. This sustainable and economical methodology provides a promising route for $CO_2$ utilization and hydrogen storage, contributing to cleaner energy generation and the advancement of carbon-neutral technologies.

**Keywords:** Carbon dioxide, Green catalysis, Copper complex, Formic acid, Sustainable

# Greener synthesis of water-soluble nanosized copper(II) complex with 1,10-Phenanthroline derivatives as catalyst for the production of hydrogen

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**Abstract**

Hydrogen has emerged as one of the most promising clean energy carriers owing to its high energy density, environmental compatibility, and renewable production potential. In the present study, a novel series of nano-sized copper(II) complexes with the general formula [CuL], where L = 1,10-phenanthroline derivative, were synthesized and thoroughly characterized using elemental and thermal analyses, molar conductance, cyclic voltammetry, magnetic moment measurements, powder X-ray diffraction (XRD), scanning electron microscopy (SEM), and spectral techniques (FT-IR, UV-Vis, and ESR). Physico-chemical and spectroscopic studies revealed that the complexes exhibit a square planar geometry around the copper(II) ion. The average crystallite size, as obtained from powder XRD data, was found to be in the range of 25-35 nm, confirming the nanoscale nature of the materials. SEM images showed uniformly distributed nano-aggregates with a quasi-spherical morphology. The complexes were evaluated for photocatalytic and electrocatalytic hydrogen evolution from wastewater, following pre-treatment with mesoporous bioadsorbents for contaminant removal. Among the synthesized complexes, the copper(II) complex containing a $\pi$-conjugated phenanthroline ligand exhibited the highest catalytic performance, achieving turnover number (TON) and turnover frequency (TOF) values of 18,200 and 9,600 $h^{-1}$, respectively, at pH 10.4 in $CH_3CN$ solution. The enhanced catalytic efficiency is attributed to the synergistic interaction between the metal center and the extended $\pi$ - system of the ligand, as well as the formation of metal–oxo species that facilitate proton reduction. Overall, the study demonstrates that nano-sized copper(II) phenanthroline complexes act as efficient and robust catalysts for sustainable hydrogen production, providing a distinct pathway for green fuel generation from wastewater under photochemical and electrochemical conditions.

**Keywords:** Electrochemical, Photochemical, Turnover, Frequency, Hydrogen

# Electrochemical synthesis of $WSe_2$ featuring abundant selenium vacancies towards efficient electrocatalytic hydrogen evolution

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**Abstract**

Water splitting has emerged as a promising approach for sustainable energy production through hydrogen ($H_2$) generation. However, the sluggish kinetics of the hydrogen evolution reaction (HER) continue to limit large-scale $H_2$ production. To address this challenge, the development of highly efficient electrocatalysts, capable of operating at low overpotentials ($\eta$) is essential. In recent years, transition metal dichalcogenides (TMDs) have demonstrated great potential as HER electrocatalysts due to their unique physicochemical properties. Among these, tungsten diselenide ($WSe_2$) has gained considerable attention for its excellent stability and catalytic performance. In $WSe_2$, selenium (Se) vacancies play a key role in tuning the adsorption energies of reaction intermediates, thereby enhancing HER activity. Moreover, the presence of vacancies increases the surface area and improve the electronic properties of the material, facilitating faster charge transfer and higher exchange current density, which are crucial for effective electrocatalysis.

In this study, $WSe_2$ was synthesized using an electrodeposition method and introduced controlled Se defects by applying different treatment potentials. The presence of vacancies was thoroughly characterized through X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and high-resolution transmission electron microscopy (HRTEM). The vacancy-induced $WSe_2$ (VI- $WSe_2$) exhibited significantly enhanced HER performance, confirming the key role of vacancies in boosting catalytic activity. This work presents a cost-effective and scalable approach to engineering high-performance electrocatalysts through defect modulation, offering a promising strategy for efficient hydrogen production.

**Keywords:** $WSe_2$, Hydrogen evolution reaction (HER), Electrocatalyst, Se vacancy

# Photophysical, solvatochromic, and electronic structure studies of fluorescent Azo-Anthracene dye for dye-sensitised solar cell applications

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**Abstract**

In this research work, a comprehensive experimental and theoretical investigation was carried out on the photophysical and electronic properties of the newly synthesized azo dye (E)-1-((3-hydroxy-2-oxo-2H-chromen-4-yl) diazenyl) anthracene-9,10-dione (E-AN). The molecule combines an anthracene-9,10-dione core with a diazenyl-linked coumarin fragment, generating a push–pull conjugated system favorable for intramolecular charge transfer (ICT). UV–visible absorption and fluorescence emission spectra recorded in solvents of varying polarity revealed pronounced positive solvatochromism, with large Stokes shifts increasing in polar and hydrogen-bonding media. Solvent–solute interactions were quantitatively analyzed using the Catalán multiparameter model, demonstrating that polarizability, dipolarity, and both acidic and basic hydrogen bonding interactions significantly stabilize the excited state ($r^2$ = 0.952). Density functional theory (DFT) calculations provided optimized ground-state geometry, revealing planarity across the azo bridge, shortened C=O and C–N bonds, and strong conjugation throughout the molecule. Frontier molecular orbital analysis indicated that the HOMO is localized on the anthraquinone moiety and the LUMO on the coumarin–azo unit, confirming ICT transitions with a calculated HOMO–LUMO gap of 3.121 eV. Global chemical reactivity descriptors suggested that E-AN is a soft electrophile with high electron affinity (EA = 2.858 eV) and an electrophilicity index ($\omega$ = 6.372$eV$), consistent with its charge-transfer character and environmental sensitivity. The molecular electrostatic potential (MEP) map further identified oxygen and nitrogen centers as dominant electrophilic sites, in agreement with solvent-dependent photophysics. The implemented in a $TiO_2$-based DSSC under AM1.5G illumination, E-AN achieved $J_{sc}$ = 19.3 mA $cm^{-2}$, $V_{oc}$ = 0.257 V, FF = 39.5%, and PCE = 1.97%, evidencing efficient light harvesting and electron injection but losses from interfacial recombination and series resistance. These findings position E-AN as a promising, tunable organic sensitizer with clear routes to performance enhancement via interfacial and architectural optimization.

**Keywords:** Oxazole derivatives, Photophysical properties, HOMO-LUMO, GCRD, DSSC

# Natural dye based memristor and ion incorporation: towards sustainable neuromorphic devices

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## Abstract

Neuromorphic devices that emulate biological brain functions are emerging as key components for intelligent computing systems. The emulation of neural activities fundamentally depends on ionic interactions that govern excitatory and inhibitory signal transmission at synapses. In this study, we report an indigo-based two-terminal artificial synaptic device in which sodium ($Na^+$) and chloride ($Cl^-$) ions play a vital role in modulating synaptic behavior. The incorporation of NaCl ions significantly enhances both the memory and synaptic characteristics of the device. Experimental results reveal that the device exhibits high sensitivity toward $Na^+$ and $Cl^-$ ions, with a detection limit ranging from (0.05 ± 0.015) mM to (0.5 ± 0.015) mM. The optimized concentration of 0.1 mM NaCl led to a sixfold enhancement in the ON/OFF ratio at 1.3 V and a twelvefold increase in both excitatory and inhibitory postsynaptic current (EPSC and IPSC) responses. These findings successfully emulate the physiological functions of $Na^+$ and $Cl^-$ ions in biological synapses, demonstrating efficient ionic modulation of synaptic plasticity. The study underscores the potential of organic molecular systems, specifically indigo, as a promising platform for developing next-generation neuromorphic technologies capable of brain-like learning, memory, and adaptive computing.

**Keywords:** Neuromorphic device, Indigo, Ionic modulation, Synaptic plasticity, Artificial synapse, Memristor, Organic electronics, Sustainable electronics

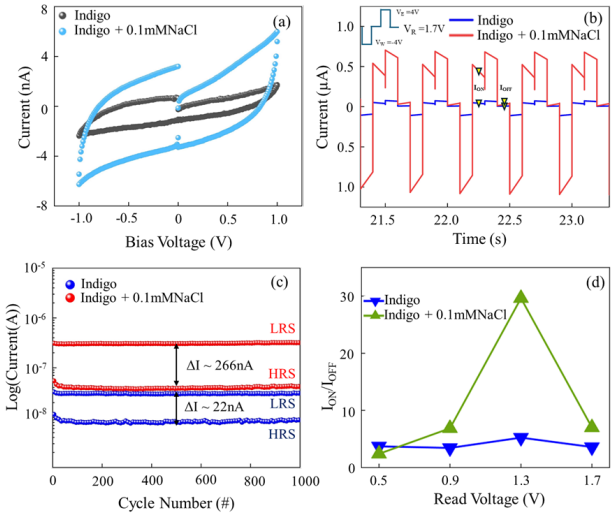


**Figure:** (a) Current-voltage characteristics of the indigo-based device without (black) and with 0.1 mM NaCl addition (blue). (b) Memory characteristics using write-read-erase-read cycles, showcasing the enhanced performance of the NaCl-added device (red line) vs the pristine indigo device (blue line). The voltage pulse sequence is indicated in the inset.

# Controlled hydrothermal synthesis of La-doped CdTe nanomaterial for enhanced optoelectronic applications

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**Abstract**

The hydrothermal synthesis approach for producing La-doped CdTe nanoparticles has been successfully carried out. Four samples have been prepared amongst which, one is undoped CdTe and other three samples are La-doped CdTe with increasing La content. Cubic phase of CdTe was established by X-ray diffraction (XRD). Peak shift towards higher theta angle has been observed due to the La incorporation in the CdTe crystal lattice. Raman spectroscopy gave important information about the vibrational modes of CdTe, and transmission electron microscopy (TEM) confirmed the CdTe phase and showed values for interplanar spacing. The X-ray photoelectron spectroscopy (XPS) inferred the electrical structure and surface composition. Increased La concentration was shown to decrease the bandgap in the 2.3-3.5 eV range using UV-Vis spectroscopy. An improved current response and significant variations in the material's rise and decay intervals under illumination were found by the photo response analysis. The photocurrent also gave good results in responsivity (R), detectivity (D) and also the I-T curves measured the rise and decay times. The nonlinear optical studies revealed significant values of the nonlinear absorption coefficient and nonlinear refractive index, indicating their potential utility in various advanced optical applications.

**Keywords:** Nanomaterials, La-doped CdTe, Hydrothermal synthesis, Optoelectronics

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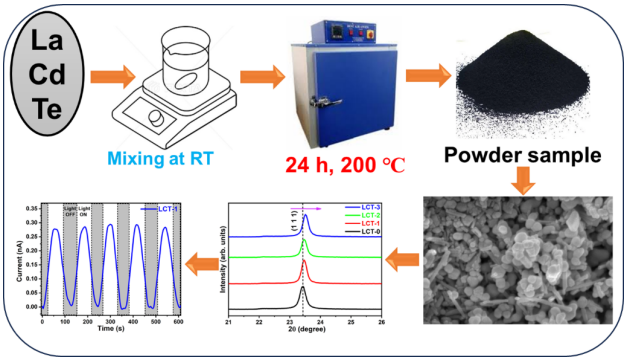


**Figure:** Controlled hydrothermal synthesis of La-doped CdTe nanomaterial for enhanced optoelectronic applications

# Dielectric, impedance, modulus spectroscopy studies of KDP – $K_2SO_4$ composite crystal system

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**Abstract**
Potassium Dihydrogen Phosphate (KDP) is well known non-linear optical (NLO) material crystal having large number of applications in laser based and opto-electronic devices. In the present study to modify and engineer the a.c. electrical properties the composite crystals of KDP and Potassium Sulfate ($K_2SO_4$) are grown. Presently to grow composite crystals 50 ml of solution of KDP is added to 75 ml $K_2SO_4$ solution and stirred for 2 hours and transferred to the water bath to maintain 270°C for slow evaporation of the solvent. Transparent, colorless, and prismatic crystals are harvested. In the same manner pure KDP crystals are grown. Powder XRD study carried out and in the composite crystals two distinct phases for KDP and $K_2SO_4$ are identified and indexed and using appropriate software their percentages are evaluated. It is found that KDP percentage in composite crystal is higher than $K_2SO_4$. From the power XRD analysis one finds that tetragonal phase of KDP present as major phase along with orthorhombic minor phase responsible to $K_2SO_4$. To identify the elemental composition of the composite crystal the EDAX analysis is performed on three different locations of the composite sample and it has been found that sulfur is present indicating the composite nature of the sample involving $K_2SO_4$. The a.c. electrical studies are carried out using 4294A Precision Impedance Analyzer, 40 Hz to 110 MHz within temperature from 27°C to 177°C by varying frequency of applied field from 100 Hz to 10 MHz. The variation of dielectric constant, dielectric loss, a.c. conductivity, real and complex part of impedance as well as modulus with applied frequency is studied for different temperatures. By applying Jonscher's power law to a.c. conductivity data and evaluating parameters *s* and *A* for different temperatures it is found that equivalent circuit model for a.c. conductivity is prevailing within the temperature range studied. The single semi-circular arc of the Nyquist plots suggests the presence of grain contribution only and which is fitted by R - CPE equivalent circuits and values of the circuit components are evaluated. The presence of grain contribution is also confirmed by single hump in the complex modulus plots of M" vs M'. The a.c. electrical study of composite crystal is compared with that of pure KDP crystal.

**Keywords:** Composite crystals, Dielectric study, Impedance and Impedance study, Jonscher analysis, Complex Impedance and Modulus study

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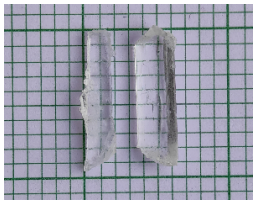

**Figure:** KDP – $K_2SO_4$ composite crystal

# First principles study of electronic structure and optical response of $Cu_2O$: effects of group-III doping and Cu vacancy – DFT+U study

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**Abstract**

Tuning the electronic and optical properties of cuprous oxide ($Cu_2O$) is essential for its applications in optoelectronic and photovoltaic devices. $Cu_2O$ is a p-type semiconductor with an electronic band gap of approximately 2.17 eV and an optical band gap ranging from 2.38 to 2.51 eV[1]. The ease of formation of two types of vacancies—simple and split—is responsible for the observed p-type conduction in $Cu_2O$. Studies focusing on doping in $Cu_2O$ in the presence of a Cu vacancy are limited. In this study, we explore the effects of group-III dopants (In, Al, and Ga) in the presence of a copper vacancy on the electronic structure and optical behavior of $Cu_2O$ using first-principles density functional theory calculations. We analyze how dopants, in combination with vacancies, influence the band structure, density of states, and optical absorption, providing insights into strategies for modifying the material's properties. Our findings demonstrate that both dopants and defects can serve as effective tools for engineering the electronic and optical characteristics of $Cu_2O$ for future device applications.

**Keywords:** Cuprous oxide, Dielectric function, Band structure

**References:**

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# Temperature dependent complex impedance spectroscopy of $SnO_2$ using SCAPS 1D

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**Abstract**

Applicability of SCAPS-1D[1] software to simulate the impedance spectroscopy of $SnO_2$ in the frequency range upto 1M Hz using FTO/$SnO_2$/Ag architecture between room temperature to 400 K range was simulated. The obtained impedance data was analysed by plotting frequency-dependent real and imaginary parts of impedance and total conductivity for all the mentioned temperatures. Also, there impedance data was fitted using RC equivalent circuits to extract resistance (R), constant phase element (CPE), Capacitance (c) and maximum of angular frequency ($\omega_{max}$) values using the software $Z_{simpwin}$. The observed behaviour reveals the conductivity increases with increase of applied temperature. Further, activation energy was estimated using Arrhenius plot[2] and it was found to be 0.66 eV and a correlation between DC and AC conductivities was also studied by analysing data using BNN relation[3-5].

**Keywords:** Tin Oxide, SCAPS-1D software, Impedance Spectroscopy, Temperature, Arrhenius plot, AC Conductivity, Activation energy, BNN relation

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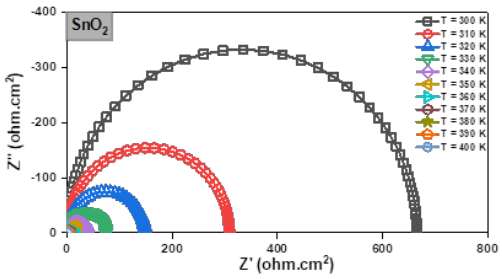


**Figure:** Numerical simulated Cole-Cole plot of FTO/$SnO_2$/Ag for various temperatures up to 400 K

# Visible blue and NIR emission in Nd doped $CaZrO_3$ perovskite

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**Abstract**

This work presents the effect of Nd doping on structural and optical properties of $CaZrO_3$. A series of samples are synthesized with varying neodymium doping concentration via the solid-state reaction method. Through x-ray diffraction (XRD) single phase of the synthesized compounds is confirmed. The oxidation states of the host compound and dopant are studied using the x-ray photoelectron spectroscopy. Further, to study the optical properties of the samples, UV-Vis spectroscopy was performed. The intra-band transitions of $Nd^{3+}$ rare earth element were distinctly observed in the UV-Vis absorption spectra. The observed absorption peak positions were considered for exciting the sample for photoluminescence studies. Upon exciting the doped samples with 358 nm, emission in the visible blue region is observed with intense peaks at 392 nm, 421 nm and 457 nm. Further, the emission from same samples in the near-infrared region is observed by exciting with 590 nm light source. This wavelength dependent emission in different regions make this functional material interesting to explore for wide range of optoelectronic applications.

**Keywords:** Calcium zirconate, Neodymium doping, Photoluminescence, Optoelectronics

# Studies on excitonic absorption and polarization property of perovskite 2-D nanoplatelets with varying thicknesses

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**Abstract**
Metal halide perovskites (MHPs) have gained attention for their potential application in numerous photonic devices, especially polarization. The optical properties of nanocrystals (3D) MHPs are easily tunable by the halide composition. However, MHPs can also be synthesized as colloidal nanoplatelets (NPLs) with monolayer (ML)-level thickness control, exhibiting strong quantum confinement effects. The thickness of these nanoplatelets directly dictates their band gap, establishing it as a critical parameter for tailoring their optoelectronic response. In our work, we precisely control the thickness of the 2D perovskite NPLs synthesized by ligand-assisted reprecipitation (LARP), a low-cost solution processable method and a significant blue shift in the excitonic absorption peak (384 to 356nm) as the thickness decreases (6 to 2ML), was observed using UV-VIS spectroscopy, confirming the strong quantum confinement effect. Phase and morphological properties were assessed by X-ray diffraction and transmission electron microscope analysis. Multiple measurements showed a decrease in polarization percentage when we go to thicker samples (2 to 6ML). The linear polarization was verified, and the 3ML sample of $Cs_xPbCl_xBr_x$ exhibited the maximum polarization of 18%, followed by the pristine $Cs_xPbCl_x$ samples. We observe distinct changes in the polarization emission response, which result from the quantum confinement effect. These novel properties of perovskites will have potential applications in optoelectronic devices like polarisation-dependent photodetectors and display technologies.

**Keywords:** Perovskites, Quantum confinement, Nanoplatelets, Linear-polarization

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# V-Shaped nano groove design for enhanced efficiency in CdS/CdTe nanowall solar cells

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**Abstract**

This study presents a novel and efficient approach to improving the performance of CdS/CdTe solar cells through the integration of *V-shaped nano groove walls (VSNGW)* within the conventional nanowall (NW) structure. The proposed VSNGW design aims to enhance optical absorption and carrier collection efficiency by optimizing light trapping and charge transport mechanisms. Comprehensive numerical simulations were carried out using **TCAD Silvaco**, and the results reveal a significant improvement in the photovoltaic characteristics of the device. The VSNGW-based CdS/CdTe solar cell exhibits an impressive enhancement of **57.5% in short-circuit current density (Jsc), 8.23% in fill factor (FF)**, and 68.94% in overall conversion efficiency (Eff) compared to the conventional nanowall configuration. Moreover, the proposed structure demonstrates an outstanding **100% Internal Quantum Efficiency (IQE)** beyond **540 nm**, along with notable improvements in the lower wavelength region (300–540 nm). These findings confirm that the VSNGW architecture effectively addresses optical and recombination losses, offering a promising pathway toward next-generation high-efficiency thin-film solar cells.

**Keywords:** CdS/CdTe Solar Cell, Nanowall, TCAD Simulation, Nanoflower, Nanodisk

# Polyaniline incorporation as a strategy to suppress surface and grain boundary defects in $MAPbI_3$ perovskite thin films

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**Abstract**

A simple and effective strategy to enhance the environmental stability of methylammonium lead iodide ($MAPbI_3$) perovskite thin films has been developed by incorporating the conducting polymer polyaniline (PANI) into the perovskite matrix. The incorporation of PANI was achieved via a solution-assisted approach, allowing uniform distribution within the MAPI lattice. The PANI molecules effectively interact with uncoordinated $Pb^{2+}$ ions and iodide vacancies, providing efficient defect passivation and forming a protective conductive network across the grain boundaries. The resulting PANI-MAPI films exhibit improved crystallinity, enhanced surface coverage, and reduced trap-assisted non-radiative recombination, as confirmed by photoluminescence (PL) and X-ray diffraction (XRD) analyses. X-ray photoelectron spectroscopy (XPS) further confirms the chemical interaction between PANI and MAPI, indicating strong bonding at the interface. The optimized PANI content leads to a denser morphology and improved moisture resistance. Under ambient conditions, the PANI-MAPI films retain their structural and optical integrity for over 48 hours, whereas pristine MAPI films degrade rapidly within a few hours. The PANI-modified device demonstrates enhanced power conversion efficiency and superior stability, highlighting the potential of conductive polymer incorporation as a promising route toward durable and efficient perovskite solar cells.

**Keywords:** Perovskite Solar cells, MAPI-PANI, Defect passivation, Grain boundary

# Thermodynamic stability and phase transition map of mixed-anion chalcogenide-halide perovskites via DFT simulation

Jonnadula Siva Venkata Pranietaa Ratna[1,*], Jarial Aarin Anil[1,*], Nair Aparna S[1,*], Binu Diya Elsa[1]

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**Abstract**

Chalcogenide perovskites have come forward as lead candidates for the next generation of photovoltaic and optoelectronic devices, providing greater chemical stability and stable electronic properties over their halide perovskite analogues. Still, the reproducible synthesis of mixed-anion systems, which can tune band gaps and improve stability, is usually hindered by thermodynamic instabilities that cause phase separation. This research utilizes density functional theory (DFT) to delve systematically into the thermodynamic stability and phase transition propensities in mixed-anion compounds $A(BX_{3-x}Y_x)$, where X is a halide (I, Br, Cl) and Y is a chalcogenide (S, Se, Te).

By means of density functional theory (DFT), we compute the formation enthalpy ($\Delta H$) for different compositions of anions in a supercell, and obtain the mixing energy $\Delta E_{mix}$ to estimate the driving force for demixing and phase instability. A positive $\Delta E_{mix}$ indicates a thermodynamic propensity for phase instability and demixing, while a negative value implies possibility to form stable or metastable solid solutions. Our findings provide a detailed $\Delta E_{mix}$ vs. composition (X) map, plotting areas of compositional stability and offering an predictive model for experimentalists designing novel mixed-anion perovskites. This research provides invaluable input for perovskite material rational design, informing future innovations in stable and sustainable energy technologies.

# Development of novel 1,10-phenanthroline-based ligands and metal complexes for high-performance organic light emitting diodes

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**Abstract**

Organic Light Emitting Diodes (OLEDs) have emerged as a leading technology for next-generation display and lighting applications owing to their flexibility, high brightness, wide viewing angles, and potential for low-cost fabrication. Nevertheless, limitations such as restricted operational stability, moderate device efficiency, and high production costs continue to challenge their large-scale implementation. In the present study, a series of novel 1,10-phenanthroline-derived ligands and their corresponding metal complexes were designed, synthesized, and characterized with the aim of enhancing OLED performance and lifetime. Structural modifications on the phenanthroline backbone were introduced to fine-tune the photophysical and electronic properties, thereby improving charge balance, exciton confinement, and energy-level alignment in the emissive layer. The synthesized materials were characterized by UV–Vis absorption, photoluminescence spectroscopy, cyclic voltammetry, and single-crystal X-ray diffraction studies. The photophysical analyses revealed strong emission in the visible region with high quantum yields ($\Phi_{PL}$ up to 0.72) and suitable HOMO–LUMO energy gaps (2.6–3.1 eV). The electroluminescent devices incorporating these complexes as emissive layers exhibited enhanced external quantum efficiency (EQE up to 12.4%), low turn-on voltage (~3.2 V), and improved color purity compared to conventional phenanthroline-based systems. These findings demonstrate that rational molecular design of 1,10-phenanthroline derivatives can significantly influence charge-transport and emissive behavior, providing a promising route for developing efficient and durable OLED materials. The study establishes a clear structure–property–performance relationship, paving the way for their potential use in flexible displays, solid-state lighting, and wearable optoelectronic devices.

**Keywords:** Phenanthroline, Ligands, Materials, Quantum, Electroluminescent

# Oxygen defect-induced polarons and electron-phonon interactions in $MoO_{3-x}$ nanostructures

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## Abstract

Revolutionary multidisciplinary discoveries in several fields of study have been mainly driven by the understanding of new physical principles and the development of innovative optical tools[1,2]. In recent years, molybdenum trioxide $MoO_3$ nanostructures have emerged as a viable candidate for solar energy conversion, optoelectronics, and thermal engineering due to their exceptional structural, optical, and electrical properties[3,4]. Polarons and intervalence charge transfer (IVCT) are crucial phenomena that occur in $MoO_3$, significantly impacting the thermal, electrical, and optical properties. Polarons and IVCT processes in this oxide arise from electron-lattice interactions and oxygen defect-induced localized electronic states, which facilitate the hopping of charge between two metal sites in different oxidation states [3]. Hence, these processes are very crucial in regulating charge carrier mobility, heat transport, and optical absorption[3-5], but thorough investigations of these phenomena have been very limited to date for $MoO_3$. Hence, our primary objective is to provide an in-depth study of these phenomena and lattice interactions in oxygen-deficient $MoO_3$. In this work, we utilize optical spectroscopy to investigate polaron-assisted intervalence charge transfer and electron-phonon interactions in $MoO_3$ nanostructures by tuning the structural phases. The study observed significant electron-phonon interactions and polaron strength in $\alpha$-$MoO_3$ compared to $h$-$MoO_3$, owing to the presence of substantial oxygen defects in $\alpha$-$MoO_3$. These investigations offer a route to develop energy-efficient materials and quantum technologies by elucidating the microscopic mechanisms that govern charge and energy transfer in $MoO_3$ nanostructures.

**Keywords:** $MoO_3$, Oxygen defects, Electron-phonon interactions, Polarons, Optoelectronics

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# The stability of micro-mechanically exfoliated 2D layered magnetic material $CrCl_3$

Paul Monson[1], Saswata Talukdar[2], S Chakravarty[3], K Saravanan[4], Haripriya Rejakumar[1], Surajit Saha[2], B Sundaravel[3], Sinu Mathew[1,*]

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**Abstract**

Two-dimensional (2D) layered magnetic materials have attracted great attention in recent years due to the the discovery of long-range magnetic order persisting down to monolayer. Chromium trichloride ($CrCl_3$) is one of the emerging 2D layered magnetic materials. In this work the stability of thick flakes of $CrCl_3$ under thermal annealing and harsh radiation environment is investigated. The samples were prepared by micro-mechanical exfoliation onto $SiO_2$/Si substrate and characterized using optical microscopy and Raman spectroscopy. The Raman spectroscopy measurements were carried out on samples annealed in ambient conditions at various temperatures ranging from 300 K to 700 K. Pristine $CrCl_3$ exhibits six Raman active Ag modes, we found that the degradation of $CrCl_3$ begins above 650 K along with the appearance of Cr-O peak at 555 $cm^{-1}$. Samples were also exposed to a 30 keV proton beam at fluences from $10^{13}$ to $10^{15}$ ions/$cm^2$ and ion-beam-induced structural modifications down to 100 K were investigated using temperature-dependent and polarized Raman spectroscopy. The thermal and radiation stability of $CrCl_3$ will be discussed by analysing the evolution of Raman features as a function of annealing temperature and ion irradiation.

**Keywords:** Raman spectroscopy, Van der Waals magnets, Thermal annealing, Ion irradiation

# Computational, spectroscopic and docking investigation of 5-(2-Methoxy-Phenylamino)-3-Phenyl-Thiazolidine-2,4-Dione by employing DFT methods – Anti-diabetic agent

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**Abstract**

The molecular structure of 5-(2-Methoxy-Phenylamino)-3-Phenyl-Thiazolidine-2,4-Dione, has been extensively investigated using Density Functional Theory (DFT) at the B3LYP/6-311++G(d,p) level of theory. The optimised geometry parameters were obtained and compared with available crystallographic data. The vibrational assignments of the compound were carried out using FT-IR and FT-Raman spectra, which showed excellent agreement with the experimentally predicted vibrational frequencies after applying appropriate scaling factors. The electronic absorption spectra were simulated using Time-Dependent DFT (TD-DFT) calculations to interpret the UV–Vis transitions, revealing $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ excitations characteristic of the Thiazolidinedione framework. The Frontier Molecular Orbital (FMO) analysis was performed to evaluate the reactivity of the molecule through the energy gap (HOMO–LUMO), chemical hardness, and reactivity of the molecule. The Molecular Electrostatic Potential (MEP) map illustrated the charge distribution, highlighting the electrophilic and nucleophilic reactive sites. Furthermore, Natural Bond Orbital (NBO) analysis provided insights into the intramolecular charge transfer and hyper-conjugative interactions, while Electron Localisation Function (ELF), Localised Orbital Locator (LOL), and Reduced Density Gradient (RDG) analyses elucidated the nature of bonding and non- covalent interactions present in the system. Overall, the theoretical results offer a comprehensive understanding of the structural, electronic, and thermal properties of the molecules, establishing a strong correlation between experimental and computational findings. The molecular docking study has proven the anti-diabetic activity with the affinity.

**Keywords:** DFT, TD-DFT, FMO, MEP and NBO

# Greener, sustainable and affordable bio integrated quantum sensor enabled by seaweed for climate monitoring device with dual carbon dioxide capture and sensing capabilities

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**Abstract**

Climate change monitoring requires sensing technologies that are not only highly sensitive but also sustainable, eco-friendly, and affordable. This work introduces a new class of bio-integrated quantum sensors that utilize *Hypnea* indica, a red seaweed native to Kanyakumari, as a multifunctional material for dual $CO_2$ capture and detection. Rich in alginates, carrageenan, and other polysaccharides, *Hypnea* indica provides a renewable, biodegradable, and naturally responsive matrix that synergistically couples with quantum sensing elements such as nitrogen-vacancy (NV) centers and graphene-based transducers. The resulting hybrid devices demonstrate enhanced selectivity and ultra-high sensitivity toward $CO_2$, while the seaweed-derived bio-layer simultaneously serves as a natural carbon sink through chemical adsorption. Compared to conventional non-dispersive infrared (NDIR) sensors, this biointegrated platform offers lower energy consumption, reduced production costs, and superior sustainability. Its compatibility with flexible form factors and ambient operation further enables continuous, in situ deployment across urban, agricultural, and marine ecosystems. By integrating indigenous marine resources with advanced quantum technologies, this approach not only advances climate monitoring but also aligns with global carbon neutrality and green technology goals, paving the way for scalable, next-generation environmental sensing solutions.

**Keywords:** Quantum sensor, Seaweed-based materials, $CO_2$ capture and sensing, Sustainable device fabrication, Climate monitoring

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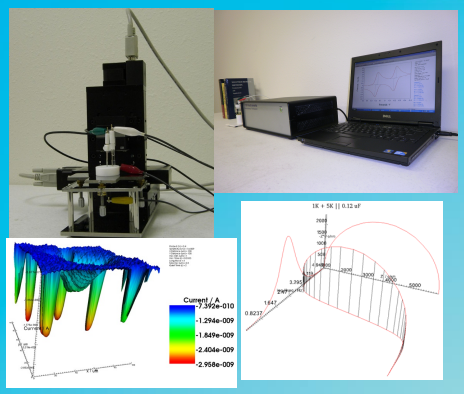

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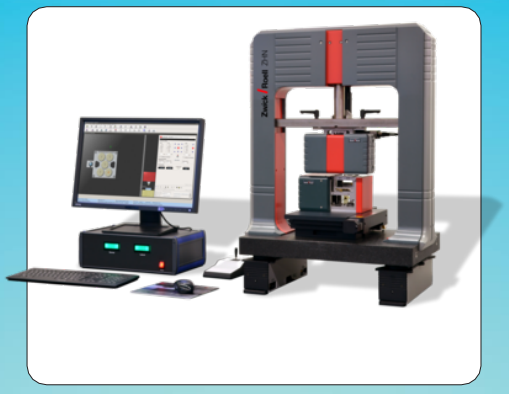

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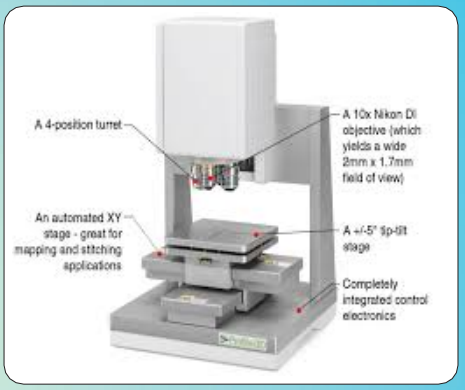


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- Program the onboard FPGA in VHDL or Verilog for custom, real-time signal processing

## Applications

- Optical metrology and spectroscopy
- Quantum computing
- Cold-atom and quantum optics experiments
- Multi-harmonic or multi-system detection
- System prototyping and simulation
- Automated test sequencing
- Closed-loop control design
- Synchronized Waveform Generators and receivers for phased-array, MIMO applications
- High-bandwidth data streaming to network storage
- High-frequency mixed domain analysis
- Implementing real-time Neural Networks


*Vacuum/Hot air oven*

*Muffle/Box furnace*

*Vacuum Induction Furnace*

*Planetary ball mill*

*Split Tube Furnace*

*CVD Furnace*

*RTA Furnace*

*Lab Table Press*

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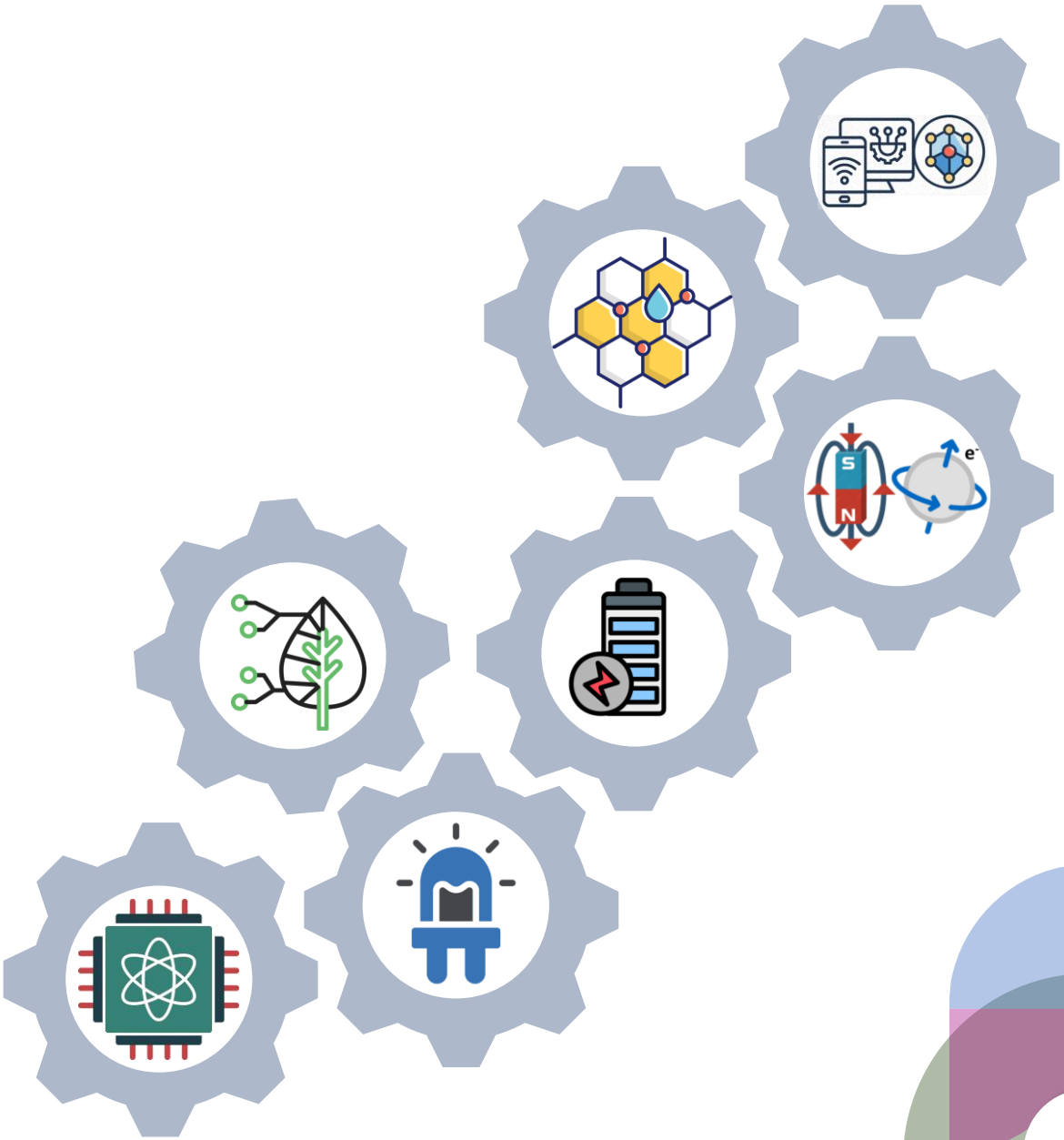


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