Department of Energy Science & Engineering, IIT Delhi

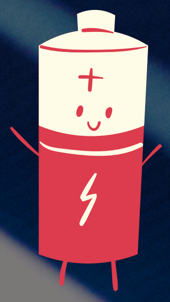
ICTN-KLC

KNOWLEDGE-LEADERSHIP-COMMERCIALIZATION

3rd International Conference on THIN FILMS AND NANOTECHNOLOGY: KNOWLEDGE, LEADERSHIP & COMMERCIALIZATION

ICTN-KLC 2025

11th-13th December



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INTERNATIONAL CONFERENCE ON THIN FILMS AND NANOTECHNOLOGY: KNOWLEDGE, LEADERSHIP & COMMERCIALIZATION (ICTN-KLC 2025)

Proceedings & Abstracts

Edited by,

Prof. Trilok Singh
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Associate Professor,
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PREFACE

Dear Colleagues,

It is my great pleasure to cordially invite you to the 3rd International Conference on Thin Films and Nanotechnology: Knowledge, Leadership & Commercialization (ICTN-KLC 2025).

The objective of this conference is to bring together researchers, scientists, and experts from academia and industry to discuss and share ideas, innovations, and recent achievements in the field. The conference will cover a wide range of topics, including thin films, advanced characterization techniques, and their translation into applied research areas such as energy generation, storage, and emerging technologies.

ICTN-KLC 2025 will be a three-day event featuring presentations and discussions led by several distinguished global leaders in thin films and nanotechnology. This conference will offer valuable opportunities to build new collaborations, address shared challenges, and explore future directions in Thin Films, Nanotechnology, Photovoltaics, Batteries, Wind Energy, Sensors, and related domains.

I am confident that ICTN-KLC 2025 will pave the way for strong scientific partnerships and contribute significantly to expanding our collective knowledge for meaningful advancements in the days ahead.

We look forward to your participation.

Prof. Trilok Singh
Chairperson

MESSAGE FROM CHIEF GUEST ICTN-KLC 2025

Advanced functional materials lie at the heart of next-generation technologies, and their successful translation from laboratory research to real-world applications is essential for societal well-being. In the context of India's strategic vision of technological self-reliance, the ability to innovate, manufacture, and deploy critical materials and devices domestically has never been more important.

There is no technological innovation without mastery of materials!

The 3rd International Conference ICTN-KLC brings together leaders from academia, industry, and policy to explore the full innovation pathway: **knowledge creation, leadership development,** and **commercialization**. These three pillars are not only essential in their own right but deeply interdependent, forming the backbone of a robust and future-ready R&D ecosystem.

I am optimistic that the outcome of the meeting will further accelerate India's progress toward secure supply chains, high-value manufacturing, and transformative technologies that directly enhance the quality of life and our societal well-being.

I extend my best wishes for a highly successful and productive conference with impactful ideas.

Prof. Sanjay Mathur
Chief Guest

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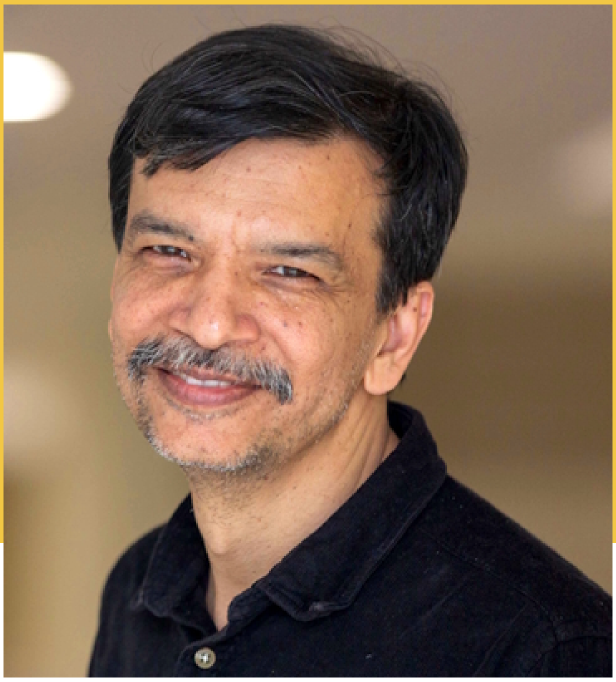
CONFERENCE PATRON

Prof. Rangan Banerjee



Director (IIT Delhi)

Prof. Rangan Banerjee is currently the Director, IIT Delhi. From February 2022 he is on lien from IIT Bombay where he served as the Forbes Marshall Chair Professor in the Department of Energy Science and Engineering - a Department that he helped start in 2007. His areas of interest include energy management, modelling of energy systems, energy planning and policy, hydrogen energy and fuel cells.

CONFERENCE ORGANIZERS

MEET THE TEAM BEHIND THE CONFERENCE ORGANIZATION

Prof. Trilok Singh

Chairperson

Dr. Trilok Singh is an Associate Professor in the Department of Energy Science and Engineering, Indian Institute of Technology Delhi (IITD.) where he is developing Novel Organic-Inorganic halide perovskite absorber layer for high-efficiency next generation solar cells. Prior joining to IIT Delhi, he worked at IIT Kharagpur as an Assistant Professor in the School of Energy Science and Engineering. Dr. Singh received Ph.D. degree from the Department of Physics IIT Delhi.

He was a post-doctoral fellow in Prof. Sanjay Mathur's group at University of Cologne, Germany. During his tenure from November 2011 till April 2015 at University of Cologne he extensively worked on the synthesis of metal oxide thin films via Chemical Vapor Deposition (CVD), Plasma Enhanced Chemical Vapor Deposition (PECVD), Atomic Layer Deposition (ALD) and Physical Vapor Deposition (PVD) and systematic modification/engineering of thin films properties for their application in solar energy driven water splitting. He also led a project on the Resistive Random Access Memory (ReRAM) to evaluate the potential of ultra thin films of metal oxide for non-volatile memory applications. In mid of 2015 he joined Prof. Tsutomu Miyasaka group at Toin University of Yokohama, Japan through JSPS fellowship where he worked on the synthesis of lead and lead-free based Organic-Inorganic halide perovskite for photovoltaic application.

His research interests include integrating micro and nanotechnology to develop innovative methods to solve energy generation problems. His interests also include the design, fabrication and development of high-efficiency flexible solar cells for various energy applications. Usage of Machine Learning tools in Energy generation for predictive analysis.

CONFERENCE ORGANIZERS

MEET THE TEAM BEHIND THE CONFERENCE ORGANIZATION

Prof. Vipin Kumar
Vice-Chairperson

Dr. Vipin Kumar is currently working as Associate Professor in the Department of Energy Science and Engineering, Indian Institute of Technology Delhi. He received his doctorate degree in Materials Science and Engineering from the School of Materials Science and Engineering, Nanyang Technological University (NTU) Singapore in 2016. During his doctoral studies, he availed exchange researcher fellowship at NTU and worked with University of Oldenburg, Germany for four months.

He worked as a research fellow for over two years at NTU Singapore, where, he developed Nanowires based gas sensor devices, and scaled-up this technology with GDS Instruments Pvt. Ltd., Singapore. He has gone through Lean Launchpad (LLP) program, which is an exercise to bring lab based research at the technology forefront, at NUS Singapore. He was awarded Inspire Faculty Award from the Department of Science & Technology (DST), India in 2017. To further excel his career in energy storage research, he moved to the Agency for Science Technology and Research (A*STAR), Singapore in 2017, and worked as a Scientist-I for nearly two years. Prior to join IIT Delhi, he worked with IIT Bhubaneswar as Assistant Professor in the School of Basic Sciences (SBS). He has contributed to various research projects, including electrochemical energy storage using carbon and oxide-nanomaterials, miniaturized gas sensor devices, and alkali metal anodes for high performance post-Li ion batteries.

Dr. Vipin Kumar’s research interests lie in electrochemical energy storage through high-energy rechargeable batteries (e.g., Sodium-Sulfur), and flexible and stretchable energy harvesting devices based on layered materials. He is also interested in developing state-of-the-art techniques to improve fundamental understanding of the nucleation and growth of the Solid Electrolyte Interphase (SEI) and metal dendrites.

CONFERENCE ORGANIZERS

MEET THE TEAM BEHIND THE CONFERENCE ORGANIZATION

Prof. Rahul Goyal
Secretary

Dr. Rahul Goyal is currently Associate Professor in the Department of Energy Science and Engineering, Indian Institute of Technology, Delhi. He received his Ph.D. in 2017 from Department of Mechanical Engineering, IIT Roorkee and Department of Engineering Sciences and Mathematics, Fluid and Experimental Mechanics, LTU Sweden. He also received his M.Tech. degree from IIT Roorkee in 2013. During his Ph.D., he worked as a Guest Researcher at Waterpower Laboratory of Norwegian University of Science and Technology (NTNU), Norway to conduct the transient flow measurements on model Francis turbine. After PhD, he worked as a Project Fellow at Department of Mechanical Engineering of Indian Institute of Technology, Roorkee from August, 2017 to March, 2018. Dr. Rahul has also worked as a Postdoctoral Fellow at Laboratoire des Écoulements Géophysiques et Industriels (Laboratory of Geophysical and Industrial Flows), Grenoble-INP, France from April, 2018 to October, 2018. Then, he worked as an Assistant Professor Grade-II in Mechanical Engineering Department of National Institute of Technology, Patna from November, 2018 to June 2019.

His research Interests are Off-design and transient operations of hydraulic machines, erosion wear and cavitation in hydraulic machines, performance assessment of hydropower plants, wind turbine performance, dynamics stall and vortex breakdown, wind and cavitation tunnel measurements, marine Propeller, hull-propeller interaction, computational fluid dynamics, fluid-Structure interactions, techno-economic analysis of floating solar, wind energy forecasting using artificial neural network, CFD analysis of single and multiphase system, atmospheric water generation.

CONFERENCE ORGANIZERS

MEET THE TEAM BEHIND THE CONFERENCE ORGANIZATION

Prof. Dinesh Pandya
Senior Advisor

Professor Dinesh Pandya earned his Ph.D. degree from IIT Delhi and before that his M.Sc. Physics and B.Sc. Hons. degrees from University of Delhi. He has a vast teaching & research experience of 50+ years that has been acquired at IIT Delhi and IIT Jammu. His expertise is in the primary area of Science and Technology of Thin Films & Nanomaterials which has been applied to the fabrication of advanced nanostructured materials tailored for novel device applications in the areas of Thin Film Solar Cells, PEC Cells, Thermoelectrics, Spintronics and Nanomagnetism, GMR sensors, Transparent Conducting Oxides, High Tc Superconducting Thin Films, Semiconducting & Optoelectronic Materials, Chemical Bath Deposition and Electrodeposition, Sputter and Ion-beam Deposition, etc. He has supervised 25 Ph.D. students in these areas and many other Masters and Bachelors students for their major projects. He has 250+ publications in journals of repute with 8400+ citations and i10 index of 103 & h-index of 36. He has been active in National Missions on Thin Film Solar Cells, High Temperature Superconductors, and Spintronics. He has been part of many international collaborations and international bi-lateral exchange programs. Prof. Pandya is former HoD Physics and Member BoG IIT Delhi. He has also undertaken the responsibility of establishing IIT Jammu and has mentored this new institution for a period of five and half years from its first day of inception by being there on-site. He has also been Member BoG, Dean of Students and Registrar IIT Jammu.

MESSAGE FROM SENIOR ADVISOR, ICTN-KLC 2025

The ICTN-KLC 2025 is the third conference in the series of conferences initiated in the memory of Late Prof. Kasturi Lal Chopra (1933-2021), the torch bearer of Thin Film Science and Technology Development activities in India as well as abroad, and to continue his legacy that was initiated by him in August 1970 with establishment of the Thin Film Laboratory at IIT Delhi after his return from the USA. His students and alumni of TFL are now serving in India and abroad in various leadership roles in academia, industry, and policy makers.

I happen to be his first batch of doctoral student who joined him in August 1970. Through close association with the research activity of Prof. Chopra, I observe that the scope of the current conference has been well designed keeping in mind the pursuit of excellence in the broad areas of Thin Films, Nano-Materials, Energy Generation and Energy Storage, including design and realization of novel devices & applications that have potential to serve society at large as well as future generations of research leaders.

The inclusion of terms Knowledge, Leadership, and Commercialization, in the title of the conference, are the special features, keeping in mind the thrust of our country for “Atma Nirbhar Bharat” and “Make in India”. It is pertinent to say that from the beginning Prof. Chopra paid special attention to development & transfer of Thin Film Technologies to Indian Industry. The Conference is in consonance with his vision. He was also the chosen leader for the advancement of Thin Film Solar Cells under the National Solar Mission initiated in 1970s.

The program of ICTN-KLC 2025 includes excellent talks by international and national leaders. All the three days will bring to the participants the current status and future pathways in the contemporary areas. There will be enough take-homes for each of the participants and for those having interest in entrepreneurship. I wish lively interactions for attendees and a successful conference. I do believe that the exciting deliberations will set the tone and benchmark for the next conference in the series.

I sincerely thank the Organizing Team of Prof. Trilok Singh for their efforts in making this event happen.

Prof. Dinesh Pandya
Senior Advisor

CO-ORGANIZERS

MEET THE CO-ORGANIZERS OF THE CONFERENCE

Prof. Pawan Kulriya

Prof. Pawan Kulriya,
Dean, School of Engineering
Associate Director, Advanced Instrumentation Research Facility (AIRF), Jawaharlal Nehru University, New Delhi
Area: Experimental condensed matter physics

Prof. Sandeep Chhoker

Prof. Sandeep Chhoker,
Jaypee Institute of Information TechnologyThe institution will open in a new tab, Noida, India
Area: Experimental condensed matter physics

Prof. Manika Khanuja

Prof. Manika Khanuja,
Centre for Nanoscience & Nanotechnology,
Jamia Millia Islamia, New Delhi
Area: 2D materials and their heterostructures

LOCAL ORGANIZING COMMITTEE

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PROF. VAMSI K. KOMARALA

Dr. Vamsi Krishna Komarala is currently a Professor in the Department of Energy Science and Engineering, IIT Delhi. His current research interests include the application of nanoscience and nanophotonics for enhancing solar cell efficiency. This involves utilizing metal nanostructures with surface plasmons to improve the absorption process in the cell, thereby increasing the baseline efficiency of solar cells.

PROF. ARIHANT BHANDARI

Dr. Arihant Bhandari is currently an Assistant Professor in the Department of Energy Science and Engineering, IIT Delhi. His present research interests are Energy conversion and storage, Multiscale modelling, Li-ion batteries, Atomistic simulations, Density Functional Theory (DFT), Electrochemistry, high-performance computing.

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Ms. Paulomi Singh
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Ms. Ankita Sao
IIT Delhi

Mr. Sidhanta Gupta
IIT Delhi

Mr. Animesh Anand
IIT Delhi

Mr. Rahul Singh
IIT Delhi

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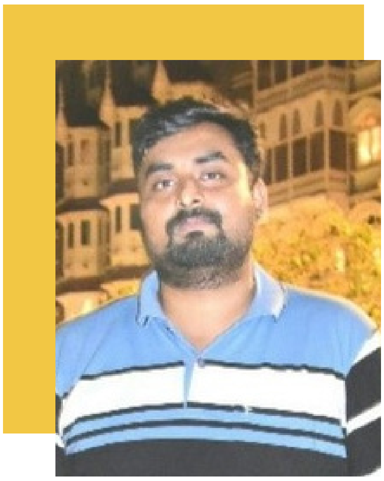
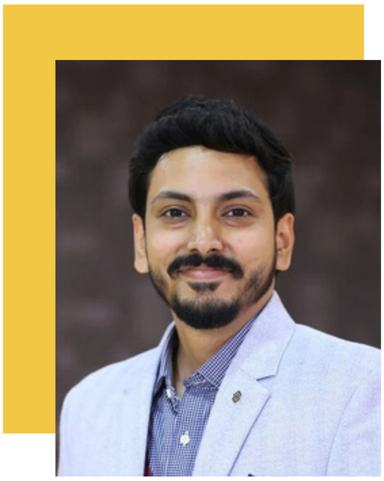
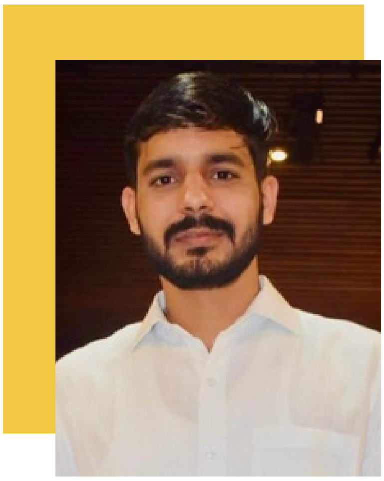


Mr. Sanjay Kumar C.
IIT Delhi

Mr. Suubi Mujuni Godwin
IIT Delhi



Mr. Dishant Sharma
IIT Delhi



Mr. Kamlesh Kumar
IIT Delhi

Mr. Subodh Singh Chauhan
IIT Delhi

Mr. Sachin Singh
IIT Delhi

PLENARY SPEAKERS

MEET THE PLENARY TEAM

1.	Prof. Dr. Sanjay Mathur	Catalysts of Change: Advanced Nanomaterials Steering Health and Energy Transition
2.	Prof. V. Ramgopal Rao	From Atoms to Applications: Translating Nanoscience into Real-World Innovation
3.	Prof. Shyam Sudhir Pandey	Facile Fabrication of Large Area Oriented Thin films and their 2D-Positional Mapping for Organic Electronic Devices
4.	Prof. Bhim Singh	Solar Photovoltaic Energy-A Sustainable Solution for Humanity

SPECIAL SESSION

MEET THE SPEAKERS

1.	Prof. Ramakrishna Ramanath Sonde	Energy transition and net zero pathway for India: Molecular Insights to Industrial Impact
2.	Prof. Gyu Min Kim	Ambient-Tolerant Mechanochemical Powder Strategy Combined with Alkali-Metal-Integrated HTLs for Stable, Solvent-Minimal Perovskite Devices

INVITED SPEAKERS

MEET OUR REVERED INVITED SPEAKERS

1.	Prof. Sanjay K. Srivastava	Efficient Organic Semiconductor-Silicon Hybrid Solar Cells Employing Effective Light Trapping Schemes
2.	Prof. Hemant Kumar	Enhancing MXene electrochemistry through spatial control of O and F termination distributions
3.	Prof. Jatin Kumar Rath	Evolution of PDS and FTPS techniques to probe the functioning of solar cells
4.	Prof. Prasanth Raghavan	Smart Textiles for Flexible and Stretchable Energy Harvesting and Storage Applications
5.	Prof. Vamsi K. Komarala	Fabrication and Characterization of HeteroJunction Solar Cells for High Efficiency
6.	Prof. Bhanu Nandan	Functionalized Textile Based Electrode Materials for Lithium Sulfur Batteries
7.	Prof. Oomman K. Varghese	Revealing the Novel Properties of Low Dimensional Semiconductors via In Situ Studies and Numerical Simulations
8.	Prof. Eswaraiah Varrla	Liquid-Exfoliated Two-Dimensional Nanosheets: Energy Efficient Approaches and Self-assembly Processes
9.	Prof. Pabitra K. Nayak	Doping of soft semiconductors for stable and efficient optoelectronics

INVITED SPEAKERS

MEET OUR REVERED INVITED SPEAKERS

10.	Prof. Arihant Bhandari	Simulations of few-layer graphene-based electrodes for electrochemical energy storage
11.	Dr. Suraj Soman	From Lightbulbs to Lifelines: Powering the Future with Indoor Light
12.	Prof. Deepak Kumar	Co-utilization strategy-based nano-composite Gr-Si anode for Li-Ion battery
13.	Dr. Bhumika Choudhary	Structurally Tunable Perovskite for Stable Thin film Optoelectronics
14.	Prof. Vanchiappan Aravinda	Materials & coating for batteries, super-capacitors and fuel cells
15.	Dr. Rashi Kedia	Solvent-Free Deposition of Copper(I) Thiocyanate Thin Film: A Sustainable Approach for the Hole Transport Layer in Perovskite Solar Cells
16.	Prof. Abhishek Sarkar	High Entropy Oxides: Opportunities and Challenges
17.	Dr. Ashish Kulkarni	Insulating Metal Oxide and Self-Assembled Monolayer Interface for Efficient Perovskite Solar Cells
18.	Prof. Raju Kumar Gupta	NASICON-Based Electrolytes for Solid-State Sodium-Ion Batteries

INVITED SPEAKERS

MEET OUR REVERED INVITED SPEAKERS

19.	Dr. Saurabh Kumar Pandey	Numerical Simulation of Bismuth-based highly efficient eco-friendly Perovskite solar cell
20.	Mr. Arup Dhar	Accurate translation of outdoor IV Measurements to STC for Photovoltaic Modules across Diverse Technologies
21.	Prof. Somnath Chandra Roy	An Exciting World of One-dimensional Metal Oxide Nanoand Hetero-structures
22.	Mr. Awatans Tripathi	Improving the pre-conditions of BIPV in India
23.	Prof. Shree Prakash Tiwari	Flexible Electronic Devices for Smart Sustainable System
24.	Prof. Upendra Pandey	Indenofluorene Dimer as an Efficient Interlayer for HighPerformance Perovskite Solar Cells
25.	Prof. Manika Khanuja	Machine Learning– Enabled Acceleration of Catalytic Reaction Pathways and Sensing Performance in 2D Nanomaterials
26.	Prof. Pankaj Yadav	Automated EIS Analysis of Metal Halide Perovskite Single Crystals Using Machine Learning for Activation Energy Prediction
27.	Prof. Ankur Goswami	Tungsten doped VO_2 thin film based resistive micro-oscillators for the application in neuromorphic systems

INVITED SPEAKERS

MEET OUR REVERED INVITED SPEAKERS

28.	Prof. Hemant Sagar	Advancing Toward 2070 Net-Zero: Hydropower Potential and Cavitation–Silt Problems Across Scales
29.	Mr. Dileep Tiwari	Unleashing Renewable Energy Opportunities: Policies, Strategies for Emerging Challenges, and the Path to Sustainable Investment in Gujarat
30.	Prof. Rishi Sharma	Cold Plasma Processing for Surface Engineering
31.	Prof. Dibyajyoti Ghosh	Designing Layered Halide Perovskites for Optoelectronics: Insights from ab initio and datadriven modeling
32.	Prof. Suresh C. Sharma	Plasma-Assisted Vertically Aligned Semiconducting 2D Graphene Field Effect Transistor Based Biosensor for Detection of Various Cancerous Bio-molecules
33.	Prof. Rajendra Singh Dhaka	Sodium-ion Batteries for Sustainable Future and Viksit Bharat
30.	Prof. Jai Singh	MoS_2 monolayer, bilayer thin films fabricated by RF sputtering and pulsed laser deposited ZnO thin-films/nanostructures
34.	Prof. Ulganathan Mani	Strategies for Enhancing Zinc-Iron Hybrid Redox Flow Battery

PLENARY SPEAKER

Prof. Dr. Sanjay Mathur

Prof. Sanjay Mathur is a Chair Professor and Director of the Institute of Inorganic Materials Chemistry at the University of Cologne in Germany. He is a Distinguished Professor at IIT Madras, India and an International Faculty at IIT Kharagpur, IIT Bhilai and IISER Tirupati. He is also the Director of the Institute of Renewable Energy Sources at the Xian Jiao Tong University, Xian, China and a World Class University Professor at the Chonbuk University in Korea. His research interests focus on application of nanomaterials and advanced ceramics for energy technologies. He holds several patents and has authored/ co-authored over 540 original research publications (h index, 83) and has edited several books. He serves as the Editor-in-Chief for Journal of Electroceramics, and Editor for Nano Energy. He is an Academician of the World Academy of Ceramics. He was awarded the Honorary Doctorate of Vilnius University in 2016. He is a Fellow of ACerS, ASM International and MRS. He was elected Fellow of the European Academy of Science in 2020 and as Foreign Fellow of National Academy of Science, India in 2021. He was awarded the Woody White Award of the Materials Research Society (MRS) in 2021 and had received the Medal of the Chemical Research Society of India (2022). He is also the recipient of the Materials Frontiers Award (2022) of the International Union of Materials Research Society (IUMRS, 2022). He has served as the President of the American Ceramic Society (ACerS, 2022-23), USA. He was recognized by the Orton Jr. Lecture (2022/23) of the ACerS. He is the Secretary of IUMRS, and he serves on the Boards of European Science Council, German Ceramic Society and German Materials Society. He was recognized with the M L Bhagat award of the Indian Ceramic Society (2024). He was elected Fellow of the European Ceramic Society (2025) and Academician of the African Academy of Science (2025).

CATALYSTS OF CHANGE:
ADVANCED NANOMATERIALS STEERING HEALTH AND ENERGY TRANSITION

SANJAY MATHUR

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Abstract

Advanced materials are driving innovation across all fields of technology, ranging from construction and mechanical engineering, automotive and electromobility, to medical technology, energy storage and conversion technologies, and microelectronics. Given their technological impact, functional materials represent an essential segment of industrial technologies with significant value creation potential for both established markets and emerging technologies. Especially in the context of sustainable production techniques, substitution of critical raw materials, and energy- and resource-efficient manufacturing, tailored surfaces and interfaces are gaining increasing importance in the future. In this context, chemical processing of nanostructured ceramics in tuning the functional and interfacial properties for better charge transport, higher corrosion protection and enhanced performance. The examples will include the role of functionalized inorganic surfaces in electrolysers for hydrogen production, and advances in photon-harvesting technologies for perovskite-based photovoltaics. Moreover, chemically functionalized SiO_2 nanoparticles acting as efficient drug-carriers to transport higher amounts of therapeutic payloads to diseased sites will be presented. Hollow nanocarriers can reduce undesired off-site effects and enable theranostic and thera-regenerative approaches. This talk will emphasize the power of chemical synthesis in designing new materials for energy and health transitions.

This talk will discuss the potential benefits of engineered nanomaterials towards energy conversion processes, and recent developments in precision drug delivery approaches.

Keywords: Sustainable development, Energy Transition, Green Hydrogen and Ammonia, Precision Drug Delivery

PLENARY SPEAKER

Prof. Dr. V. Ramgopal Rao

Prof. V. Ramgopal Rao is the Group Vice-Chancellor of the Birla Institute of Technology and Science, Pilani, overseeing its campuses in Pilani, Hyderabad, Goa, Dubai and Mumbai. He earlier served as the Director of IIT Delhi for 6 years and as Chair Professor at IIT Bombay and IIT Delhi. An internationally acclaimed nanoelectronics researcher, he has published over 500 papers and holds 50 patents, with technologies licensed globally and used in hundreds of millions of chips. He co-founded two successful deep-tech startups in India, Nanosniff and Soilsens, which have commercial products in the market. A Fellow of IEEE, TWAS, INSA, IASc, INAE and NASI, Prof. Rao has guided 53 Ph.D. scholars and received over 40 national and international awards, including the Shanti Swarup Bhatnagar Prize in Engineering Sciences, the Infosys Prize, and the IEEE EDS Education Award. He serves on the Editorial Advisory Boards of leading international journals such as ACS Nano Letters, AIP Applied Physics Reviews, and the IEEE Journal on Flexible Electronics, and has delivered over 200 plenary, keynote, and invited lectures worldwide.

FROM ATOMS TO APPLICATIONS: TRANSLATING NANOSCIENCE INTO REAL-WORLD INNOVATION

V. RAMGOPAL RAO

Fellow of IEEE, TWAS, INAE, IASc, INSA, NASI
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Abstract

Nanotechnology has moved from a laboratory curiosity to a powerful enabler of new products and solutions across sectors. From advanced semiconductor devices and sensors to healthcare diagnostics, energy systems and environmental applications, nanoscale science is reshaping every aspect of modern life. As this field matures, the focus is shifting from what is possible to what is useful for society.

This talk will reflect on the journey of nanotechnology research in India and elsewhere, and how ideas born at the nanoscale translate into impactful innovations when coupled with entrepreneurship, policy support and a strong ecosystem for commercialization. Drawing on experiences from academic research, industry partnerships and startup efforts, the discussion will highlight lessons in time to market, IP creation, scaling pathways and the importance of interdisciplinary collaboration. In the end, nanotechnology is not just about manipulating matter at atomic and molecular levels. It is about using that knowledge to build a safer, healthier and more sustainable world.

PLENARY SPEAKER

Prof. Dr. Shyam Sudhir Pandey

Prof. Shyam S. Pandey completed PhD from, National Physical Laboratory, New Delhi, India in 1997 in the area of synthesis, characterization and application of organic conjugated polymers. He came to Japan as post-doctoral fellow in 1998. He worked as Fukuoka IST sponsored post-doctoral fellow in the Kyushu Institute of Technology from 1998-2001 in the area of photo-functional materials and devices. He was JSPS post-doctoral fellow from 2001-2003 (Soft-actuators & Artificial Muscles) and Knowledge Cluster invited researcher from 2003-2007 (Protein Biochips). He has received National Technology Award from National Research Development Corporation, Government of India in 2005 for the development of Glucose Biosensors, which is currently being manufactured and marketed. He worked in Kyushu Institute of Technology as assistant professor form 2009-2012 in the area of design and development of novel photofunctional materials for their application in the area of next generation solar cells. As an Associate Professor, he started his Organic Photofunctional Materials Devices research group in the same institute from April 2012-March and worked in the area of reserach and development of Next Generational Cells, Organic Electronic Devices and Bio-image sensors. Currently he is a Professor in the Green Electronics department of Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology. He has published more than 230 papers in international refereed journals and about 30 patents in India, Japan Europe and USA. His research interests deal with the Dye-Sensitized and Organic Solar Cells, Quantum Chemical Calculations, Organic Electronics & optoelectronics, Organic Conducting Polymers, Biosensors and Protein Biochips.

FACILE FABRICATION OF LARGE AREA ORIENTED THIN FILMS AND THEIR 2D-POSITIONAL MAPPING FOR ORGANIC ELECTRONIC DEVICES

SHYAM S. PANDEY

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Abstract

Solution processable organic semiconductors play a pivotal role for the practical realization of flexible and wearable electronics. High performance organic electronic devices utilizing organic molecular semiconductors have been although demonstrated utilizing vacuum deposition for thin-film fabrication but such thin-films processing is not suitable for the mass production of organic electronic devices. Although spin-coating has been most widely used for thin film fabrication of conjugated polymers (CPs), huge material wastage and challenges for multi-layer coating are intriguing issues. To circumvent these issues, we have developed and improvised a facile and highly cost-effective technique to fabricate large-area anisotropic thin films of CPs known as the floating film transfer method (FTM). It has been demonstrated that FTM is capable of fabricating large area (> 20 cm x 2 cm) and oriented thin films of several well-known CPs. Using NR-P3HT, we have recently demonstrated that FTM processed thin films not only exhibit very similar spectral features like its regioregular counterpart but also a remarkable increase (> two orders of magnitude) in the charge carrier mobility upon orientating the thin films by FTM. Utilizing highly edge-on oriented thin film thin films of PBTTT-C14 processed by FTM, we have not only demonstrated a very high optical dichroism of >10 but also an OFET mobility of 1.24 cm^2/Vs, which is one of the highest reported mobility values for this class of CPs. In spite of enhanced solubility long chain substituted P3ATs in common organic solvents, serious fall in the carrier mobility as a function of increasing alkyl chains confined the utilization of P3HT extensively. We have recently demonstrated that FTM is capable to solve this issue amicably, where such detrimental influence of alkyl chain length for planer charge carrier transport was not observed making the freedom for the selection of any of P3ATs for OFET applications. Although the molecular orientation in FTM films can be tuned by parametric optimizations, it is important to probe the film homogeneity in terms of thickness and extent of the molecular orientation. To provide an amicable solution, we have developed 2-dimensional positional mapping system for a facile and swift profiling of thickness as well as the molecular orientation. At the same time, the validity of the newly designed 2D positional mapping system was also proved using several CPs fabricated by different thin-film fabrication methods such as FTM, friction transfer and spin coating. Details about large area facile thin film fabrication, their implementation to a variety of CPs and their impact on the anisotropic charge carrier transport will be discussed.

Keywords: Conjugated Polymers; Oriented Thin Films; 2D-Positional Mapping; Organic Electronics

PLENARY SPEAKER

Prof. Dr. Bhim Singh

Professor Bhim Singh received his B.E. from the University of Roorkee (1977) and his M.Tech. and Ph.D. from IIT Delhi (1979, 1984). He began his career at the University of Roorkee in 1983 and joined IIT Delhi in 1990, becoming Professor in 1997. He has served as ABB Chair Professor, CEA Chair Professor, Head of Electrical Engineering, Dean Academics, JC Bose Fellow, and is currently an ANRF National Science Chair and Emeritus Professor at IIT Delhi. He is also Chairperson, BOG, SVNIT Surat (2023–2026). He has supervised 149 Ph.D. and 184 Master's theses, filed 109 patents, executed over 90 projects, and co-authored a textbook on Power Quality. His research spans renewable energy systems, power electronics, electric drives, microgrids, and power quality. He is a Fellow of FNAE, FNA, FNASc, FASc, FTWAS, FIEEE, FIET, FIE, FIETE, and a Life Member of ISTE, SSI, NIQR. His major honors include the Rashtriya Vigyan Puraskar – Vigyan Shri (2024), IIT Roorkee Distinguished Alumnus Award (2023) and the Goyal Prize (2021–22), along with several notable IEEE, INAE, and national awards. Prof. Singh has held leading roles in major IEEE conferences, chaired IEEE Delhi Section, served as an IEEE Distinguished Lecturer, and contributed to national committees including SERB-DST and NAMPET. He has delivered over 300 invited lectures and chaired 100+ sessions. He also mentors successful start-ups such as Quanteon, HyperX Energy, Intellicon, Tadpole Projects, and Tsuyo Manufacturing.

SOLAR PHOTOVOLTAIC ENERGY-A SUSTAINABLE SOLUTION FOR HUMANITY

BHIM SINGH

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Abstract

The global shift towards renewable energy has become imperative in addressing the challenges posed by climate change, environmental degradation, and the depletion of finite fossil fuels. This talk will explore how solar photovoltaic energy, offers a sustainable solution for humanity. By analysing current technological advancements, policy frameworks, and economic impacts, the talk highlights the potential of solar PV energy to provide a reliable, cost-effective, and environmentally friendly alternative to conventional energy sources. Additionally, the talk covers the socio-economic benefits of solar PV energy adoption, such as job creation, energy security, and reduced greenhouse gas emissions. As the world moves towards a low-carbon future, solar PV energy emerges not only as a necessity but as a cornerstone for sustainable development and a cleaner, more resilient future for all.

The large-scale development and deployment of solar energy technologies are essential to global pursuit of decarbonizing the energy sector. To effectively harness variable and intermittent solar PV source, and to integrate the electricity generated by these plants, power electronics plays a crucial role. Developing, testing, and commercializing appropriate power electronic devices, such as voltage source converters and DC-DC converters, are key to maximizing the benefits of solar PV energy. The challenges involved are complex and require a comprehensive understanding of solar PV energy resource characteristics, electric machines, electricity generation, transmission, distribution, utilization systems, circuit analysis, and power electronics. This talk will also cover several applications of solar photovoltaic power generation such as rooftop, solar water pumping and electric vehicle charging infrastructure.

Keywords: Solar PV Rooftop Generation, Solar PV Water Pumping, Solar PV Integration in Electric Vehicle Charging Infrastructure, Power Quality, Control and Configurations.

SPECIAL SESSION

Prof. Ramakrishna Ramanath Sonde

Prof. R. R. Sonde (PhD, FNAE) is a Professor at IIT Delhi–Abu Dhabi, and Visiting/Adjunct Professor at IIT Roorkee, IIT Jodhpur, IIT Jammu, and IIT Gandhinagar. A distinguished technologist and former Executive Vice President, CTO, and Board Member at Thermax Ltd., he has also served as Outstanding Scientist, Atomic Energy Commission of India, and Executive Director at NTPC Ltd. He began his career at BARC, where he topped his batch and received the Dr. Homi Bhabha Gold Medal, contributing significantly to heavy-water technology, isotope separation, and nuclear process engineering. At NTPC, he established the pioneering Energy Technologies (now NETRA) division, advancing clean coal, IGCC, carbon capture, hybrid solar-thermal systems, and efficiency enhancement platforms. Prof. Sonde is a Fellow of the Indian National Academy of Engineering, Chairman of major national programs including the DST CCUS initiative and NITI Aayog Task Force on Methanol, and Advisor to JSPL, IIT Jodhpur's Hydrogen Valley, Ahmedabad University, and several national committees on energy, innovation, and sustainability. His corporate and academic leadership spans hydrogen energy, fuel cells, sodium–sulfur batteries, carbon capture, CDI-based water purification, and energy transition technologies, supported by deep collaborations with global research institutions. He has founded multiple technology start-ups in mobility, AI/ML, and hydrogen fuel cells at IIT Delhi and IIT Gandhinagar. Prof. Sonde's contributions have been recognized with numerous honors including the Dr. M. Visvesvaraya Gold Medal, Dr. Homi Bhabha Gold Medal, Dr. Doraswami IIChE Medal, and the INS Gold Medal. He currently teaches process simulation, process integration, and technology commercialization at IIT Delhi, and continues to drive India's clean energy mission through research in hydrogen, methanol economy, CCUS, clean coal gasification, biomass-derived hydrogen, advanced batteries, and next-generation fuel cell systems.

ENERGY TRANSITION AND NET ZERO PATHWAY FOR INDIA: MOLECULAR INSIGHTS TO INDUSTRIAL IMPACT

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Abstract

Humanity is at a turning point in its long history of evolution, where on one hand, due to positive disruptive science, it has created an enormous amount of wealth and an economy for a better living standards and on the other hand, the same science has created a negative disruption in ecology and climate change to the extent the existential crisis is nearly upon us! The cheap access to energy (fossil mainly) is the disruptor-in-chief for both. For a nation like India in its exponential trajectory where in next 25 years leading to our Viksit Bharat@2047 India will reach an economy of 35 trillion $ economy and its energy demand will grow from current 8500 TWh to 32000 TWh and India is committed to bring down the CO_2 emissions from current 3100 Million tons to under 1300 million tons for its net zero by 2070 means an enormous challenge no developed nations had ever to face.

The time has come to reset the science with new models to bring speed and scale for sustainability. Energy transition is the biggest transition for humanity in its long history for the very existence of homo sapiens and hence the need for speed and the scale.

The big solutions lie in integrating multiphysics in one device, discovery of new molecules, rendering the new molecules on many different surfaces and substrates and building devices as basic building blocks for a scaled up system. The talk gives an insight into how to do such deep science and then push the boundaries for making industrial scale impact.

SPECIAL SESSION

Prof. Gyu Min Kim

Prof. Dr. Gyu Min Kim is an Associate Professor in the Department of Chemical Engineering at Hankyong National University (Republic of Korea). He earned his Ph.D. in Applied Chemistry from the University of Tokyo in 2017 and subsequently carried out postdoctoral research as a JSPS Research Fellow in Prof. Tsutomu Miyasaka’s group — a leading lab in perovskite photovoltaics. Dr. Kim’s research centers on developing high-performance, durable perovskite solar cells through careful crystallization control, interfacial engineering, solvent and additive design, and advanced transport layers (e.g., ALD-SnO_2); he also works on dopant-free hole-transport materials, antisolvent-free fabrication, photocurrent-enhancing plasmonic architectures, rapid/scale-friendly processing, and photodetector devices. His work includes high-impact contributions such as the JACS report on achieving $V_{OC} > 1.4$ V in tin-oxide-based dopant-free $CsPbI_2Br$ cells (2020), a widely cited Energy & Environmental Science review on the open-circuit voltage in perovskite cells (2022), and multiple recent articles (2023–2025) on process optimization, MACl/Ge-doping strategies, and ALD-SnO_2 roles in device performance and stability. Dr. Kim combines fundamental studies of film formation and interfacial chemistry with practical, reproducible fabrication methods aimed at improving device lifetime and manufacturability, and his collaborations with leading groups have advanced both the scientific understanding and technological readiness of perovskite photovoltaics for real-world and even space applications.

AMBIENT-TOLERANT MECHANOCHEMICAL POWDER STRATEGY COMBINED WITH ALKALI-METAL-INTEGRATED HTLS FOR STABLE, SOLVENT-MINIMAL PEROVSKITE DEVICES

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Abstract

Perovskite photovoltaics continue to face reproducibility and stability bottlenecks as long as liquid-phase dopants and trace additives remain indispensable for both the perovskite and hole-transport layers. We replace this paradigm with a fully solid-state route that embeds MACl into mechanochemically synthesized perovskite powder, steering crystallization and suppressing compositional drift from the outset. The resulting powder retains structural integrity even after prolonged exposure to 85% RH and 100 °C, dissolves cleanly into precursor inks, and reliably evolves into α-phase films without reliance on solution-side precision. In parallel, alkali-metal-integrated carbazole-based Hole Transport Layers (HTLs) provide dipole alignment and moisture-tolerant hole extraction without Li-TFSI or t-BP, eliminating the most instability-prone steps in conventional HTL doping. Under solvent-minimal fabrication with ultra-low anti-solvent loading (<10 μL), devices consistently exceed 20% PCE, and the fully powder-based configuration reaches 24.33% while retaining 96.8% of its initial efficiency after 800 h of continuous operation (AM1.5G, 25 °C, dry air). By transposing both the absorber formation and interfacial energetics into intrinsically defined powders, this approach renders perovskite fabrication markedly less sensitive to ambient humidity, operator handling, and dopant chemistry pushing the technology closer to reproducible, industrial-scale deployment.

Keywords: Perovskite powder; Mechanochemical synthesis; Alkali-metal HTL; Dopant-free

INVITED SPEAKER

Prof. Sanjay K. Srivastava

Prof. Sanjay K. Srivastava is a Principal Scientist at CSIR–National Physical Laboratory (NPL), New Delhi, and an Associate Professor at AcSIR. He joined CSIR-NPL in 2007 and works in the Photovoltaic Metrology and Advanced Materials & Device Metrology divisions. His research focuses on photovoltaic metrology, high-efficiency silicon solar cells, thin and flexible Si photovoltaics, and silicon nanostructure-based light-trapping schemes. He has significantly contributed to developing novel silicon nanowire architectures, hybrid and heterojunction Si solar cells, and next-generation PV device concepts. He holds a Ph.D. in Physics from IIT Delhi (2007), an M.Tech in Materials Science & Engineering from IIT Bombay (2001), and an M.Sc. in Physics from Banaras Hindu University (1999). Over the years, he has worked on materials science, carbon nanostructures, and advanced silicon photovoltaic devices, including a BOYSCAST Fellowship at the Max Planck Institute, Germany, where he researched silicon nanowires for thin optical materials. Prof. Srivastava has published more than 90 research works, including over 55 SCI journal papers, 10 book chapters, and several conference publications. He also holds granted US and EU patents related to silicon nanostructure-based PV technologies. His contributions have earned him notable recognitions such as the CSIR Young Scientist Award (2013) and the Young Investigator Award (2011). At AcSIR, he plays an active academic role in teaching, curriculum design, doctoral advisory committees, and mentoring PhD students in advanced photovoltaic research.

EFFICIENT ORGANIC SEMICONDUCTOR-SILICON HYBRID SOLAR CELLS EMPLOYING EFFECTIVE LIGHT TRAPPING SCHEMES

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Abstract

Solar photovoltaic (PV), which is dominated by silicon (Si) homojunction solar cells, is one of the most reliable technologies for harvesting solar energy. However, these PV cells are based on high thermal budget dopant-diffusion and annealing processes (≥850 °C). Naturally, these processes are time consuming, complex and in turn increase per unit power cost of the PV devices. This has driven significant research interests towards combining the best of both organic and inorganic systems. Organic carrier selective layer with Si is a promising approach for the next generation solar cells owing to their unique properties like light weight, cost effectiveness and environment friendly. The organic-Si hybrid solar cells (HSCs), in principle, can achieve comparable efficiency to that of a conventional Si homojunction solar cell as light absorption and photo-carriers generation take place in the Si wafer only in such architecture. Most commonly, an inexpensive, highly conducting and transparent polymer namely, poly(3,4-ethylenedioxythiophene)-poly(styrene sulfonate) (PEDOT:PSS), which acts as a p-layer (carrier selective hole transport) is coated over n-type crystalline Si surfaces resulting into a Schottky junction at the PEDOT:PSS/Si interface. The HSCs based on PEDOT:PSS/n-Si, have attracted a lot of attention toward the development of low-cost and efficient PV devices. However, it requires extensive control and optimization of the photoelectric property of the PEDOT:PSS thin films, Si surface properties, PEDOT:PSS/n-Si hetero-interface, n-Si/rear electrode contact, and so on. Effective surface engineering of the Si wafers, can play important role in achieving not only effective light harvesting but also a quality PEDOT:PSS/n-Si hetero-interface leading to high efficiency HSCs. For example, highly efficient PEDOT:PSS/Si HSCs (with photo-conversion efficiency >12.25%) could be achieved via an effective surface micro-engineering of the as-cut, low-cost solar-grade thin Si wafers, by a simple one-step aqueous KOH process. The process reduces the weighted surface reflectivity from >35% to <9% in broad spectral range in addition to removing the surface saw-damages of the wafers completely. The combined effect in turn improves the PEDOT:PSS/Si interface (junction) property leading to a highly efficient PEDOT:PSS/Si HSCs even in its simplest possible device architecture. The talk will discuss few such examples of efficient hybrid solar cell architectures including flexible solar cells employing simple yet effective light trapping schemes involving random micro-pyramids, Si nanowires and silver nanoparticles (Ag NPs) plasmonic effect, developed at CSIR-NPL during past 5 years.

INVITED SPEAKER

Prof. Hemant Kumar

Dr. Hemant Kumar is an Assistant Professor in the Department of Physics at IIT Bhubaneswar, specializing in computational materials science, multiscale modelling, and energy-storage materials. He obtained his Ph.D. in Physics from IISc Bangalore and completed postdoctoral research at the University of Pennsylvania before joining IITBBS in 2019. His research focuses on 2D materials and van der Waals heterostructures, flexible and solid-state battery materials, nanomaterials, and confined biomolecular systems, integrating multiscale simulations and machine-learning approaches. He leads multiple funded projects, including Development and Applications of Multiscale Modelling Methods for 2D Material Heterostructures (IITBBS), Rational Design of Flexible Energy Storage Devices Using Multiscale Simulations and Machine Learning (SERB India), Integrated Clean Energy Material Acceleration Platform for AI/ML-Assisted Development of Solid-State Batteries (DST India), and Room-Temperature Sodium–Sulfur Batteries for Stationary Storage Applications (ReNew Power). Dr. Kumar has an extensive publication record across leading journals such as Nature Physics, Advanced Energy Materials, ACS Nano, Nano Letters, Langmuir, Scientific Reports, and Physical Chemistry Chemical Physics, covering topics including strain solitons in 2D materials, MXene magnetism, magnesium-ion and sodium-ion battery anodes, catalytic HER activity in Janus TMDs, confined water dynamics, and transport phenomena in nanostructures. His work, combining theory, simulation, and materials design, contributes significantly to the advancement of computational materials physics and next-generation energy-storage technologies.

ENHANCING MXENE ELECTROCHEMISTRY THROUGH SPATIAL CONTROL OF O AND F TERMINATION DISTRIBUTIONS

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Abstract

MXenes have attracted considerable attention as potential electrode materials due to their adjustable chemical properties while retaining excellent metallic conductivity. Mixed surface functionalization, exemplified by O and F terminations on $Ti_3C_2O_{2(1-x)}F_{2x}$ MXenes, dictates electrochemical performance, yet the specific role of their spatial arrangement is poorly understood. This study utilizes a synergistic combination of density functional theory (DFT), kinetic Monte Carlo (KMC), and ab-initio molecular dynamics (AIMD) to investigate how the nanoscale distribution of surface terminations governs Li transport and storage. DFT calculations identify distinct local neighbourhood environments characterized by unique Li diffusion barriers, challenging the simplification inherent in weighted-average compositional models. KMC simulations over 100 random O/F configurations show a 147-fold variation in Li diffusivity at room temperature, despite identical compositions. Furthermore, a composition-dependent analysis indicates that F-rich mixed-terminated surfaces facilitate faster Li diffusion compared to O-rich counterparts. The accuracy of the KMC model itself is validated by AIMD results, ensuring reliable dynamic predictions. Additionally, we show that the theoretical Li storage capacity is sensitive to these local termination environments. These findings reveal that, even at constant composition, the spatial configuration of surface terminations critically impacts electrochemical behaviour. This underscores the limitations of averaging approaches and highlights local termination structure as a key design parameter. Nanoscale control of termination patterns can significantly enhance MXene performance, enabling a new approach to modelling and optimizing 2D materials.

Keywords: MXene, Mix-termination, DFT , Ion transport, LIB

INVITED SPEAKER

Prof. Jatindra Kumar Rath

Prof. Jatindra Kumar Rath is a Professor in the Department of Physics at the Indian Institute of Technology Madras, where he leads a broad research program in applied physics focused on photovoltaics, thin-film solar cells, nanomaterials and device/optical engineering. He earned his Ph.D. from IIT Madras (2007) and has built a prolific publication record on topics that include quantum-dot and nanorod-based solar absorbers, metal-oxide and chalcogenide heterojunctions, silicon heterojunction passivation and light-management strategies for thin-film/heterojunction devices. His recent work (2024–2025) covers SnS quantum-dot–TiO_2 heterojunctions and hybrid SnS QD solar cells, electrical modelling of TiO_2–SnS heterojunctions, Sb_2Se_3/CdS substrate-configured heterojunctions, Fe_2O_3–WS_2 heterojunctions for enhanced photoelectrochemical conversion, and studies on V_2O_x and SnO_2 electron-transport/passivation layers for perovskite and silicon devices — contributions that illustrate his emphasis on materials-to-device translation and scalable processing. Prof. Rath has authored well over ~244 papers, contributed several high-impact reviews and book chapters, and his work has attracted thousands of citations (profile lists ~5,111 citations with an h-index in the 30s), reflecting sustained international influence and numerous collaborations in photovoltaics and nanotechnology. He is also active in experimental device fabrication, optical/electrical characterization and modelling, and in supervising students and collaborative projects that bridge academic and applied energy research.

EVOLUTION OF PDS AND FTPS TECHNIQUES TO PROBE THE FUNCTIONING OF SOLAR CELLS

JATINDRA KUMAR RATH

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Abstract

One of the important phenomena that controls the working of a solar cell is carrier generation and recombination under light conditions. To explain this behavior, an accurate estimation of the electronic density of states (DOS) in the subgap region is required. Among many techniques, photothermal deflection spectroscopy (PDS) and Fourier transform photocurrent spectroscopy, the two techniques which were mainly developed for amorphous and nanocrystalline silicon based materials, have now evolved as powerful tools to probe the quality of not only many inorganic materials, e.g., CdTe, GaN, CZTS, etc, but also organic based materials e.g., metal halide perovskites used in solar cells. From a series of data on Urbach tail energies (E_0) of absorber materials, a correlation with the voltage loss in solar cells has been established. It explains why high voltages are achieved in perovskite solar cells. Due to improvements in PDS detection technique, the DOS of extremely thin layers of high bandgap metal oxides, e.g., MoO_X, TiO_X, Al_2O_X, etc., has been evaluated. The role of E_0 and the midgap states, which include defect states and polarons, of these materials for the selective carrier transport at the interface with c-Si has been simulated. This is important information towards the development of carrier-selective contact (CSC) silicon heterojunction solar cells. The specialty of FTPS is that the absorber materials in a solar cell structure, even the subcells in a tandem cell, can be probed. The technique is further developed to record the quantum efficiency of a solar cell. The Fourier transform technique makes FTPS a fast measurement process compared to more time-consuming photo current methods, e.g., constant photocurrent measurement or dual beam photocurrent techniques. The measurement in a cell structure is a great advantage while probing perovskite materials, which are prone to ambient. With the help of FTPS, the role of SAM, alkaline materials and various chemical treatments, etc., on the structure, midgap defects and stability of the perovskite solar cell is evaluated.

INVITED SPEAKER

Prof. Prasanth Raghavan

Prof. Dr. Prasanth Raghavan is a Professor in the Department of Polymer Science and Rubber Technology at Cochin University of Science and Technology (CUSAT); he earned his B.Tech and M.Tech from CUSAT and completed his Ph.D. in engineering at Gyeongsang National University, Republic of Korea (2009) under the BK21 fellowship, finishing his doctoral work in under three years. His research portfolio spans 3D printing, carbon materials, energy storage, nano-composites and nano-engineered materials, polymer synthesis and processing, and recycling/waste management, and he has authored some 50+ publications including recent articles on recycling medical face masks, gel polymer electrolytes, TiO_2 fillers for solid polymer electrolytes, and reviews on graphene and MXenes for energy devices. Dr. Raghavan is also the author/co-editor of several books with CRC/Taylor & Francis and Springer — notably Graphene and Carbon Nanotubes for Advanced Lithium-Ion Batteries (CRC Press, 2018), Polymer Electrolytes for Energy Storage Devices (CRC Press, 2021), Ceramic and Specialty Electrolytes for Energy Storage Devices (CRC Press, 2021), and Electrospinning for Advanced Energy Storage Devices (Springer, 2021). He has received institutional and student-award recognitions and leads research and training activities at CUSAT aimed at translating nano-engineered polymers and carbon materials into safe, high-performance energy-storage technologies.

SMART TEXTILES FOR FLEXIBLE AND STRETCHABLE ENERGY HARVESTING AND STORAGE APPLICATIONS

PRASANTH RAGHAVAN

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Abstract

Smart textiles have wide range of applications in energy sectors to improve the safety and electrochemical performance of energy storage devices and harvesters. Electrospinning is a simple and versatile method which is gaining importance in recent years as the textile prepared by employing this method have controlled properties. The electrospun polymer nonwoven textile consist of thin fibers of micron/sub-micron diameters with high specific surface area. The interlaying of fibers generates large porosity with fully interconnected pore structure that facilitates easy transport of ions, and serves as flexible and stretchable electrolyte and electrode in batteries and supercapacitor for the advanced energy storage solutions especially for electric vehicles and stationary power source applications. Due to the high porosity and robustness these smart textiles also explored for the harvesting energy which is outperform than other electrodes. The smart textiles prepared from different polymers such as PAN, PVdF and their blend with other polymers such as PMMA or their nanocomposite are employed in different energy storage devices such as lithium ion batteries, sodium ion batteries and super capacitors and energy generator such as triboelectric nanogenerators. The smart textiles are explored for flexible and stretchable textile/fiber supercapacitors, the next generation energy storage solutions. The schematic illustration on the fabrication of smart textile based energy storage device is displayed in Figure 1. The employment of these smart textiles not only enhanced the electrochemical properties and charge discharge cycling orate capability of the batteries but also significantly improved the thermal stability and safety of the batteries, which can safely operate at very high temperature above 200 ℃.

INVITED SPEAKER

Prof. Vamsi K. Komarala

Vamsi K. Komarala is a professor at the Department of Energy Science and Engineering, IIT Delhi. He received M. Sc. degree in Physics from the Sri Venkateswara University, Tirupati, in 1996; M. Tech. degree in Energy Science and Technology from the Jadavpur University, Kolkata, in 1999; and Ph. D. in thin-film heterojunction solar cells from IIT Delhi, in 2004. He worked as a post-doctoral fellow in the School of Physics of Trinity College Dublin, Ireland for 3 years, and as a research associate at the Dept. of Physics, University of Arkansas, USA for 3 years on the topics; Quantum dots' excitons and metal nanoparticles' surface plasmons interaction, and Resonant energy transfer between excitons and plasmons for enhancing quantum dots' photoluminescence efficiency.

After this experience, he has been associated with IIT Delhi since 2010. His primary interest initially was in implementing Plasmonics and Nanophotonics concepts to enhance solar cell performance under third-generation solar cell concepts. Now, his present research interest is in silicon heterojunction solar cell fabrication and characterization. He has co-authored around 85 articles in peer-reviewed international journals and 15 papers in conference proceedings on the above-mentioned topics. He teaches solar photovoltaic devices and direct energy conversion methods to inspire and provide knowledge/understanding to the students.

FABRICATION OF HIGH-EFFICIENCY SILICON HETEROJUNCTION SOLAR CELLS

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Abstract

Energy harvesting from the sunlight has been one of the widely explored research areas with the built-in-potential creation from a simple pn-junction, followed by charge carrier collection. The primary goal of the photovoltaic community is to develop low-cost solar cells and systems for harnessing abundant solar energy, thereby ensuring future energy production is secure and contributes to global prosperity through climate-neutral energy resources. In the case of solar cell fabrication, to achieve the goal, the approach has been either to improve power conversion efficiency or to find simple fabrication steps.
Amorphous/crystalline silicon heterojunction (SHJ) solar cells are well known for their inherent high open-circuit voltage (V_{OC}) potential, better temperature coefficient, higher bifaciality, simpler fabrication process, and low thermal-budget manufacturing. The front emitter and the back surface field are formed by low-temperature deposition of doped a-Si:H(*p* or *n*) layers. This eliminates the need for high-temperature dopant diffusion and the complexity of local metal contact formation on the silicon wafer. As photovoltaic electricity is set for terawatt-scale deployment, new investors are now considering high-volume manufacturing of high-efficiency SHJ solar cells, which currently offer the highest module efficiency among c-Si PV technologies. It should be noted that despite the seemingly simple cell structure and lean processing, it has been challenging for researchers to realize the formation of exceptionally well-passivated a-Si:H/c-Si interfaces and SHJ cells with high V_{OC} and efficiency.

This talk will focus on SHJ solar cells fabrication and characterization to reach >23% power conversion efficiency; (a) front-end process; crystalline silicon surface preparation, (b) c-Si surface passivation with i-a-Si:H; process parameters optimization with the plasma enhanced CVD, (c) device characterization to enhance power conversion efficiency.

INVITED SPEAKER

Prof. Bhanu Nandan

Dr. Bhanu Nandan is a Professor in the Department of Textile Technology and Fibre Engineering at IIT Delhi, renowned for his extensive contributions to polymer science, nanostructured fibres, and self-assembly in polymeric systems. He earned his Ph.D. from DMSRDE, Kanpur University, followed by highly productive postdoctoral and research appointments at National Tsing Hua University (Taiwan) and the Leibniz Institute of Polymer Research Dresden (Germany). His research spans self-assembly in block copolymers and supramolecular systems, polymer crystallization under confinement, electrospinning and nanostructured fibre fabrication, organic–inorganic hybrid nanofibres, and structure–property relationships in advanced polymeric materials, supported extensively by small-angle scattering techniques. Dr. Nandan's work has led to over 73 journal publications, more than 70 conference papers, several patents, and impactful contributions in areas such as polymer nanotemplates, block copolymer morphologies, hybrid nanofibre architectures, and confined crystallization phenomena. His innovative studies have been featured in leading journals including ACS Applied Materials & Interfaces, Angewandte Chemie, Soft Matter, PCCP, Journal of Colloid and Interface Science, and Advanced Functional Materials. He has been honoured with the Hitachi Best Paper Award, a Gold Medal for academic excellence, the Award of Honor at GJUST Hisar, and inclusion in Marquis Who's Who in Science and Engineering. With a strong international research footprint and expertise across polymer nanostructures, fibre science, catalysis-related materials, and functional nanofibres, Dr. Nandan continues to advance fundamental science and application-driven innovation in textile materials, nanotechnology, and polymer engineering.

FUNCTIONALIZED TEXTILE BASED ELECTRODE MATERIALS FOR LITHIUM SULFUR BATTERIES

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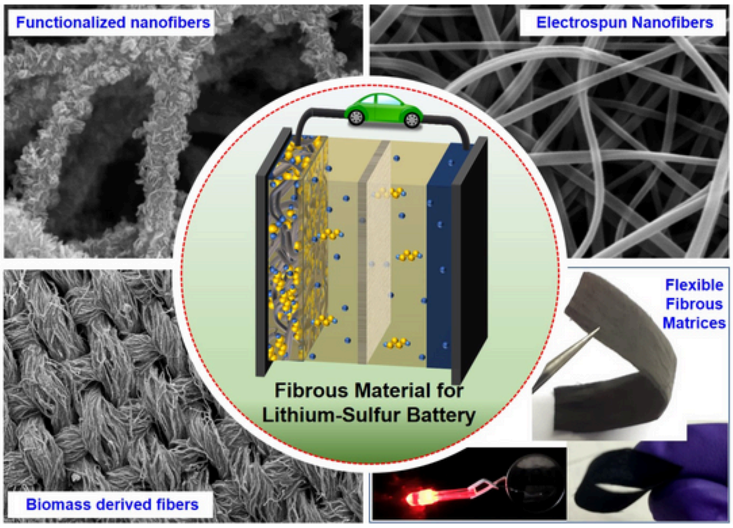
Abstract

The overconsumption of global energy resources to meet the rapid industrial growth and technological advancement have led to the search for clean energy alternatives to supplant the fossil fuels. In this direction, electrochemical energy storage systems such as Lithium based batteries and supercapacitors have attracted significant attention in last few years. Furthermore, the focus on increasing the energy/power densities of these electrochemical devices has catalyzed the search for novel active materials as well as their rational design. Here, fibre/textile based functional fibrous materials are being increasingly considered for designing the required components of these devices. The fact that the fibrous materials have high surface area, could be easily functionalized and fabricated in a variety of shapes further enhances the utility of these materials in energy storage devices. Moreover, with increasing attention on wearable electronics, the use of fibrous materials readily helps in fabricating energy storage devices which could be integrated with wearables. In this talk, the focus will be on the work done by our research group in fabricating such functional fibrous materials for sustainable and flexible electrode materials for Lithium Sulfur bateries. The talk will also focus on the utilization of biomass-based fibres for designing such functional fibrous materials which provides a more sustainable route for the materials required in electrochemical energy storage systems.



Keywords: Fibrous materials, Lithium sulfur battery, energy storage

INVITED SPEAKER

Prof. Oomman K. Varghese

Dr. Oomman K. Varghese is a Professor in the Department of Physics at the University of Houston, where he heads the Nanomaterials and Devices Laboratory. He completed his Ph.D. in Physics at the Indian Institute of Technology Delhi (IIT Delhi). Dr. Varghese's research is dedicated to designing and developing nanostructured inorganic and carbon-based materials — especially sustainable, earth-abundant and environmentally friendly materials — for applications in solar energy conversion, solar-fuel generation, environmental sensing, and medical/clinical diagnostics. His work aims at using nanoscale architectures to overcome limitations in cost, toxicity and scalability, while enabling clean energy solutions (e.g., hydrogen generation, CO_2 recycling to fuels) and accessible environmental and health-related sensors. On the recognition front, Dr. Varghese has received several honours: he was ranked 9th in the 2011 list by Thomson Reuters of "World's Top 100 Materials Scientists in the Past Decade."

He has also been named a "Highly Cited Researcher" (i.e. among the top 1% by citation) in 2014 and 2015 by Thomson Reuters, and his name appeared among the "World's Most Influential Scientific Minds" in those years. Beyond research, his professional activities include serving as Associate Editor, Research for a journal published by the American Association for the Advancement of Science (AAAS) / Science Partner Journal, and as Honorary Editor of the Journal of Nanomedicine Research. He is a member of several major professional societies: the American Physical Society (APS), the Materials Research Society (MRS), and the Institute of Electrical and Electronics Engineers (IEEE) — reflecting his interdisciplinary engagement across physics, materials science and device engineering.

INVITED SPEAKER

Prof. Eswaraiah Varrla

Dr. V. Eswaraiah is an Assistant Professor in the SRM Research Institute and the Department of Physics and Nanotechnology at SRM Institute of Science and Technology, Kattankulathur, where he has been a faculty member since 2017. With more than eleven years of post-PhD research experience, he leads a group focused on developing energy-efficient, scalable production and advanced processing techniques for low-dimensional materials — particularly graphene and other 2D materials — for applications in sensing, printed and flexible electronics, polymer nanocomposites, thermal management, energy generation and conversion, and solution-processed electronic materials. His research has contributed significant advances to the high-yield production, surface engineering, and device integration of 2D materials, and his group has reported important findings in graphene processing, including three co-invented technologies in graphene synthesis and strain-sensor nanocomposites. His scientific interests span sustainable manufacturing routes, green hydrogen technologies, self-assembly of nanomaterials, thermal interface materials, and the development of next-generation flexible and energy devices using environmentally benign processes. Through a combination of fundamental materials design and application-driven device development, Dr. Eswaraiah's work aims to accelerate the translation of sustainable nanomaterials into real-world technologies across electronics, energy, and advanced composites.

LIQUID-EXFOLIATED TWO-DIMENSIONAL NANOSHEETS: ENERGY EFFICIENT APPROACHES AND SELF-ASSEMBLY PROCESSES

ESWARAIAH VARRLA

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Abstract

Two-dimensional materials are highly versatile in composition, bonding characteristics and exhibit layer dependent physical properties with wide range of thermal stabilities. For example, the thermal conductivity of single layered graphene with 100% Carbon is ~3000 W/mK whereas thermal conductivity of single layered phyllosilicate nanosheet with multiple elements with different oxidation states is <0.1 W/mK. Recently we have developed a sustainable and liquid-phase exfoliation and stabilization of series of two-dimensional nanosheets from bulk layered materials using natural surfactants in aqueous media. The exfoliated nanosheets are characterized by microscopy and spectroscopy techniques. Delamination of vermiculite yields thermally insulating nanosheets that, when incorporated into epoxy matrices, form nanocomposite coatings exhibiting excellent fire-retardant properties on wood and polymer substrates, including flame self-extinguishing exhibiting V_0 rank, reduced flame spread, decreased thermal degradation, and minimal toxic smoke release. Hexagonal boron nitride (h-BN) nanosheets, produced with high yield as well-dispersed fillers for thermal interface materials for cooling electronic devices. Biopolymer-modified h-BN nanosheets dispersed in silicone oil yield non-curing thermal compounds with improved filler dispersion and reduced Kapitza resistance, achieving thermal conductivity as high as 1.16 W m-1 K-1 at 50 wt%. Liquid-phase exfoliated molybdenum disulfide (MoS_2) nanosheets stabilized by natural surfactant achieve aqueous dispersions that exhibit superior aqueous lubricant performance, notably reducing friction and wear significantly, at optimized low filler contents. These energy efficiency approaches and indigenous solid precursors show enormous potential for scaling 2D materials in large scale. Collectively, these studies illustrate multifunctional 2D nanosheet-based composites for advanced fire retardancy and thermal management applications. I will briefly discuss about our latest results in self-assembly of 2D nanosheets for developing tiled thin-films of individual sheets at micron-nanoscale.

Keywords: Graphene; 2D Materials; Exfoliation; Energy Efficiency.

INVITED SPEAKER

Prof. Pabitra K. Nayak

Dr. Pabitra K. Nayak is the Principal Investigator at the Tata Institute of Fundamental Research – Hyderabad (TIFR-Hyderabad), where he leads a highly interdisciplinary research program in advanced optoelectronic materials, with a strong focus on organic, inorganic, and hybrid halide perovskites. He earned his Ph.D. in Natural Sciences from TIFR Mumbai in 2009, following an M.Sc. and B.Sc. in Chemistry from Utkal University, and went on to build an internationally distinguished career through postdoctoral fellowships at the Weizmann Institute of Science (2010–2013) and at the University of Oxford (2014–2015), later serving as a Marie Skłodowska-Curie Fellow (2015–2017) and Group Leader in Oxford's Department of Physics (2017–2019). Dr. Nayak's research spans fundamental photophysics, charge transport, exciton dynamics, defect physics, energy-loss mechanisms, and device-limiting phenomena in emerging semiconductors, leading to influential contributions on perovskite structure–property relationships, ion migration, ultrafast exciton processes, electronic coupling at hybrid interfaces, and performance limits in photovoltaic technologies. He has authored numerous high-impact publications in Nature Reviews Materials, Nature Communications, Energy & Environmental Science, Advanced Materials, JACS, ACS Photonics, PRB, and the MRS Bulletin, including widely cited perspective articles and multiple Research Highlights for the Materials Research Society. His work continues to shape the global understanding of next-generation solar materials, optoelectronic devices, and fundamental excitonic processes, positioning him as one of the leading contributors to modern perovskite science.

DOPING OF SOFT SEMICONDUCTORS FOR STABLE AND EFFICIENT OPTOELECTRONICS

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Abstract

Organic conjugated compounds and halide perovskite materials are driving progress in low-cost optoelectronics. To expand their use, electronic doping is crucial. Typically, molecular and metal complex dopants are employed, but their high costs, limited efficiency, and stability issues necessitate alternative approaches. We have thus developed a variety of dopants suitable for numerous organic semiconductors, enabling effective and durable doping of organic transport layers in perovskite devices. We also showcase how this innovative doping technique can be applied in metal halide perovskite solar cells, organic thin-film transistors, and organic light-emitting diodes.

INVITED SPEAKER

Prof. Arihant Bhandari

Arihant Bhandari was a bachelor student at Indian Institute of Technology Kanpur (IITK) from 2009-2013. He got a patent and best B.Tech. project award for making an enhanced water purification system based on solar still. He also got a doctorate (Ph.D.) from IITK on simulation of electrochemical energy storage in Li-ion batteries. He was a postdoctoral research fellow (2019-2024) of the multiscale modelling project (batterymodel.co.uk) of the Faraday Institution (faraday.ac.uk), a consortium of 27 UK universities and 50 companies for electrochemical energy storage research. There he developed theory and software tools for multiscale simulations and demonstrated its applications in designing better energy materials. He joined the department of Energy Science and Engineering at IIT Delhi in 2024. He is interested in multiscale simulations at electronic, atomistic, microscopic and macroscopic length and time scales. The research group is open to all interested in interdisciplinary research at the intersection of various subjects including engineering, physics, materials, chemistry and high-performance computing.

Research Interests: Energy conversion and storage, Multiscale modelling, Li-ion batteries, Atomistic simulations, Density Functional Theory, Electrochemistry, high-performance computing

SIMULATIONS OF FEW-LAYER GRAPHENE-BASED ELECTRODES FOR ELECTROCHEMICAL ENERGY STORAGE

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Abstract

Electrochemical devices such as supercapacitors can store charge in the electrode as well as in the electrode-electrolyte interface. The electrons are stored in the empty bands of electrode while the electrolyte ions are stored in the form of electric double layer at the interface. The number of electrons transferred to the electrode depends on the applied potential. As the charge is stored on the electrode, there is a build-up of opposite charge in the electric double layer. We develop a novel grand canonical model to simulate charge storage in such electrochemical devices under potential control. The electrons are modelled using density functional theory, while electrolyte ions are modelled using Poisson-Boltzmann theory. The method is demonstrated for few-layer graphene-based electrodes. The predicted differential capacitance agrees well with experimental measurements.

Charge storage in Li-ion batteries (LIBs) requires intercalation of Li^+ ions in the layers of electrodes (apart from the above processes). While intercalation is the desired reaction in a Li-ion battery, often surface deposition of Li^+ ions and their reduction to metallic Li (Li plating) is found to occur at similar voltages. Li plating leads to loss of reversible capacity and formation of dendrites which can cause short-circuit and fires, thereby posing a significant safety hazard. We apply our novel grand canonical model to study Li plating on graphite anode under potential control for identifying conditions which lead to onset of Li plating and recommend measures for safe operation of LIBs.

INVITED SPEAKER

Dr. Suraj Soman

Dr. Suraj received his Ph.D. from Dublin City University, Ireland, and pursued postdoctoral research at Caltech and Michigan State University, USA. He joined CSIR-NIIST in 2014 and currently serves as a Senior Scientist at the Centre for Sustainable Energy Technologies (C-SET). His research focuses on the indigenous development of indoor solar cells using third-generation molecular light-harvesting technologies such as dye-sensitized and perovskite solar cells, aiming to replace one-time use primary batteries realizing self-powered gadgets. He established a state-of-the-art indigenous dye solar module manufacturing facility at CSIR-NIIST and has authored over 50 publications as corresponding author in this area. He has also developed innovative self-powered products integrating the indoor solar cells made indigenously at NIIST, which are undergoing field trials at various locations. Dr. Suraj is a recipient of several prestigious awards, including the Solar Challenge Award (2023), CSIR Young Scientist Award (2020), INSA Medal for Young Scientist (2020), Kerala State Young Scientist Award (2018) and BRICS Young Scientist Award (2017).

FROM LIGHTBULBS TO LIFELINES: POWERING THE FUTURE WITH INDOOR LIGHT

SURAJ SOMAN, SENIOR SCIENTIST

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Abstract

In the realm of third-generation molecular light-harvesting technologies, our focus is on efficiently capturing and recycling diverse light sources, including indoor, artificial, ambient and diffused sunlight using custom engineered dye-sensitized solar cells (DSCs). DSCs stand out for their high efficiency, exceeding 40%, and their suitability for indoor use due to their lower cost, stability and ease of production.1-2 Recent innovations, such as co-sensitization approach, introduction of dual-species copper-based electrolytes replacing traditional iodide systems, use of bilayer TiO2-ZnO nanostructured electrodes, have addressed recombination issues, enhancing performance of these innovative nano-photovoltaic devices under indoor and ambient lighting conditions.1-4 These advancements not only improve efficiency but also promote environmentally friendly practices, positioning DSCs as a viable option to replace conventional one-time-use primary batteries for powering electronic devices, facilitating self-powered applications thereby reducing the carbon footprint.

My presentation will highlight CSIR-NIIST's pursuit of self-reliance in indoor light-harvesting technologies underscored by advancements in the domain of DSCs and the fascinating lab to land transition being realized developing indigenous scale-up production equipment's, innovative self-powered products over the past decade in my research lab at CSIR-NIIST. At NIIST, our endeavors extend to the custom design and optimization of these indoor light harvesters, utilizing tailor-made molecules, materials, and device architectures realizing efficiencies of 40% and above. By nurturing capabilities, CSIR-NIIST strives to establish a formidable position in the global indoor photovoltaic landscape, and propelling India towards self-sufficiency in emerging photovoltaic sectors.

INVITED SPEAKER

Prof. Deepak Kumar

Dr. Deepak Kumar is a Professor in the Centre for Automotive Research and Tribology (CART) at IIT Delhi, with a progressive academic career at the institute from Assistant Professor (2013–2018) to Associate Professor (2018–Feb 2022) and Professor (March 2022–present); prior to joining IITD he was a Postdoctoral Fellow at ETH Zurich (2011–2013) and a Research Associate at IISc Bangalore (2010–2011). He earned his Ph.D. in Mechanical Engineering from the Indian Institute of Science, Bangalore (2005–2010) after completing an M.Tech. in Metallurgical & Materials Engineering at IIT Roorkee (2003–2005) and a B.Tech. in Production Engineering from G.B. Pant University (1996–2000). His research spans energy-storage materials, tribology, surface and interface analysis, environmentally friendly lubricants (metalworking fluids and nanocomposite greases), wear- and corrosion-resistant coatings, and light metals and alloys; he leads and has led numerous industry- and government-funded projects (including SERB DST, BRNS DAE, CSIR, FIRP IRD IITD and industry partnerships with Schlumberger, Bharat Forge, LG Soft, Stanvac and RITES) on thermal-sprayed and HVOF/ HFFS coatings, nano-greases, high-entropy alloy coatings, and tribo-materials for transportation and industrial applications. Dr. Kumar's scholarly output includes several journal articles and extensive conference contributions on topics such as HVOF and hybrid ceramic coatings, eco-friendly greases from vegetable oils and natural emulsifiers, rGO-doped alumina coatings, Mg and Al alloy composites, and tribo-mechanisms in zirconium and steel systems; his doctoral work and subsequent research have earned him recognitions including the Young Faculty Fellowship at IIT Delhi (Kusuma Trust) and the Prof. B. K. Subba Rao Medal for best Ph.D. thesis in Mechanical Engineering at IISc (2010–2011). He is also the author (with S. K. Biswas) of the book Nanotribology of Emulsified Lubricants (LAP, 2011) and routinely presents at major international forums such as the World Tribology Congress, ICMCTF and IndiaTrib, translating fundamental studies in surface science into practical solutions for wear mitigation, sustainable lubricants, and advanced protective coatings.

CO-UTILIZATION STRATEGY-BASED NANO-COMPOSITE GR-SI ANODE FOR LI-ION BATTERY

BHAVYA NIDHI VATS AND DEEPAK KUMAR

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Abstract

Capacity fading in Li-ion batteries is a significant issue typically arising from the substantial volume changes occurring during lithium insertion and extraction. This issue is particularly pronounced for silicon, which, despite its high theoretical capacity of 4200 mAh/g, experiences significant volume fluctuations. This can lead to physical damage, such as cracking and crumbling of the silicon electrode, ultimately compromising its structural integrity and reducing capacity over time. To address these challenges, nanostructured electrode materials gained significant attention. Unlike bulk silicon, these materials offer advantages such as a high surface area, enhanced mechanical strength, and improved electrical conductivity. These properties facilitate better ion transport, increase electrode/electrolyte contact, and enhance overall charge/discharge performance. However, there are some disadvantages, such as a more complex synthesis process for the nanostructured material. Therefore, a critical challenge is to synthesize these materials with efficient and economical methods that reduce both time complexity and cost. This study reports the developed a core-shell structure nanoparticles; silicon as the core and titanium dioxide (TiO_2) as the shell. This core-shell (Si@TiO_2) material was used as reinforcement to graphite to develop the composite anode in a 2016-coin cell configuration. The material and structural characterization (FESEM, TEM, XRD) confirm the elemental composition and validate the structural integrity of the core-shell material. The Si@TiO_2 anode achieved an initial specific capacity of 2213 mAh/g with 55% capacity retention after 100 cycles and showed a 37% improvement over bare silicon. The developed material can effectively absorb and manage the stresses induced by volume fluctuations, thereby preserving the overall integrity and stable performance of the electrode.

INVITED SPEAKER

Dr. Bhumika Choudhary

Dr. Bhumika Chaudhary, Senior Researcher, University of Turku, Finland, pursued her master's degree from the Indian Institute of Technology (IIT), Roorkee in chemistry and Ph.D. at the Interdisciplinary Graduate School, Energy Research Institute (ERI@N), Nanyang Technological University (NTU), Singapore on perovskite photovoltaics. Later, she worked on photon-up conversion application at the Agency for Science, Technology, and Research, Singapore. She has also worked as a postdoc researcher at the Institute for Photovoltaics, University of Stuttgart, Germany on slot die coating of perovskite for large area fabrication and in-situ thermal stability via X-ray diffraction. Her research interest includes materials development, thin film/device fabrication, and characterizations for optoelectronic applications. Her technical background is in chemistry and materials science, and her research is interdisciplinary, where she searches for novel and feasible solutions for efficient optoelectronics devices. Outside of research, she likes doing sports (running, playing badminton etc.), volunteering, and public speaking.

STRUCTURALLY TUNABLE PEROVSKITE FOR STABLE THIN FILM OPTOELECTRONICS

BHUMIKA CHOUDHARY, SENIOR RESEARCHER

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Abstract

The Organic-Inorganic Halide Perovskite (OIHP), with many salient optoelectronic properties, has gained enormous attention for various applications such as solar cells, LED, photodetector, laser, and sensors etc. Despite possessing excellent optoelectronic properties, the perovskite material still needs to overcome the challenge of long-term stability, which is the primary hurdle to obtaining stable and scalable photovoltaic devices. In the highlight of the current challenges, this talk will include the research background regarding the role of structural dimensionality in influencing the stability and optoelectronic properties of perovskites. Based on this, the choice of novel strategies to boost the perovskite stability and optoelectronic properties will be discussed. Furthermore, the talk would emphasize the role of interfacial, solvent, and dimensional engineering in altering the structural and morphological properties, which thus impacts the degradation and properties of the perovskites. Finally, the talk will underline the future perspectives for next generation stable perovskite thin film optoelectronics.

INVITED SPEAKER

Prof. Vanchiappan Aravinda

Dr. Vanchiappan Aravindan is an Associate Professor at the Indian Institute of Science Education and Research (IISER) Tirupati, where he leads a research program focused on scalable synthesis and application of low-dimensional and carbonaceous materials for next-generation energy storage and conversion. Since joining IISER Tirupati (Assistant Professor, 2017–2023; Associate Professor, 2023–present), Dr. Aravindan's work has centered on high-performance supercapacitors, Li- and Na-ion batteries and hybrid/ion-capacitor systems, with particular strengths in biomass-derived carbons, graphene/reduced-graphene oxide architectures, ternary metal-selenide and metal-nitride nanosheets, conversion–insertion electrode chemistries, solid-state and composite electrolytes, and strategies for reuse and recycling of spent Li-ion battery materials. His group develops solution- and carbothermal-based routes to produce electrode and electrolyte materials at scale, investigates structure–property relationships that govern capacity, rate and cyclability, and translates these findings into flexible and solid-state device prototypes with improved energy and power density. Dr. Aravindan's publications span high-impact journals and collaborative, multidisciplinary teams (including international partners), addressing practical challenges such as long-cycle durability, electrode/electrolyte interface engineering, and circular-economy approaches to battery materials—positioning his lab at the intersection of materials chemistry, electrochemistry and sustainable energy technology.

HYBRID CATHODES FOR LI-ION BATTERIES FROM RECYCLING

VANCHIAPPAN ARAVINDAN

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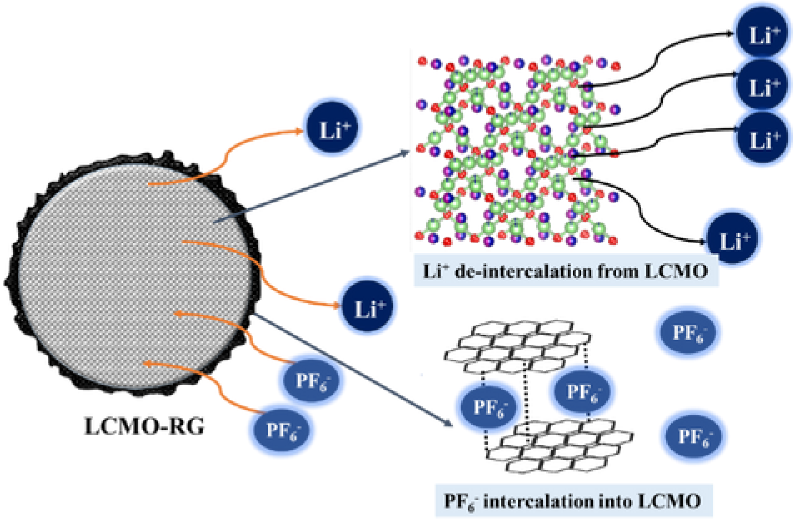
Abstract

With increasing environmental concerns, spent lithium-ion batteries (LIBs) have attracted significant attention, prompting the investigation of various metal oxide crystal structures and a range of carbon-based materials as affordable alternatives to conventional components, particularly for energy storage applications. Graphite, long established as the standard anode material in LIBs, continues to see growing demand regardless of the cathode chemistry used. The rise of graphene-related technologies has further boosted global graphite consumption, underscoring the urgent need for sustainable sources of battery-grade graphite. Despite graphite's essential role, most industrial recycling methods for spent LIBs fail to recover it, missing a valuable opportunity. Recycling graphite not only decreases dependence on virgin raw materials but also allows its reuse in manufacturing new LIBs. Recovered graphite has demonstrated excellent electrochemical performance when used as a cathode in dual-ion batteries. Furthermore, when combined with high-voltage cathode materials (>4.5 V vs. Li) such as $LiNi_{0.5}Mn_{1.5}O_4$ and $LiCoMnO_4$, the graphite electrode can undergo partial or full anion intercalation and extraction, diverging from its typical lithium insertion and extraction behavior seen with lithiated components. Additionally, full-cell designs have been developed using $Li_4Ti_5O_{12}$ as the anode, including configurations that omit the anode entirely—known as anodeless cells.



Keywords: Recycling; Li-ion Battery; Hybrid Cathodes; Graphite; Anion-intercalation

INVITED SPEAKER

Prof. Rashi Kedia

Dr. Rashi Kedia is an Assistant Professor at the Amity Institute of Nanotechnology, Amity University Uttar Pradesh, specializing in nanoscience, nanotechnology, and energy materials. She earned her Ph.D. from CSIR–National Physical Laboratory (AcSIR) in 2024 and subsequently completed a Postdoctoral Research Fellowship at Chung-Ang University, Seoul (2024–2025). She has been awarded prestigious national fellowships, including the CSIR-JRF (2020–21) and CSIR-SRF (2022–24), and received international travel grants from SERB and CSIR for presenting her work at PSCO-2023 (Oxford, UK) and IPEROP-24 (Tokyo, Japan). In 2025, she was honored as a DST-INSPIRE Faculty Awardee and represented India at the 74th Lindau Nobel Laureate Meeting (Chemistry). Her teaching portfolio includes Nanoscience and Nanotechnology as well as Nano Chemistry, with broader interests in Chemistry and advanced nanomaterials. Her research focuses on organic solar cells, energy applications, conductive polymers, and solution-processed device interfaces. Dr. Kedia has published over 15 papers in leading journals such as ACS Applied Polymer Materials, Journal of Materials Chemistry A, ACS Sensors, and Energy Advances, and has contributed to one funded research project. She has received several accolades, including second prizes at CSIR-NPL's National Science Day 2023 and the 76th Foundation Day Poster Competition, and a third prize at National Science Day 2022. Her work continues to advance modern material architecture, optoelectronics, and sustainable energy technologies.

SOLVENT-FREE DEPOSITION OF COPPER(I) THIOCYANATE THIN FILM: A SUSTAINABLE APPROACH FOR THE HOLE TRANSPORT LAYER IN PEROVSKITE SOLAR CELLS

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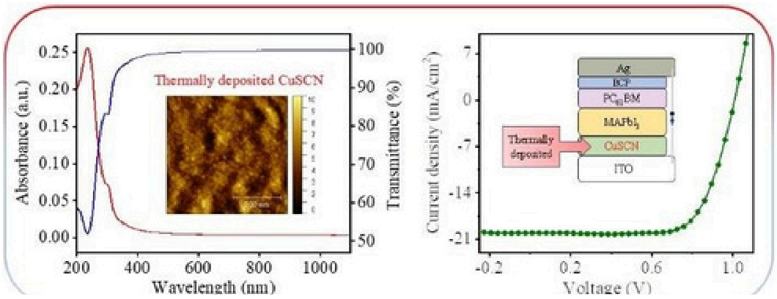
Abstract

Copper(I) thiocyanate (CuSCN) is an air-stable and inexpensive material that has been widely used as a hole transport layer (HTL) in perovskite solar cells. For CuSCN thin film as a HTL, the various deposition methods such as doctor blading, electrodeposition, spin coating, and spray coating have been widely reported in the literature. However, the commonly used solvents for its solution-processable deposition often have unpleasant smell, are toxic and inadvisable to use in glove-box, which can restrict their possible practical applications in the upcoming future. To address this issue, herein, we report thermally deposited CuSCN thin film as an alternative and solventless approach to the conventional solution-processed methods for the HTL in inverted perovskite solar cells.

In this work, the thermal deposition of CuSCN, a solvent-free and sustainable approach have been reported for the fabrication of CuSCN thin film as an HTL on ITO surface. The structural, electrochemical, optical, and morphological properties of the CuSCN films were characterized. The effect of CuSCN film thicknesses (20, 30, 40, 60, and 100 nm) and annealing temperatures (RT, 50, 100, 150, and 200 °C) of CuSCN films on the photovoltaic performance were investigated. The optimized device configuration ITO/CuSCN/$MAPbI_3$/PC61BM/BCP/Ag with 30 nm thin CuSCN film annealed at 100 °C for 10 min exhibits the maximum power conversion efficiency (PCE) of 15.71% with Voc = 1.01 V, Jsc = 20.2 mA/cm2, and FF = 0.77. For reference, perovskite solar cells without HTL have been also fabricated simultaneously. Importantly, the thermally deposited CuSCN based devices show the excellent reproducibility and stability up to 240 h with ∼89% retention of the initial PCE. This study demonstrates a new methodology for obtaining the better CuSCN thin film by thermal deposition technique for efficient, sustainable and scalable electronic device applications.



Keywords: CuSCN, Thermal deposition, Hole transport layer, Perovskite solar cells

INVITED SPEAKER

Prof. Abhishek Sarkar

Abhishek received his B.Tech (2014) and M.Tech (2016) in Metallurgical and Materials Engineering from NIT Durgapur and IIT Madras, respectively. He pursued his master's thesis at Karlsruhe Institute of Technology (KIT), Germany, availing the DAAD-IIT Master Sandwich fellowship. Subsequently, he was employed as a doctoral research associate jointly between KIT and Technical University (TU) Darmstadt, Germany, and received his Ph.D. from TU Darmstadt in 2020. He continued as a postdoc at KIT and TU Darmstadt until 2023. During this time, he also spent 4 months as a visiting scientist at the University of California (UC) Irvine, USA. Following this, he joined the Department of Metallurgical and Materials Engineering at IIT Kharagpur as an Assistant Professor in September 2023. He moved to the Department of Materials Science and Engineering at IIT Delhi as an Assistant Professor in April 2024.

His research work focuses on functional ceramics. His main research contributions have been to the development of the emerging field of high entropy oxides (HEOs), which includes discovering new HEO classes, identifying the unique magneto-electronic phase separation in HEOs, and importantly, establishing the use of HEOs as electrodes for Li-ion batteries. The topics of his current interest are: (a) Electrode design of Li-ion and post-Li batteries, (b) Design and phase stability of HEOs, (c) Effect of chemical disorder on magneto-electronic properties of complex oxides, and (d) Electrochemistry-driven tuning of magnetic properties in materials.

HIGH ENTROPY OXIDES: OPPORTUNITIES AND CHALLENGES

ABHISHEK SARKAR

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Abstract

High entropy oxides (HEOs) represent an emerging class of single-phase oxide solid solutions consisting of multiple cations in near-equiatomic proportions occupying a specific sub-lattice. HEOs were first reported in 2015, and over the last five years, the field has witnessed rapid growth. Within the framework of our research work, we have addressed several fundamental and applied aspects of HEOs, which have been pivotal in the development of this research topic. This presentation will initially focus on the discovery of HEO classes (and compositions), and their diverse synthesis and thin-film fabrication routes. The extensive compositional flexibility of HEOs offers the possibility to tailor a plethora of functionalities. In this context, initial case studies pertaining to three unique/improved functionalities of HEOs such as enhanced electrochemical cyclic stability, tunable optical properties, and exotic magneto-electronic properties, will be presented. While these opportunities hold potential for future applications, researchers working on HEOs face multiple challenges in terms of precisely identifying the local atomistic features of HEO in single-crystal thin films. Hence,some of the possible approaches to tackle these challenges will be discussed. In summary, the presentation will provide an overview of the versatility of the multicomponent high entropy-based design approach for engineering the structure and properties of oxide systems.

Keywords: Single-phase stabilization; Energy storage; Magnetoresistance; Single-crystal films

INVITED SPEAKER

Dr. Ashish Kulkarni

Dr. Ashish Kulkarni is an Assistant Professor in the Department of Chemistry at the Indian Institute of Technology (IIT) Tirupati, India. He specializes in the field of halide perovskite solar cells, focusing on the development of both lead-based and lead-free perovskite materials for next-generation photovoltaic technologies.

Dr. Kulkarni earned his Integrated Master of Science (M.Sc.) in Chemistry from the Indian Institute of Technology (IIT) Roorkee, India, and completed his Ph.D. under the supervision of Prof. Tsutomu Miyasaka, the inventor of perovskite solar cells, at Toin University of Yokohama, Japan. His doctoral work centered on lead and lead-free halide perovskite solar cells, combining fundamental materials chemistry with applied photovoltaic research.

Following his Ph.D., Dr. Kulkarni gained extensive international research experience. He served as a JSPS Postdoctoral Fellow at Toin University of Yokohama, and later as a Postdoctoral Scientist at Forschungszentrum Jülich GmbH, Germany, working with Prof. Thomas Kirchartz and Prof. Michael Saliba on advanced perovskite optoelectronic materials. He also held a DAAD PRIME Fellowship (2023–2024), conducting research with Prof. Sanjay Mathur at the University of Cologne, Germany, and Prof. Shahzada Ahmad at the Basque Center for Materials, Applications and Nanostructures, Spain.

His research contributions have been recognized through several prestigious awards, including the Japan Society for the Promotion of Science (JSPS) Fellowship (2017–2019), the “Emerging Young Scientist Award” from the Materials Research Society of Japan (2017), and the Best Research Article Award from the Bulletin of the Chemical Society of Japan (2018).

At IIT Tirupati, Dr. Kulkarni continues to advance research in perovskite photovoltaics, materials design for sustainable energy conversion, and nanostructured semiconductor systems, contributing to the global pursuit of efficient and eco-friendly solar energy technologies.

INSULATING METAL OXIDE AND SELF-ASSEMBLED MONOLAYER INTERFACE FOR EFFICIENT PEROVSKITE SOLAR CELLS

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Abstract

Perovskite solar cells (PSCs) have shown rapid rise in power conversion efficiency owing to their interesting optoelectronic properties such as diffusion length, low exciton binding energy, tuneable bandgap, and ambipolar charge mobility. Among various device structures, p-i-n structured device employing self-assembled monolayer (SAM) as hole transport layer is promising as all the device stack layers can be deposited at low temperature and is also suitable for silicon-perovskite tandem solar cells. However, device incorporating SAM suffers from hydrophobic issue and prohibits the uniform perovskite layer formation (at the perovskite SAM interface). This talk will present strategy to overcome the aforementioned issue by incorporating the insulating metal oxide layer at the interface of SAM and perovskite. This metal oxide layer acts as scaffold to promote uniform perovskite layer formation on top of the SAM. Interestingly, spectroscopic studies reveal that SAM layer has a strong tendency to bind with the metal oxide layer, thereby, interfacing directly with the perovskite layer while simultaneously promoting uniform perovskite layer formation. As a result of this, solar cell incorporating low bandgap (Eg = 1.53 eV) perovskite with a composition of $FAPbI_{3-x}Br_x$ delivered a power conversion efficiency of ~23% with high stability. The present talk will discuss the insights into the SAM/metal oxide (SAM)/perovskite interface and highlights the underlying mechanism of promoting a uniform perovskite layer. The present strategy is universal as it helps in obtaining a uniform perovskite layer with enhanced crystallinity with different SAMs which have different symmetry and orientations.

Keywords: Perovskite, solar cells, self-assembled monolayer, high efficiency

INVITED SPEAKER

Prof. Raju Kumar Gupta

Prof. Raju Kumar Gupta is a Professor of Chemical Engineering at the Indian Institute of Technology (IIT) Kanpur), India. His research focuses on photocatalysis, green nanomaterials synthesis, perovskite solar cells, supercapacitors, and electrospun nanocomposites for energy and environmental applications.

He earned his B.Tech. in Chemical Engineering from IIT Roorkee (2005) and Ph.D. from the National University of Singapore (2010). His group develops hybrid nanostructures for sustainable energy and clean water solutions, emphasizing charge transport, film formation, and device stability in perovskite-based systems.

Prof. Gupta is a Fellow of the Royal Society of Chemistry and recipient of several honors, including the Distinguished Alumnus Award (IIT Roorkee, 2021), P.K. Kelkar Fellowship, DST Inspire Faculty Award, and Young Engineer Award. He serves on the Advisory Board of RSC's Molecular Systems Design & Engineering and the Editorial Board of IET Nanodielectrics.

NASICON-BASED ELECTROLYTES FOR SOLID-STATE SODIUM-ION BATTERIES

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Abstract

Solid-state batteries (SSBs) are attracting increasing attention as promising alternatives to conventional liquid-based systems due to their superior safety. NASICON-type (Sodium Superionic Conductor) materials are promising solid electrolytes for solid-state sodium-ion batteries owing to their high ionic conductivity, excellent chemical stability, and wide electrochemical window. In this talk, I will present our group's recent work over compositional tuning, aliovalent doping, and microstructural optimization strategies for enhancing the electrochemical performance of NASICON electrolytes. NASICON-type solid-state electrolytes were synthesized with various dopants (e.g. Ru, V, Ta etc.), achieving ionic conductivities in the order of mS cm^{-1} at room temperature. Using theoptimized cathode and solid-state electrolyte, solid-state sodium ion batteries were fabricated in 2032 coin-cell configurations. The assembled cells demonstrated an initial discharge capacity of 85 mAh g^{-1} at 0.5 C and 55 mAh g^{-1} at 1 C, along with excellent long-term stability, retaining over 80% of their capacity after 1000 cycles at 0.5 C. Further, to address the poor interfacial contact typically associated with rigid ceramic electrolytes such as NASICON, flexible solid polymer electrolytes were developed using polyethylene oxide (PEO) as the polymer matrix and doped NASICON as a ceramic filler. While pure PEO exhibits a low room-temperature ionic conductivity (~10^{-7} S cm^{-1}), the composite electrolyte achieved enhanced conductivity (~10^{-4} S cm^{-1}) due to improved ion-conduction pathways at the polymer–ceramic interfaces. This design improves mechanical flexibility, electrode compatibility, and overall electrochemical performance, paving the way for high-performance sodium-ion solid-state batteries.

Keywords: NASICON electrolyte, Solid-state sodium-ion battery, Ionic conductivity, Aliovalent doping

INVITED SPEAKER

Dr. Saurabh Kumar Pandey

Dr. Saurabh Kumar Pandey is an Associate Professor in the Department of Electrical Engineering at the Indian Institute of Technology (IIT) Patna), where he has been serving since 2015 (Assistant Professor: 2015–2023; Associate Professor: 2023–present). He previously held academic positions at the National Institute of Technology (NIT) Hamirpur, the Military College of Telecommunication Engineering, and S.V.I.T.S. Indore. His research focuses on semiconductor device modeling, perovskite and double perovskite solar cells, resistive switching devices (memristors), nanoelectronics, and optoelectronic sensors. Dr. Pandey has published extensively in leading journals such as IEEE Transactions on Electron Devices, IEEE Journal of Photovoltaics, Applied Materials Today, and Energy Technology, contributing over 100 high-impact papers on topics including eco-friendly solar cells, memristor-based neuromorphic systems, and thin-film optoelectronics. He has also co-authored several book chapters published by Springer. A Senior Member of IEEE, he is actively involved in numerous professional societies, including ISTE, IAAM, IETE, OSA, and IEEE Nanotechnology Council. Dr. Pandey has delivered invited lectures at prestigious institutes such as IITs, NITs, and international conferences, and received numerous recognitions including the Albert Nelson Marquis Lifetime Achievement Award, Best Research Paper Awards, and selection for the BRICS Young Scientist Conclave. His research group at IIT Patna focuses on developing sustainable electronic and photonic materials for next-generation energy and neuromorphic computing technologies.

NUMERICAL SIMULATION OF BISMUTH-BASED HIGHLY EFFICIENT ECO-FRIENDLY PEROVSKITE SOLAR CELL

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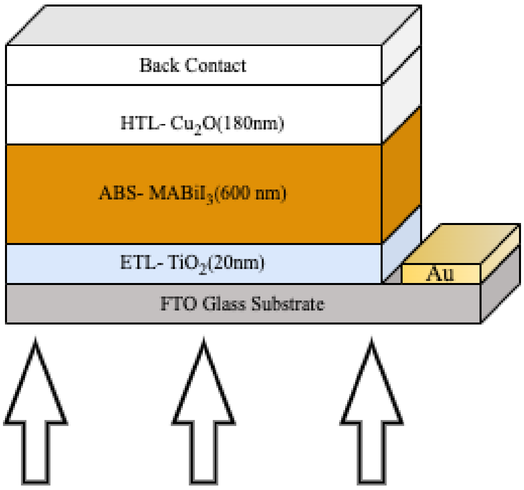
Abstract

In last few decades, with the advancement of technology, Perovskite solar cell have gained attention with substantial application-oriented research. This work focuses on comprehensive numerical modelling and analysis of an efficient lead-free perovskite-based solar cell (PSC) using device simulation software. Rigorous theoretical investigation has been performed for optimization of device parameters more specifically absorber layer. We have conducted a numerical simulation to investigate the possibility of the $CH_3NH_3BiI_3$ absorber layer with TiO_2 as an electron transport layer and Cu_2O as a hole transport layer. The cell structure of FTO/Cu_2O/$MABiI_3$/TiO_2/Au has been considered the solar cell's key component. Maximum power conversion efficiency (PCE) of 29.61% has been achieved with an open circuit voltage (V_{OC}) of 1.11 V, a short circuit current (J_{SC}) of 31.93 mA/cm², and a fill factor (FF) of 83.26% under photo illumination of AM 1.5. This study will aid researchers for reasonably selecting material for highly efficient perovskite solar cell.



Keywords: Lead free; Simulation; $MABiI_3$; acceptor density

INVITED SPEAKER

Mr. Arup Dhar

He is currently serving as Deputy Director (Technical) at the Solar Cell and Solar Photovoltaic Module Laboratory, National Institute of Solar Energy (NISE). He holds an M.Tech in Renewable Energy Science and Technology from the Indian Institute of Engineering Science and Technology, Shibpur, and previously worked as a research fellow at IIT Kharagpur in the field of solar photovoltaics. His research focuses on the design of high-efficiency solar cells, module performance reliability, and degradation analysis. At NISE, he leads efforts on indoor and outdoor performance assessment of various PV technologies and their influence on energy generation in solar power plants. He has presented and published his work in several reputed international conferences and journals.

ACCURATE TRANSLATION OF OUTDOOR IV MEASUREMENTS TO STC FOR PHOTOVOLTAIC MODULES ACROSS DIVERSE TECHNOLOGIES

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Abstract

Accurate performance evaluation of photovoltaic (PV) systems under real-world conditions is critical for energy yield estimation, long-term reliability assessment, and large-scale deployment. However, outdoor I V measurements are affected by varying environmental factors such as solar irradiance, module temperature, angle of incidence (AoI), spectral distribution, and the direct-to-diffuse irradiance ratio, complicating direct comparison with standardized benchmarks. To enable consistent performance assessment, field data must be translated to Standard Test Conditions (STC), defined as 1000 W/m² irradiance, 25°C cell temperature, and AM1.5 spectrum. Standard correction procedures, including IEC 60891 and ASTM E1036, rely on irradiance and temperature-based interpolation and extrapolation. However, these methods often produce significant deviations under actual field conditions due to limited consideration of spectral and angular effects. This study assesses the effectiveness of various correction models in translating I-V characteristics of PERC, TOPCon, HJT & CdTe PV modules to STC. I-V data were collected both in outdoor and indoor conditions using a calibrated I-V tracer and solar simulator, respectively. Standard correction methods IEC 60891 and ASTM E1036 were applied, and the resulting deviations from STC were analyzed. Results indicate that outdoor translated data exhibit greater deviation from STC due to angular, spectral mismatches, and temperature, whereas indoor-translated data align more closely with STC. Procedure 1 of IEC 60891 and ASTM E1036 model demonstrated the higher accuracy during outdoor translated results as compared to procedure 4 of IEC 60891. The ASTM E1036 model is defined for only Isc, Voc and Pm translation. The model has been modified by incorporating the temperature coefficient of fill factor, which considers the effect of Rs and is able to generate the complete I-V curve. The modified ASTM E1036 model demonstrated the higher translation accuracy and significantly reduced deviations in outdoor data translation, enhancing the precision of field-based PV performance and degradation assessments. Further, the work incorporates the effect of AoI and spectral mismatch to enhance the accuracy of translation to a greater extent, along with the translational distance and uncertainty analysis.

INVITED SPEAKER

Prof. Somnath Chandra Roy

Prof. Somnath C Roy, completed his BSc and MSc degrees in Physics from the Banaras Hindu University, Varanasi in 1997 and 1999, followed by PhD from IIT Delhi in 2005. After a brief stint as a Lecturer in the Amity University Noida, he joined the Materials Research Institute at Pennsylvania State University, USA in 2006 as a post-doctoral researcher. In 2010, he joined the Department of Physics, IIT Madras, and became a professor in 2021. During the past 14 years at IIT Madras, he has been involved in the growth and study of 1D nanostructures for solar energy and gas sensing applications and has guided 10 PhD students so far. At present his research group called Semiconductor Oxide Materials, Nanostructures and Tailored Heterojunctions (SOMNaTH) Lab, is comprising of 12 PhD students, 2 post docs and a number of UG and PG project students. He had been selected for the Bhaskara Advanced Solar Energy (BASE) Fellowship and also the Shastri Indo Canadian Institute's (SICI) Faculty Travel and Internationalization (FTI) award. In the year 2023, he was awarded with Australia Award Fellowship hosted by the University of Sydney and high risk high reward (HRHR) travel grant award from the office of global engagement (OGE), IIT Madras for initiating collaborative research with University College London. Recently. the energy consortium at IIT Madras has awarded Trend-Setter grant award for pioneering work on solar powered CO_2 conversion to fuel.

AN EXCITING WORLD OF ONE-DIMENSIONAL METAL OXIDE NANOAND HETERO-STRUCTURES

SOMNATH CHANDRA ROY

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Abstract

One dimensional nanostructures hold special importance in nanosciene because of directional charge transport and higher specific surface area, that make them useful for reduced recombination of photogenerated charges. In particular, vertically aligned structures directly grown from an underlying substrate offer high flexiblity and advantage in device design and implementation. In this talk, I shall discuss fabrication of three metal oxide systems such as TiO_2 nanotubes/nanorods, CuO nanowires and $BiFeO_3$ nanorods in vertically oriented morphology and their heterostructures. Further, the charge transport mechanisms in single/individual nanostructure has been studied and their photo-electrochemical properties are explored. Also, our work on ion beam irradiated TiO_2 nanorods will be discussed. In the final part, I will present recent developments on photocatalytic CO_2 reduction using TiO_2-Graphene oxide nanocomposites and our innovations in both materials engineering and reactor design.

INVITED SPEAKER

Mr. Awatans Tripathi

Awatans Tripathi is an energy professional specializing in renewable energy, building performance, and sustainable design. He currently serves as a Junior Energy Advisor at GIZ India, where he works at the intersection of solar energy deployment, BIPV integration, policy analysis, and government collaboration to advance India’s clean-energy transition.

Previously, Awatans worked as an Energy Analyst at Smart Joules, leading data-driven energy-efficiency initiatives focused on HVAC optimization, energy simulation, and sustainability outcomes. His earlier roles at CARBSE, GRIHA Council, GIZ, and architectural consultancies strengthened his expertise in building performance modeling, green building frameworks, and climate-responsive architectural design.

Awatans holds an M.Tech in Building Energy & Performance from CEPT University and a Bachelor of Architecture from Jamia Millia Islamia, enabling him to combine architectural insight with advanced energy analytics in developing high-performance building and renewable-energy solutions.

IMPROVING THE PRE-CONDITIONS OF BIPV IN INDIA

AWATANS TRIPATHI

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Abstract

India has committed to significantly boosting its renewable energy capacity to 500 GW by 2030. With electricity demand projected to grow by nearly 5% annually until 2040 and an urgent need for climate change mitigation, scaling up innovative solar photovoltaic (PV) applications across the country is crucial. The Ministry of New and Renewable Energy has identified building-integrated photovoltaics (BIPV) as key new and innovative solar applications for proliferation under the Indo-German Solar Energy Partnership-Innovative Solar (IGSP IN-Solar).

Despite the immense potential of BIPV (estimated at 309 GW) in India's urban development and infrastructure expansion plans, stakeholder confidence in these technologies is low. This is due to significant knowledge and awareness gaps regarding costs, benefits, technical feasibility, and potential applications. Additionally, there is a scarcity of skilled professionals and training programs, lack of economically sustainable business models, and an absence of a well-defined and supportive regulatory framework.

To support this objective, the German Federal Ministry for Economic Cooperation and Development (BMZ) is funding a project through its Development Partnership with the Private Sector (develoPPP) program. The project, implemented by Deutsche Gesellschaft für Internationale Zusammenarbeit (GIZ), partners with Ornate Agencies Private Limited to facilitate the widespread adoption of BIPV in India. The discussion will revolve around the efforts of the project and briefly touch upon the technical aspects of BIPV- the processes and challenges the project has gone through the journey.

Keywords: BIPV, Innovative Solar, Renewable Energy

INVITED SPEAKER

Prof. Shree Prakash Tiwari

Shree Prakash Tiwari is currently working as Professor in Department of Electrical Engineering. Prior to joining IIT Jodhpur as a faculty member in 2011, Prof. Tiwari had worked as a Postdoctoral Fellow in School of ECE at Georgia Institute of Technology, Atlanta, USA, for 3 years (2008-2011). He had done his Ph.D. from EE Department, IIT Bombay from 2003 to 2008, during which he had also worked at NTU Singapore for about 7 months. Prof. Tiwari is a Senior Member of IEEE and serves as selected member of technical committees on “Flexible Electronics and Displays” and “Electronic Materials” of IEEE Electron Devices Society. Prof. Tiwari was Visvesvaraya Young Faculty Research Fellow of Ministry of Electronics and Information Technology, Government of India, for 2018-2023. He was part of Indian Delegate to attend Indo-German Frontiers of Engineering Symposium in Bremen, Germany (2022) organized by Alexander von Humboldt Foundation and Department of Science and Technology, followed by CONNECT Follow-up Programme Award by Humboldt Foundation and IGSTC-CONNECT Plus Award to visit and work in Germany in 2023. At IIT Jodhpur, he leads the Flexible Large Area Microelectronics (FLAME) Research Group, with focus towards biodegradable electronics. He was recently conferred with “Institute Award for Research Excellence-2024, Senior Researcher Award (Engineering)” from IIT Jodhpur. He has co-authored over 160 research articles, including more than 80 in journals of high repute with many in IEEE, ACS, and Wiley Journals

FLEXIBLE ELECTRONIC DEVICES FOR SMART SUSTAINABLE SYSTEMS

SHREE PRAKASH TIWARI

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Abstract

Flexible electronics has become an enormously explored contender for next-generation low-cost electronics due to its applicability in a broad range of applications towards smart textiles and wearable electronics. Moreover, in recent times, devices are being explored for eco-friendly electronics, to eventually reduce the impact of increasing E-waste on environment, which has become a severe issue for earth, ecology, and health. Organic devices, specifically transistors receive significant attention as a key device for flexible electronics due to their potential use for multifunctional, circuit, and sensing applications. Developing low-cost flexible sensing devices has become very important for wearable electronics specifically for monitoring physiological parameters. Incorporation of organic, natural, and biocompatible materials in devices can be an excellent way towards sustainability. Moreover, adding synaptic and energy harvesting capabilities lead these efforts towards energy autonomous smart wearable systems. In this talk, firstly, approaches for designing high performance, multifunctional, and biodegradable organic transistors will be presented. Fabricated p-channel transistors on these substrates with natural gate dielectrics exhibit high electrical stability and exceptional synaptic characteristics resembling a biological synapse. Quest to replicate complex cognitive functions with these fabricated devices helped towards the advancement of brain-inspired computing, which mimics the biological brain to achieve superior performance through parallel computing. Demonstration of use of natural proteins for development of flexible biodegradable substrates can also help in developing transient electronics. Complete dissolution of these devices in aqueous environments without any alteration to temperature or pH has been shown to confirm excellent biodegradability of these devices leading towards transient neuromorphic circuits and systems that adhere to the concepts of circular economy. In addition, some strategies for development of IoT enabled low-cost wearable and smart systems will also be discussed. Devices for human-machine interaction and energy harvesting demonstrated through sustainable ways will be discussed. In one of the demonstrations, a unique biocompatible composite of abundantly available natural arid zone (Sewan grass) and xanthan gum (XG) as a tribo-positive layer is demonstrated for high-performance flexible TENG devices exhibiting impressive electrical output with peak-to-peak voltage exceeding 200 V and efficient energy conversion. Continuous motion sensing of body joints is successfully demonstrated through direct application of these devices on human body, specifically on the knee, elbow, and fingers. Long-term durability over 12,000 cycles (4000 s), high reliability, and real-time human-machine interaction (HMI) are also demonstrated through distinct electrical signals generated by finger movements of human hand, which are effectively used to produce intuitive and direct control over the movements of a robotic hand. The presented proof-of-concept highlights the versatility of these devices for sustainable and smart wearable electronics.

These investigations highlight the promise towards implementation of low-cost, flexible, and smart sustainable systems.

Keywords: Flexible Electronics; Synaptic Transistors; Sustainability; Energy Harvesting

INVITED SPEAKER

Prof. Upendra Pandey

Prof. Upendra Pandey is an accomplished academic and researcher specializing in organic and perovskite photovoltaics, organic semiconductors, and flexible electronics. His research focuses on device architecture, evaluation of novel donor–acceptor materials for organic solar cells (OSCs) to improve performance and stability, and detailed stability and degradation studies of both OSCs and perovskite solar cells. His work also includes charge carrier transport and mobility measurements in organic semiconductors, along with the study of alternative hole and electron transporting materials for perovskite devices.

He earned his Ph.D. from the University of Calabria, Italy, and completed postdoctoral research at both the University of Calabria, Italy, and the University of St. Andrews, Scotland, UK. He has also served as a DST INSPIRE Faculty Fellow at the Indian Institute of Science (IISc), Bangalore. Currently, he is an Assistant Professor in the Department of Electrical Engineering, School of Engineering, Shiv Nadar University, Delhi-NCR.

He holds an M.Tech degree from Rajiv Gandhi Proudyogiki Vishwavidyalaya, Bhopal, and has prior industry experience as an Engineer at Quantalase Enterprises Pvt. Ltd., Indore. His achievements include the prestigious DST-INSPIRE Faculty Fellowship (Engineering) and recognition as a JACS Young Investigator (2020).

INDENOFLUORENE DIMER AS AN EFFICIENT INTERLAYER FOR HIGH-PERFORMANCE PEROVSKITE SOLAR CELLS

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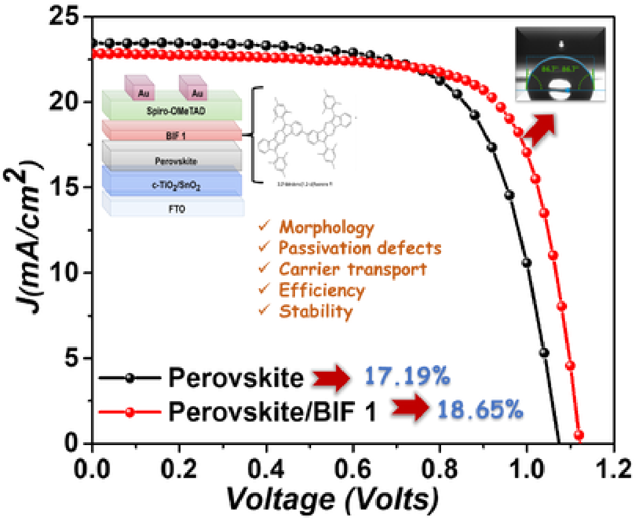
Abstract

Perovskite solar cells (PSCs) have achieved high power conversion efficiencies, yet their commercialization is hindered by instability and interfacial defects, especially at the perovskite/hole transport layer (HTL) interface. The commonly used HTL, Spiro-OMeTAD, induces trap-assisted recombination and charge extraction losses, accelerating degradation during operation. To overcome these limitations, we introduce 3,3'-biindeno[1,2-b]fluorene-1 (BIF-1) as a functional interlayer between the perovskite absorber and Spiro-OMeTAD. BIF-1 effectively passivates interfacial trap states, suppresses non-radiative recombination, and improves hole mobility, resulting in enhanced charge extraction and reduced recombination losses. PSCs incorporating BIF-1 show an ~8.5% increase in efficiency and improved device-to-device reproducibility. Furthermore, the modified devices retain ~86% of their initial efficiency after 1400 hours of ambient storage, compared to ~57% for control cells. This work demonstrates the potential of BIF-based molecular interlayers as a scalable strategy to simultaneously boost efficiency and long-term stability in PSCs.



Keywords: Interlayer, Perovskite solar cells, interfacial defects, stability

INVITED SPEAKER

Prof. Manika Khanuja

Dr. Manika Khanuja is a materials scientist and nanotechnology researcher at the Centre for Nanoscience and Nanotechnology, Jamia Millia Islamia, New Delhi. She holds a Ph.D. in Nanoscience and Nanotechnology from the Indian Institute of Technology (IIT) Delhi, along with an M.Sc. in Physics from IIT Delhi and a B.Sc. (Hons.) in Physics from the University of Delhi. She completed her doctoral research in 2009 on palladium nanoparticles and bimetal layers for enhanced hydrogenation, where she discovered a novel pulse-like, concentration-specific hydrogen sensing response.

Dr. Khanuja has extensive international research exposure, having delivered over 20 invited talks, authored 4 books and 8 book chapters, and published around 40 international research papers with more than 780 citations. Her expertise lies in the fabrication and characterization of nanomaterials for applications in gas and biosensing, antimicrobial technologies, water disinfection, energy storage, photocatalytic water splitting, and agricultural applications. She has hands-on experience with advanced characterization techniques including XRD, TEM, FESEM, AFM, UV-Vis spectroscopy, and XPS.

She is currently serving as an Assistant Professor at Jamia Millia Islamia since 2016. Previously, she held academic and research positions at Amity University (Noida), University of Delhi, and as a Project Scientist at IIT Delhi. She also worked as a Guest Scientist at the University of Duisburg-Essen, Germany, under the CENIDE program, where she specialized in the gas-phase synthesis and size-selected deposition of palladium and rare-earth nanoparticles.

Dr. Khanuja continues to advance cutting-edge research in two-dimensional materials, nanostructured heterostructures, photocatalytic water disinfection, and sustainable energy and environmental nanotechnologies.

AMACHINE LEARNING–ENABLED ACCELERATION OF CATALYTIC REACTION PATHWAYS AND SENSING PERFORMANCE IN 2D NANOMATERIALS

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Abstract

Two-dimensional (2D) materials such as MXenes, TMDs, and MOF-derived nanosheets have shown promising applications in the fields of electronics, optoelectronics, environmental remediation and energy storage owing to their tunable electronic structure, high surface activity, and exceptional physicochemical properties. However, optimizing the reaction parameters and deploying them in real-time sensing and catalytic activity remains limited by slow experimentation cycles. Integrating machine-learning (ML) frameworks can accelerate application pipelines for 2D materials by facilitating the development of insights and discoveries from a large amount of data in a short time, and the use of supervised learning and feature-importance analysis to uncover the dominant reaction drivers. By employing data-driven ML models, one may predict and optimize performance through material concentration, band gap, surface area and other parameters, thereby reducing the number of required experiments significantly. ML algorithms such as Support Vector Machine (SVM), XGBoost, Multilayer Perceptron (MLP) and others can be used to explore the reaction parameters and shorten the development cycles. Case studies on colorimetric/optical sensing and catalytic activity illustrate how ML can uncover hidden descriptors, accelerate catalyst design, predict performance, and guide parameter optimisation toward target functionalities. This talk highlights a pathway toward autonomous labs, digitally twinned materials platforms, and the rapid translation of 2D materials into sensing and environmental applications.

Keywords: 2D materials, Machine learning, environmental remediation

INVITED SPEAKER

Prof. Pankaj Yadav

Dr. Pankaj Yadav is an Associate Professor at Pandit Deendayal Petroleum University (PDPU) in Gujarat, India. Before joining PDPU, he worked as a Swiss Excellence Fellow under Prof. Michael Grätzel at École Polytechnique Fédérale de Lausanne in Switzerland. His work has been recognized through prestigious awards, including the Fulbright Fellowship, Swiss Excellence Fellowship, Nawa Fellowship (Poland Govt), and Overseas Postdoctoral Fellowship.

Dr. Yadav has authored over 100 papers in top international journals, establishing himself as an influential voice in the field of material technology for energy applications. He engages actively with the public, students, and policymakers, discussing the latest advances and future trends in energy technologies.

At PDPU, Dr. Yadav's research explores the fundamentals and practical applications of advanced materials for energy harvesting and storage devices. His work spans thin-film technologies, solar photovoltaics, perovskite solar cells, hydrogen generation, and fuel cells. Additionally, he has a strong focus on electroanalytical characterization, enhancing the efficiency and performance of energy devices. Dr. Yadav collaborates internationally with research groups in Switzerland, the UK, Sweden, Germany, and the US, aiming to drive innovations in sustainable energy technologies and contribute to global advancements in this crucial field.

AUTOMATED EIS ANALYSIS OF METAL HALIDE PEROVSKITE SINGLE CRYSTALS USING MACHINE LEARNING FOR ACTIVATION ENERGY PREDICTION

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Abstract

Metal halide perovskite single crystals (MHP SCs) hold great potential for optoelectronic applications, but their long-term stability is compromised by ion migration, which impacts performance. A crucial aspect of understanding this instability is the calculation of activation energy under varying conditions like illumination, applied bias, and heat. While Electrochemical Impedance Spectroscopy (EIS) is a powerful tool for distinguishing ionic and electronic processes, its traditional analysis is labor-intensive, requiring extensive data collection, circuit fitting, and manual interpretation. This study introduces a machine learning (ML)-driven approach that automates the entire EIS analysis workflow. By analyzing EIS data for $MAPbI_3$ and $MAPbBr_3$ across a temperature range of 263K to 343K, we generated a large database to train ML models. These models predict EIS spectra at unknown temperatures, fit electrical circuits, and automatically extract passive component values to calculate activation energy via an Arrhenius plot. This automated process significantly reduces analysis time and offers reliable activation energy predictions, even when temperature data is incomplete. Our ML-based approach streamlines EIS analysis, enhancing the understanding of MHP SC stability and performance.

Keywords: Metal Halide Perovskites, Single Crystals, Activation Energy, Machine Learning, Impedance Spectroscopy

INVITED SPEAKER

Prof. Ankur Goswami

Prof. Ankur Goswami is currently Associate Professor at the Department of Materials Science and Engineering at IIT Delhi, India. Before joining IIT Delhi, he was a postdoc fellow at Department of Chemical and Materials Engineering and Electrical and Computer Engineering at the University of Alberta, Edmonton, Alberta, Canada. He did his B.Tech in Ceramic Technology from West Bengal University of Technology, Kolkata in 2006, India. He completed his Ph.D. in Materials Science and Engineering from Indian Institute of Science (IISc.), Bangalore in 2013. Following to his Ph.D., he was Unilever postdoc fellow at Centre for Nanoscience and Engineering at IISc, Bangalore. His current research interest includes fabrication of MEMS devices, novel energy harvesting devices, electronic and optical switch using smart materials, use of scanning probe microscopy to investigate electronic properties of materials at the surface. He is author or co-author of several international peer reviewed journal paper, conference proceedings and book chapter. He is reviewer of several international reputed journals. He has mentored four PhD students and several interns till date.

TUNGSTEN DOPED VO_2 THIN FILM BASED RESISTIVE MICRO-OSCILLATORS FOR THE APPLICATION IN NEUROMORPHIC SYSTEMS

ANKUR GOSWAMI

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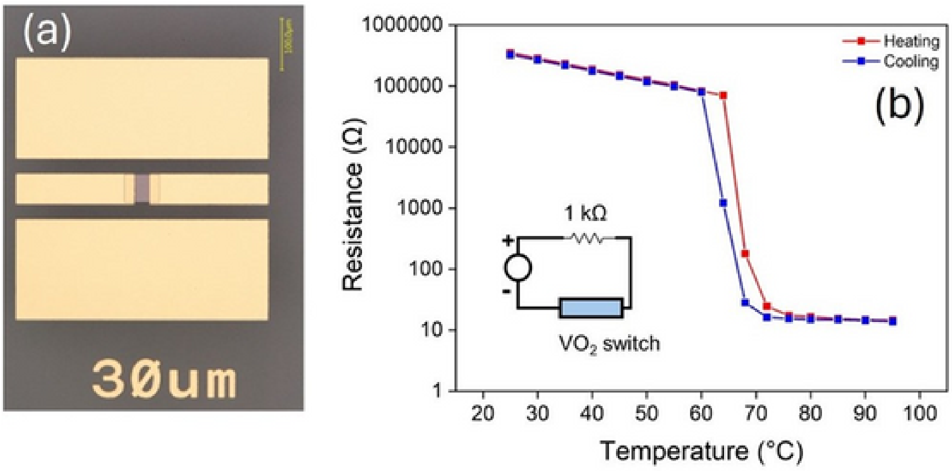
Abstract

The drawbacks of the conventional Von-Neumann computing systems can be circumvented by utilizing Vanadium dioxide (VO_2) based resistive oscillators and neuromorphic circuits, owing to their low operational temperature close to room temperature, frequency modulation, and the ability to integrate as both neuron and synaptic devices. Regardless of these advantages, the deviation in activation voltage and resistive states of the metal-insulator transition (MIT) results in switching stochasticity, while higher operational voltage results in filament destruction in VO_2 and device failure. This withholds the application of low-power and room-temperature VO_2 oscillatory neural circuits. This work presents tungsten (W) doped VO_2 film oscillators capable of generating high-frequency oscillations at room temperature with minimal external line resistance. W doping enables low power oscillators while maintaining effective switching states and good device reliability (switch threshold deviation < 1%). We present a series of co-sputtered W:VO_2 films and devices with differing switch lengths to investigate the impacts of VO_2 negative differential resistance (NDR) development and oscillation frequency. We further characterize these films to understand the effect of doping on the structural polymorphs and further investigate first principal calculations to explain underlying physics related to the doping effect. We believe these micro-oscillators show a promising future for artificial neurons in neuromorphic circuits along with applications in sensing and memory devices.



(A) W DOPED VO_2 DEVICE FOR STUDYING NDR, (B) MIT OF THE GROWN W DOPED VO_2 FILM.

Keywords: Metal Halide Perovskites, Single Crystals, Activation Energy, Machine Learning, Impedance Spectroscopy

INVITED SPEAKER

PROF. HEMANT SAGAR

Prof. Hemant Sagar is an Assistant Professor (Grade-I) in the Department of Hydro and Renewable Energy at the Indian Institute of Technology (IIT) Roorkee, India. He is an internationally trained researcher with extensive expertise in multiphase flow, cavitation dynamics, fluid–structure interaction, hydroelasticity, and underwater hydrodynamics. Prior to joining IIT Roorkee, he served as a Research Group Leader at the University of Duisburg-Essen, Germany, and as a Postdoctoral Fellow at Harbin Engineering University, China.

Prof. Sagar earned his Doctorate in Mechanical Engineering from the University of Duisburg-Essen, where his research focused on numerical and experimental investigations of laser-induced cavitation bubbles and associated material damage. He has led and contributed to several international research collaborations and is the Principal Investigator of multiple funded projects. He has published widely in high-impact journals such as Physics of Fluids, Ocean Engineering, and Journal of Fluids and Structures, and regularly serves as a reviewer for leading international journals.

INVITED SPEAKER

Mr. Dileep Tiwari

Dileep Kumar Tiwari is an Executive Officer at the Gujarat Energy Development Agency (GEDA), where he has been leading renewable energy initiatives since 2016. He specializes in renewable energy policy, regulations, techno-commercial project evaluation, and climate action planning, with substantive contributions to the implementation of policies underpinning more than 30 GW of commissioned renewable energy capacity in Gujarat.

He holds an M.Tech in Energy Systems from PDEU and a B.Tech in EEE from AKTU. With extensive experience in solar, wind, hybrid systems, PM-KUSUM, and state-level policy development, he contributes to Gujarat’s clean energy leadership through policy formulation, project execution, and sustainability planning.

UNLEASHING RENEWABLE ENERGY OPPORTUNITIES: POLICIES, STRATEGIES FOR EMERGING CHALLENGES, AND THE PATH TO SUSTAINABLE INVESTMENT IN GUJARAT

DILEEP TIWARI

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Abstract

Unleashing Renewable Energy Opportunities: Policies, Strategies for Emerging Challenges, and the Path to Sustainable Investment in Gujarat.
Gujarat's renewable energy transition is redefining its developmental landscape by advancing sustainability, energy independence, and inclusive economic growth. This presentation delivers a comprehensive perspective on the state's policy evolution, regulatory frameworks, and investment strategies under the Electricity Act, 2003, highlighting emerging opportunities across both utility-scale and distributed renewable energy projects.
The discussion explores key project models—including competitive bid-based utility initiatives, open access systems (captive and third-party), and hybrid renewable projects integrated with Battery Energy Storage Systems (BESS)—illustrating Gujarat's strategic agility in overcoming implementation challenges and strengthening investor confidence.
Showcasing Gujarat as a national benchmark, the session delves into replicable best practices in policy design, financial structuring, and investor facilitation, which have positioned the state as a leader in India's clean energy transformation.
Further, the presentation emphasizes the integration of circular economy principles, green job generation, and pathways to carbon neutrality. It outlines a forward-looking roadmap for achieving India's 500 GW renewable energy goal by 2030 and advancing toward the Net Zero vision by 2070 through innovation, collaboration, and strategic implementation.

INVITED SPEAKER

Prof. Rishi Sharma

Dr. Rishi Sharma is an Assistant Professor in the Department of Physics at Birla Institute of Technology (BIT), Mesra, where he has been serving since 2008. He holds M.Sc., M.Tech., and Ph.D. degrees and brings more than 15 years of teaching experience and 18 years of research experience in the areas of materials science and nanotechnology. His research expertise includes cold plasma processing of materials, thin film technology, graphene, nanocrystalline diamond and diamond-like carbon coatings, solid lubricant coatings, and dye-sensitized solar cells.

Dr. Sharma has worked as a Visiting Scholar at the University of Duisburg-Essen, Germany, under the DST–BMBF Indo-German bilateral program. He has successfully led several nationally funded research projects supported by DST-SERB, DRDO, BRNS-DAE, UGC-DAE CSR, and industry partners, and holds a granted Indian patent in diamond-like carbon film deposition. With a strong publication record in leading international journals, he actively contributes to the scientific community through professional societies, editorial boards, and conference leadership roles.

COLD PLASMA PROCESSING FOR SURFACE ENGINEERING

RISHI SHARMA

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Abstract

Cold plasma processing has emerged as a transformative technique in surface engineering, offering a versatile, low-temperature approach to modify surface properties without compromising the integrity of bulk materials. This non-equilibrium plasma, distinguished by high-energy electrons and low gas temperatures, enables precise control over surface chemistry, morphology, and functionality across a broad spectrum of substrates, including metals, polymers, ceramics, and composites. Plasma-assisted techniques are increasingly adopted in diverse industrial sectors such as automotive, aerospace, biomedical, and microelectronics manufacturing, where surface modification and thin film deposition are critical for performance and reliability. The expanding demand for tailored surface properties has accelerated the use of plasma technologies for thin film deposition, etching, and functionalization. Consequently, a growing community of engineers and scientists from multidisciplinary backgrounds is actively engaged in plasma-assisted processing, driving innovation in both manufacturing and research and development.

Keywords: Cold plasma; Surface processing; Thin film deposition

INVITED SPEAKER

Prof. Dibyajyoti Ghosh

Dibyajyoti finished his Bachelor's in Science (Chemistry Hons.) from Dept. of Chemistry, Visva Bharati University, Shantiniketan, West Bengal in 2009. He joined JNCASR, Bangalore as an Integrated Ph.D. student in the Chemistry and Physics of Materials Unit. He completed his Master's in Science degree in 2012 and moved to the Theoretical Sciences Unit of the same institute to undertake his Ph.D. under the supervision of Prof. Swapan K Pati. His Ph.D. was primarily focused on two topics, the charge and heat transport in molecular-devices and magnetism in low-dimensional materials. He completed his Ph.D. in 2016 and moved to the Dept. of Physics and Chemistry, University of Bath, UK as a post-doctoral research associate for 2 years. He worked with Prof. Saiful Islam and Prof. Alison Walker there. The main topics of his research were computational investigation of structural stability, ion migration and photovoltaic properties of halide perovskite solar cells. Following that, from November 2018 to July 2021, Dibyajyoti was a research associate at Los Alamos National Laboratory, USA. His mentors were Dr. Sergei Tretiak and Dr. Amanda Neukirch. There he was involved in several projects, (1) in-silico compositional engineering of optoelectronic materials, (2) adiabatic and non-adiabatic carrier dynamics for solid-state lighting and photocatalysis and (3) machine learning for energy materials design and optimization. He joined the IIT Delhi as an assistant professor in July 2021.

DESIGNING LAYERED HALIDE PEROVSKITES FOR OPTOELECTRONICS: INSIGHTS FROM AB INITIO AND DATA-DRIVEN MODELING

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Abstract

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

Keywords: Layered halide perovskites; ML; excited-state dynamics; carrier lifetime

INVITED SPEAKER

Prof. Suresh C. Sharma

Suresh C. Sharma received the M.Sc. (Physics, Specialization in Electronics) and M.Phil. (Physics and obtained 2nd position in Agra University) from Agra University, Agra, in 1986 and 1989, respectively. He joined the Department of Physics, IIT Delhi, as a Senior Research Assistant in the month of September 1990 and worked till December 1996. In the meantime, he received Ph.D. degree in Plasma Physics from Agra University, Agra in 1994 (Research work carried out at Physics Department, IIT Delhi during tenure of Senior Research Assistant). He was awarded the Young Scientist project as a Principal Investigator by the Department of Science and Technology (DST), Govt. of India for a two-year duration (1997-99) and worked with the Department of Physics and Astrophysics, University of Delhi from Jan. 6, 1997 to Oct. 14, 1997. He was a Monbusho Postdoctoral Fellow under Japanese Govt. fellowship, Department of Physics, Faculty of Science, Ehime University, Matsuyama, Japan from October 1997 to March 1999. In addition, he has been a JSPS (Invitation) Postdoctoral Fellow and visiting researcher from May 2004 to October 2005 with the Centre for Atomic and Molecular Technologies (CAMT), Osaka University, Japan. Besides, he was awarded Senior Research Associate under the Scientist's Pool Scheme by CSIR, Govt. of India for 3 years duration (1999-2002) and worked in the Department of Physics and Astrophysics, University of Delhi from April 1999 to January 2002. He has worked on several research projects in India and abroad. He has guided numerous Ph.D., M. Tech & B. Tech students. He has delivered several invited and oral talks in India and abroad. He established a Plasma and Nano simulation research Lab. He has guided 20 Ph.D. students. He has published 222 research papers in Journals of International & National repute and Proceedings of International & National Conferences. He was awarded commendable Research Award for Excellence in Research by DTU, Delhi for 7 consecutive years i.e., March 21, 2018; March 19,2019; March 13, 2020, Feb.15, 2021 , March 3, 2022 , April 6,2023 and Sept 5, 2024.

Currently, Dr. Sharma has been working as Professor with the Department of Applied Physics, DTU Delhi since June 13, 2012 and Dean (Academic -PG) from September 2, 2019 to August 31, 2022. He was Head, Department of Applied Physics, DTU, Delhi from August 1, 2012 to September 30, 2018; Chairman, Department Research Committee (DRCs) [Applied Physics], DTU from November 29, 2017 to August 15, 2023 . Prior to joining DTU, he has worked as Professor, Department of Physics, MAIT (GGS Indraprastha University, Delhi), Delhi from November 1, 2009 to June 12, 2012.

Prof. Sharma is a Member of the American Physical Society (APS), USA; Senior Member of the Institute of Electrical and Electronics Engineers (IEEE), USA; Member of the International Association of Engineers (IAENG), Hong Kong; Member & designated delegate of Asian African Association for plasma Training (AAAPT); Member of the Association of Asia Pacific Physical Societies-Division of Plasma Physics (AAPPS-DPP); Member of the National Academy of Sciences (MNASc), India; Life Member - Plasma Science Society of India (PSSI); Life Member- Indian Science Congress Association (ISCA) and Life Member -Indian Society for Technical Education (ISTE), New Delhi, India.

PLASMA-ASSISTED VERTICALLY ALIGNED SEMICONDUCTING 2D GRAPHENE FIELD EFFECT TRANSISTOR BASED BIOSENSOR FOR DETECTION OF VARIOUS CANCEROUS BIO-MOLECULES

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Abstract

Graphene field-effect transistors (g-FETs) have shown great potential for highly sensitive biosensing applications due to their outstanding electrical characteristics. Here, vertically aligned semiconducting 2 D Graphene synthesized using Plasma-Enhanced Chemical Vapor Deposition (PECVD) technique is implemented as the channel. This research focuses on the analytical modeling and numerical simulation of a plasma-assisted g-FET fabricated through the plasma-enhanced chemical vapor deposition (PECVD) process. A detailed analysis is conducted to evaluate how different plasma parameters influence the device's electrical behaviour and overall performance.

The simulation results indicate that optimizing plasma power and pressure enhances the transistor's functionality by increasing drain current, improving output conductance, and lowering the cutoff frequency. These results emphasize the importance of precise plasma control in maximizing device efficiency. The proposed g-FET design aligns strongly with experimental observations, confirming its feasibility for real-world biosensing applications. This study provides critical insights into the role of plasma-assisted fabrication in advancing g-FET technology for next-generation biosensors.

INVITED SPEAKER

Prof. Rajendra Singh Dhaka

Prof. Rajendra Singh is a Professor in the Department of Physics, IIT Delhi, and the Principal Investigator of the Advanced Semiconductor Materials and Devices Group. He also serves as Joint Faculty in the Department of Electrical Engineering, IIT Delhi. He earned his Ph.D. from Jawaharlal Nehru University, New Delhi (2001), following an M.Sc. in Physics (1995), with doctoral research focused on the effects of swift heavy ion irradiation on Si and GaAs. He pursued post-doctoral research at the Technical University of Munich and the Max Planck Institute, Germany, specializing in InP-based HBTs, wafer bonding, layer splitting, and SOI technologies.

Prof. Singh joined IIT Delhi in 2006 and leads cutting-edge research in GaN and gallium oxide devices, semiconductor nanowires, 2D–3D interfaces, quantum materials, and advanced semiconductor growth and nanofabrication techniques. He has published around 200 research papers, played a key role in establishing the Nanoscale Research Facility at IIT Delhi, and is the recipient of the MRSI Medal Award (2017) and the IIT Delhi Teaching Excellence Award (2018).

SODIUM-ION BATTERIES FOR SUSTAINABLE FUTURE AND VIKSIT BHARAT

RAJENDRA SINGH DHAKA

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Abstract

In recent years, energy storage devices especially rechargeable batteries have become part of our daily life in portable electronic devices like mobiles, laptops as well as being used at large scale in electrical vehicles (EV), etc. Among various types of batteries, the only commercially established and feasible technology is based on Li-ion intercalation, mainly due to the advantage of its high energy density, good rate kinetics and light weight. However, the main concern comes from the limited availability and uneven distribution of Li in the earth crust. More importantly, the unavailability of Li in India motivates us to search for alternative avenue, and the Na-ion batteries are one of the potential candidates particularly for grid level storage due to its low cost and abundance on the globe, and therefore extensive research has been started in this field over past few years. In this direction, it is vital to find suitable and high-performance electrode materials. However, there are many challenges due the larger size of the Na-ion as compared to the Li. Therefore, constant efforts are going on to search new electrode materials (negative as well as positive) for improving the electrochemistry.

Recently, we have developed few cathode and anode materials and tested their electrochemical performance to understand the diffusion kinetics, stability, rate capability and coulombic efficiency in sodium ion batteries. In the talk, I will present some of our effort towards development of cost-effective/high-performance sodium-ion batteries for energy storage applications.

INVITED SPEAKER

Prof. Jai Singh

Dr. Jai Singh is working as a Professor, Dept of Pure and Applied Physics, Guru Ghasidas Central University, Bilaspur, C.G, India. Before joining GGU Bilaspur, I was worked as Assistant Professor in the Department of Physics, Dr. Harisingh Gour Central University, Sagar, India. He did Doctoral degree in the field of II-VI oxide nanomaterails from Dept. of Physics, Banaras Hindu University, Varanasi, India. Soon after completing his Ph.D., he joined Cologne University, Cologne, Germany to carry out post-doctoral research work in the area of 2-D materials (Graphene ,Graphene oxide, MoS_2 and WS_2), Transparent Conducting Oxide (TCO) materials, Energy materials and then after Pusan National University, Busan, South Korea and Sejong University, Seoul ,South Korea to work on the same field. Dr. Singh has published more than 148 research publications in refereed international journals of repute that have been cited over 4386 times, and his publication H-index is 37. He has been awarded number of prestigious National and International awards, like GATE Fellowship from Ministry of HRD, Govt of India, CSIR-Junior Research Fellowship and Senior Research Fellowship by the Council of Scientific & Industrial Research, Government of India, Postdoctoral Fellowship, Busan National University , NSC Postdoctoral Fellowship Taiwan, Visiting fellowship Cologne University ,Germany, etc. Dr. Singh is also serving as a guest editor and editorial board member for several journals and International Conference of international repute.

MOS$_2$ MONOLAYER, BI-LAYER THIN FILMS FABRICATED BY RF SPUTTERING AND PULSED LASER DEPOSITED ZNO THIN-FILMS/NANOSTRUCTURES

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Abstract

In this talk, I will discuss about MoS$_2$ and ZnO thin films/nanostrctures. One of the most practical methods to produce MoS$_2$ is chemical vapor deposition (CVD). I will discuss a simple and mass-scalable approach for thin MoS2 films via RF sputtering combined with the post- deposition annealing process. We have prepared as-sputtered film using a MoS2 target in the sputtering system. The as-sputtered film was subjected to post-deposition annealing to improve crystalline quality at 700 °C in a sulfur and argon environment. The analysis confirmed the growth of continuous bilayer to few-layer MoS$_2$ film. The mobility value of ~29 cm^2/Vs and current on/off ratio on the order of ~104 were obtained for bilayer MoS2. The mobility increased up to ~173–181 cm^2/Vs, respectively, for few-layer MoS$_2$. Well-aligned ZnO nanocones/films have been grown successfully on Si substrate without using any catalyst through a high-pressure pulsed laser deposition method. The influence of substrate temperature and growth time on the structure, microstructure, optical, and field emission properties of ZnO nanostructures have been investigated. It demonstrates that as the growth temperature increases from 500 to 8000C during 30 min, the spherical particle-like nanostructures transform into aligned nanocone. The field emission (FE) measurement of these aligned ZnO nanocones signifies a stable field emission with a low threshold field (2.40 V/μm) and a high field enhancement factor (2786). Their tapered morphologies and small tip diameters suggest as-deposited samples to be highly reproducible and henceforth as-deposited ZnO nanocones bearing excellent FE properties, through high-pressure PLD growth method without using any catalyst offer usage in various futuristic electronic applications.

INVITED SPEAKER

Prof. Ulganathan Mani

Dr. Ulaganathan is an Associate Professor in the Department of Physics, School of Physical Sciences, at Amrita University, Coimbatore. He holds B.Sc., M.Sc., and Ph.D. degrees and is actively engaged in teaching and advanced research in the field of energy storage technologies.

His primary research interests lie in electrochemical energy storage systems, with a strong focus on secondary batteries (Li-ion and beyond lithium), supercapacitors, hybrid capacitors, and redox flow batteries. His work emphasizes the design and development of electrodes, electrolytes, flow cells, and stack-level engineering for high-performance and long-life energy storage devices.

STRATEGIES FOR ENHANCING ZINC-IRON HYBRID REDOX FLOW BATTERY

ULGANATHAN MANI

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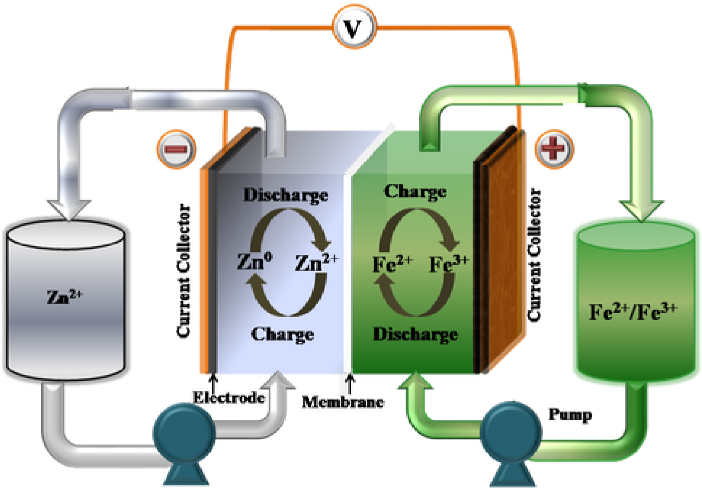
Abstract

Redox flow Batteries (RFBs) have attracted much attention due to their modular scalability, intrinsic safety, decoupling of energy and power, good cycle life, and large-scale energy storage range (>MWh). In recent times, Zn-based RFBs, specifically Zn-Fe, have been widely investigated for their high capacity and cell voltage, as well as for the earth-abundant Zn & Fe and low cost. However, the zinc dendrite formation, dead Zn-ion formation, hydrolysis of the Fe^{3+} reaction, hydrogen evolution, and unbalanced reaction kinetics, etc., are constraining further development of these Zn-Fe RFBs. To improve cell performance, the electrode and electrolytes have been modified, along with a suitable flow design. As a result, the Zn-Fe flow cell performance has been enhanced. However, it still needs further investigation to meet the commercial domain. Therefore, in this work, we aim to modify the electrode and optimize the electrolyte performance to improve the flow cell performance. The schematic representation of the Zn-Fe system (Figure 1) is shown below. The metal oxide attached to the graphite electrode shows significantly improved electrode kinetics, thereby improving the rate current and cycle life of the RFB cell.temperature increases from 500 to 8000C during 30 min, the spherical particle-like nanostructures transform into aligned nanocone. The field emission (FE) measurement of these aligned ZnO nanocones signifies a stable field emission with a low threshold field (2.40 V/μm) and a high field enhancement factor (2786). Their tapered morphologies and small tip diameters suggest as-deposited samples to be highly reproducible and henceforth as-deposited ZnO nanocones bearing excellent FE properties, through high-pressure PLD growth method without using any catalyst offer usage in various futuristic electronic applications.



Keywords: Redox Flow cell; High energy; Electrolyte; Electrode Modification

PARTICIPANT ABSTRACTS

(Abstract Domain: 1. Thin films/Nano-materials Growth, Novel techniques, and concepts)

Laser-Driven Conversion of Fullerene Dispersions to Graphullerene: A Liquid-Phase Approach

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ABSTRACT

Graphullerene, a graphene-like carbon nanostructure derived from fullerene molecules, has recently drawn significant attention for its unique optoelectronic properties and potential applications in nanoelectronics and catalysis. This study presents a facile and efficient synthesis route for graphullerene achieved via pulsed laser irradiation of liquid-phase (LIL) C_{60} fullerene dispersions in isopropyl alcohol (IPA). The process utilizes laser-induced photothermal and photochemical effects to promote polymerization and structural reorganization of fullerene molecules into extended covalently bonded frameworks.

Laser irradiation with nanosecond UV pulses induces a pronounced colour change in the fullerene solution, visually marking the molecular transformation. A schematic illustration, Fig.1, depicting this colour evolution from pristine fullerene dispersion to polymerized graphullerene solution is included to elucidate the experimental procedure.

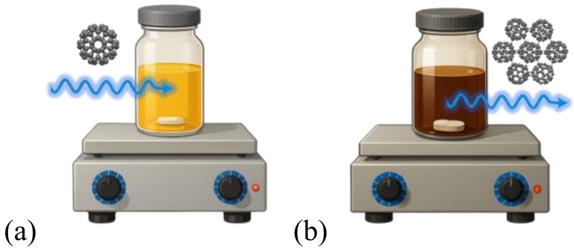
(a) (b)

Fig.1. Schematic of (a) before and (b) after irradiation experimental set up

Raman spectroscopic analysis reveals the coexistence of vibrational modes from both intact fullerene cages and graphene-like structures. Characteristic fullerene peaks are observed alongside distinct D and G bands at approximately 1350 cm^{-1} and 1590 cm^{-1}, respectively, indicative of sp^3 and sp^2 carbon domains respectively. This dual signature confirms the generation of hybrid graphullerene architectures integrating fullerene cages within graphitic networks.

X-ray diffraction (XRD) data show broadening and reduced intensity of typical C_{60} crystalline peaks, indicating polymerization-induced loss of long-range crystalline order and evidence of intermolecular covalent bonding. High-resolution transmission electron microscopy (HRTEM) images display morphological changes corresponding to covalent bond formation between fullerene molecules, validating the formation of a polymerized graphullerene phase.

This liquid-phase laser-assisted method offers a scalable, environmentally benign pathway for polymerization and partial graphitization of fullerenes in solution. The combination of Raman, XRD, and HRTEM analyses firmly establishes laser irradiation in IPA as a powerful technique for crafting graphullerene nanostructures with tailored structural and electronic properties. These graphullerene materials hold promise for future applications in nanoscale electronic devices, sensors, and catalytic systems.

Keywords: Fullerene; Laser Irradiation of Liquid phase; Graphullerene;

(Abstract Domain: 4)

DFT INSIGHTS INTO AMINO ACID FUNCTIONALIZED BORON NITRIDE NANOTUBE FOR EFFICIENT TARGETED DRUG DELIVERY

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ABSTRACT

Cancer remains one of the most critical global health challenges, with conventional therapies such as chemotherapy often limited by poor solubility, low bioavailability, systemic toxicity, and the emergence of multidrug resistance. These challenges have driven the development of targeted drug delivery strategies, where nanocarriers play a central role in enhancing therapeutic efficacy while minimizing off-target effects. Among available nanomaterials, boron nitride nanotubes (BNNTs) are particularly attractive owing to their high mechanical strength, chemical and thermal stability, and intrinsic biocompatibility. However, their hydrophobic nature and poor aqueous solubility restrict direct biomedical applications. Surface functionalization provides an effective route to overcome these limitations by improving dispersibility, polarity, and biomolecular interactions. In this study, density functional theory (DFT) simulations were employed to investigate the covalent functionalization of armchair (5,5) BNNT with three representative amino acids: arginine, valine, and phenylalanine. These molecules were selected for their distinct side-chain properties, enabling electrostatic, van der Waals, and π-π stacking interactions. Both single and double functionalizations were systematically analyzed to assess their impact on geometry, binding affinity, thermodynamic stability, electronic structure, and solvation behavior. The results reveal that amino acid attachment induces a shift from sp^2 to sp^3 hybridization, accompanied by bond distortions that increase surface reactivity and polarity. Thermodynamic analyses confirm the stability of all functionalized systems, with phenylalanine showing the strongest binding energy. Furthermore, solvation studies highlight significant improvement in aqueous compatibility, with double functionalized BNNT with phenylalanine (BNNT-2Phe), displaying the most favorable Gibbs free energy of solvation. Drug interaction studies with resveratrol on the BNNT-2Phe system demonstrate strong noncovalent adsorption and favorable charge redistribution, underscoring its potential for efficient drug loading and controlled release. Overall, this work establishes amino acid functionalization as an effective strategy to tune the structural, electronic, solvation, and drug-interactive properties of BNNT, providing a robust theoretical foundation for their application as efficient and biocompatible nanocarriers in targeted drug delivery.

Keywords: Thermodynamic stability; Solvation behaviour; Biomolecular interactions; Resveratrol.

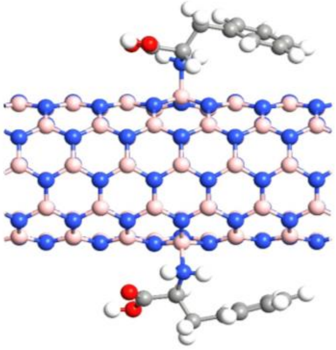

Fig.1 Optimized structure of BNNT-2Phe

(Abstract Domain: 4)

Dual-Side Functionalized AlNNTs for Enhanced 5-Fluorouracil Delivery: A DFT Investigation

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ABSTRACT

Targeted nanocarrier-based drug delivery offers a powerful strategy to overcome the limitations of conventional chemotherapy, including nonspecific biodistribution, systemic toxicity, and limited therapeutic selectivity. Among emerging nanomaterials, one-dimensional (1D) aluminum nitride nanotubes (AlNNTs) have attracted considerable interest due to their wide bandgap, high thermal conductivity, chemical stability, mechanical strength, and intrinsic biocompatibility, making them excellent candidates for engineered drug delivery platforms. In this work, first-principles density functional theory (DFT) is employed to investigate armchair (5,5) AlNNT that are dual-side functionalized to enhance drug-loading capacity and therapeutic performance. One terminus of the AlNNT is covalently modified with sorbic acid and butyric acid, biologically active organic acids with antimicrobial, anticancer, and histone deacetylase (HDAC) inhibitory properties, while the opposite terminus is decorated with amine ($-NH_2$) and carbonyl (C=O) groups to improve hydrophilicity, hydrogen bonding, and dipole–dipole interactions. This rational functionalization strategy enhances aqueous dispersibility, colloidal stability, and chemical reactivity, all of which are critical for efficient drug adsorption. Comprehensive DFT analyses, including structural optimization, binding-energy calculations, charge-transfer evaluation, density of states (DOS), and frontier molecular orbital (HOMO–LUMO) characterization, were conducted to probe the structural stability and electronic properties of the functionalized AlNNTs. Notably, among the surface chemistries examined, the sorbic acid functionalized AlNNT with dual carbonyl termination exhibits the highest aqueous solubility and the most favorable interaction with 5-fluorouracil (5-FU), underscoring the pivotal role of carbonyl-rich functionalization in enhancing drug–carrier affinity and stability. These findings demonstrate that the synergistic effects of dual-side organic acid functionalization, combined with terminal $-NH_2$ and C=O modification, substantially improve the drug-binding affinity and electronic tunability of AlNNTs. Overall, this work provides atomic-level insights into drug–nanotube interactions and highlights sorbic acid– and dual-carbonyl–functionalized AlNNTs as robust, biocompatible nanocarriers for next-generation precision oncology applications.

Keywords: Density Functional Theory (DFT), Functionalization, Nanocarriers, 5-Fluorouracil.

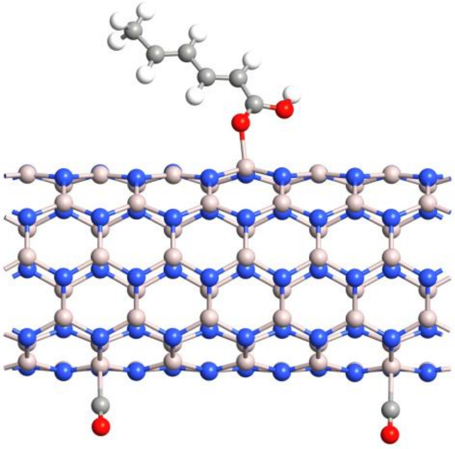

Fig 1: Sorbic acid functionalized AlNNT with dual carbonyl

Magnetic and Transport Properties of ordered $LaSrMnRuO_6$ double perovskite thin Films

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Abstract:

Double perovskite (DPs) oxides have a general formula $A_2BB'O_6$ or $AA'BB'O_6$. They show various interesting properties such as ferromagnetism, antiferromagnetic, tunnelling-type magnetoresistance (TMR) with half metallicity and some unusual magnetic states such as spin glass [1-3]. Bulk $LaSrMnRuO_6$ (LSMRO) has an orthorhombic structure with a *Pnma* space group and Mn/Ru disorder at the B-site [4]. XPS measurement reveals mixed valency of Mn (+2, +3) and Ru (+4, +5) in the system. M-T measurement on bulk LSMRO sample shows that ZFC curve displays two transitions in 100 Oe field at ~223 K, followed by a cluster glass transition at ~32 K., whereas FC curve shows a transition at 218 K. Also, at 5 K, the magnetic moment lacks saturation, and has a maximum value of $\sim 2.3\ \mu_B/f.\ u$ under 70 kOe field, which is less than theoretically predicted value of B-site ordered sample i.e $\sim 6.6\ \mu_B/f.\ u$ for Mn^{3+} and Ru^{4+} [5]. Therefore, the ordered double perovskites are considered to be better for improving magnetic and transport properties such as Curie temperature and magnetization, etc [6]. In this work, we have fabricated epitaxial LSMRO thin films STO (111) substrate using the pulsed laser deposition technique. We observed the (111) and (333) superlattice peaks at ~19° and ~61° angle in the x-ray pattern of the film, respectively, for various thicknesses, which indicates B-site ordering. From the XRR data fit, the average roughness is 0.9, 1.09 nm, corresponding to 32.4 nm and 66.4 nm thin films, were found, respectively. RSM measurement around the (330) asymmetric plane confirms compressive strain in the thin films. From ZFC magnetic measurement, we observe transitions at ~207 K, followed by a peak at ~200 K for the 66.4 nm film, and ~197 K, followed by a peak at ~190 K for the 32.4 nm film. At a high value of the magnetic field, the value of the transition temperature at ~207 K and ~197 K for both films remains the same. Whereas peak at 200 K and 190 K for both films shifts toward lower temperatures. There were no peaks observed corresponding to the cluster glass transition in bulk. Further, magnetic memory measurement at 20 K and 90 K halt temperature confirms the absence of any glassy transition. Also, at 5 K, an increase in magnetisation was observed in both thin films compared to bulk, which also confirms an increase in B-site ordering. In-

plane and out-of-plane Magnetic measurements suggest the presence of anisotropic magnetoresistance. Further, a thorough analysis of structural, magnetic, and transport properties will be presented [7].

References:

1. K. L. Kobayashi, T. Kimura, H. Sawada, K. Terakura, and Y. Tokura, Nature 395, 677 (1998).
2. J. Willem, G. Bos, and J. P. Attfield, J. Mater. Chem. 15, 715 (2005).
3. B. D. Battle, T. C. Gibb, C. W. Jones, J. Solid St. Chem. 78, 281 (1989).
4. P. M. Woodward, J. Goldberger, M. W. Stoltzfus, H. W. Eng, R. A. Ricciardo, P. N. Santhosh, and P. Karen, J. Am. Cerum. Soc. 96 (6), 1796 (2008).
5. Manuscript to be submitted.
6. J. E. Kleibeuker, E. M. Khoi, E. D. Jones, T. M. Yu, B. Sala, B. A. MacLaren, D. Kepaptsoglou, D. H. Maldonado, Q. M. Ramasse, L. Jones, J. Barthel, I. MacLaren, and J. L. M. Driscoll, NPG Asia Material 9, 406 (2017).
7. Manuscript under preparation.

A COMPREHENSIVE DFT STUDY ON UNRAVELING THE POTENTIAL OF SILICON DOPED GRAPHDIYNE NANOSHEET AS DRUG DELIVERY NANOCARRIERS

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The development of efficient nanocarriers remains a crucial step in advancing targeted drug delivery strategies for neurological disorders. Graphdiyne (GDY), a novel two-dimensional carbon allotrope with intrinsic *sp–sp²* hybridization, offers outstanding stability, tunable electronic properties, and versatile functionalization potential, making it an excellent candidate for biomedical applications. In this study, we systematically investigated the effect of nine dopants (Si, Ge, Sn, S, O, P, Cu, Ag, Au) on GDY to enhance its properties. Among them, silicon doping at site-1 emerged as the most favorable, demonstrating superior biocompatibility and stability. A silicon-doped graphdiyne (Si-GDY) nanocarrier was designed by constructing and optimizing its primitive cell using density functional theory (DFT). The pristine GDY system exhibited a direct band gap of 0.44 eV, while the stability of Si-GDY was confirmed through detailed formation energy ($E_{F.E}$) analysis. To further probe its suitability for drug delivery, solubility characteristics were examined via dipole moment and Gibbs free energy of solvation. In addition, global quantum chemical descriptors—including chemical potential, global hardness, softness, and electrophilicity—were employed to evaluate the intrinsic reactivity of the nanocarrier. Collectively, these findings provide a strong theoretical foundation for subsequent drug adsorption and loading studies, highlighting the promise of Si-GDY as a next-generation nanoplatform for targeted neurotherapeutic applications.

Thin films/Nano-materials Growth, Novel techniques and concepts

Challenges in Development of Silver Coating for Space Applications

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ABSTRACT

Silver based high reflectance coatings are widely used in astronomical telescopes and optoelectronic devices due to their high reflectance and low emissivity in the visible and infrared spectral bands. The working environment has significant influence on the durability of silver based coatings. In order to achieve the high reflectance along with environmental durability for space based telescope optics, the process parameters, coating material selection and coating design optimization to be studied thoroughly. In this present work, we are reporting all the challenges faced during the development of high reflectance protective silver coating for space applications. By successfully overcoming all the challenges, the protective silver coated mirrors are fabricated with required high reflectance and environmental durability.

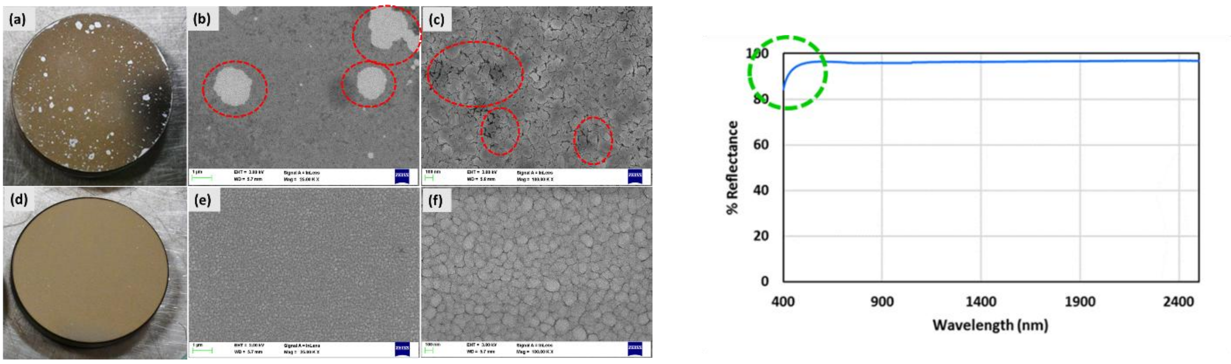

Figure. Coating failures and respective SEM images (a, b &c) & Final high reflectance protective silver coating and its SEM images (d, e & f) & Spectral reflectance vs wavelength graph of the high reflectance protective silver coating

Keywords: High reflectance; design optimization; durability; space qualification

High-Performance VOC Detection via Ru and Rh-Tailored $Ti_3C_2O_2$ MXene: A DFT and NEGF-Based Insight into Breast Cancer Sensing

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Abstract

Early detection of breast cancer, the most prevalent malignancy in women, is constrained by invasive and insensitive conventional diagnostics, prominence the crucial need for non-invasive methods. Exhaled breath analysis, leveraging volatile organic compounds (VOCs) as molecular fingerprints, has developed as a promising approach. Here, density functional theory (DFT) joined with non-equilibrium green function (NEGF) method is employed to explore Ru and Rh adatom tailored $Ti_3C_2O_2$ MXene as innovative nano-biosensors. Both tailored surfaces demonstrate strong thermodynamic stability, with formation energies of –8.519 eV and –8.505 eV. AIMD simulations at 300 K confirm the structural stability of Ru and Rh- tailored $Ti_3C_2O_2$, with adsorption configurations conserved under thermal fluctuations. Ru and Rh-Tailored $Ti_3C_2O_2$ exhibits significantly stronger adsorption of BC associated VOCs 3,3-dimethylpentane,2-methylpentane and heptanal induces pronounced charge transfer, orbital hybridization and magnetic modulation. Remarkably, 2-methyloctane on Ru tailored $Ti_3C_2O_2$ and heptanal on Rh tailored $Ti_3C_2O_2$ exhibits the highest magnetic moment induced of 1.74 and 1.73 μ_B, with consistent sensing response of 89% and 78%, respectively. Transport calculation further discloses distinct modulation of transmission spectra and low-bias I-V curve characteristics with optimal sensitivity attained at bias voltages of 0.4 V and 0.1 V, respectively. By analysing adsorption strength, charge transfer, electron difference density (EDD), electron localization function (ELF), recovery time and transmission spectra, these insights establish Ru and Rh tailored $Ti_3C_2O_2$ as a robust platform for breath based and early-stage breast cancer detection in women.

Keywords: Breast Cancer, volatile organic compounds, density functional theory, Rhodium, Ruthenium, ab into molecular dynamics, non-equilibrium green function,

Dual-Metallic NiNd-MOF with MoS_2 Composite: A Powerhouse for Supercapacitor Applications.

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Abstract

The design of bimetallic metal-organic framework (MOF) composites with layered transition metal dichalcogenides presents a compelling route toward advanced energy storage materials. Herein, we report a streamlined solvothermal synthesis of NiNd-MOF/MoS_2 composites, wherein MoS_2 nanosheets are seamlessly integrated within a redox-active NiNd-MOF matrix. Detailed structural and morphological investigations via XRD, FTIR, and SEM confirm the uniform incorporation of MoS_2 and homogenous dispersion of bimetallic nanoparticles. Electrochemical evaluation reveals an exceptional specific capacitance of 813 F g^{-1}, surpassing individual constituents and reflecting pronounced synergistic effects. Electrochemical impedance analysis indicates markedly reduced charge transfer resistance and enhanced ion diffusion, while cycling tests demonstrate the composite's remarkable stability. This work highlights the strategic assembly of MOF-derived architectures with conductive chalcogenides, establishing NiNd-MOF@MoS_2 as a robust and efficient electrode for high-performance supercapacitors, and advancing the frontier of sustainable energy storage technologies.

Keywords: NiNd-MOF, MoS_2 nanosheets, Metal-organic framework composite, Supercapacitor electrode, Electrochemical energy storage, Redox-active materials, Charge transfer resistance, Ion diffusion kinetics, Solvothermal synthesis, Bimetallic nanoparticles

Probing Interfacial Charge Transfer in Diketopyrrolopyrrole/Perovskite Quantum Dots, an Organic and Inorganic Hybrid Heterostructure

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ABSTRACT: Small molecule-based organic semiconductors have attracted attention for electronic applications due to their features such as flexibility, low-cost fabrication, and effective solution processing. On the other hand, all inorganic perovskite quantum dot (QD) semiconductors are renowned candidates for their excellent optoelectronic properties. Despite these strengths, their overall performance is limited owing to shortcomings such as the low intrinsic conductivity of organic semiconductors and the processability challenges associated with the inorganic semiconductors. Thus, to understand the combined effect of the two semiconductors, a heterostructure is developed. Herein, a diketopyrrolopyrrole-based organic chromophore and an inorganic halide perovskite QD are combined to form a hybrid heterostructure. The crystallographic analysis, such as single-crystal and powder X-ray diffraction, X-ray photoelectron spectroscopy (XPS), and high-resolution transmission electron microscopy (HR-TEM), are employed to confirm the formation of the heterostructure. Furthermore, from optical analysis, the phenomenon of interfacial charge transfer from inorganic to the organic semiconductor is observed. The frontier molecular orbital obtained from the cyclic voltammogram (CV) exhibits realignment in the hybrid heterostructure to generate a type-I heterojunction. Finally, the improvement in the photo-response of the hybrid heterostructure is discussed using AC conductivity measurements.

Keywords: Hybrid heterostructure, interfacial charge transfer, heterojunction, photo-response

A comparative study of the multifunctional role of a heterocyclic organic compound in organic-inorganic halide perovskite

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Abstract: Surface defects in metal halide perovskite single crystals (SCs) often cause charge recombination and degradation, reducing their optoelectronic performance. In this context, to overcome the materials limitations, various organic molecules, either as a passivator for the existing perovskites or as a principal A-site cation, have been explored. Therefore, this study examines a heterocyclic organic compound in both roles: as a passivator for methylammonium lead bromide ($MAPbBr_3$) SCs and as an A-site cation in the perovskite structure. LC-MS, ^1H-NMR, ^{13}C-NMR, FT-IR and XPS were employed to confirm the presence of the heterocyclic compound on $MAPbBr_3$ SCs and study interactions between the heterocyclic compound and Pb^{2+} ions. From P-XRD and SC-XRD, it was observed that the heterocyclic compound-based perovskite crystallized in a one-dimensional chain-like structure, distinct from the three-dimensional $MAPbBr_3$. Furthermore, from optical analysis, it was found that when used as the A-site cation in the perovskite crystal lattice, the heterocyclic compound-based perovskite resulted in the highest solid-state PLQY of 3.59%, which is higher than that of both $MAPbBr_3$ analogues. Also, the role of the heterocyclic compound in defect passivation was systematically investigated through positron annihilation spectroscopy in both the passivated and the low-dimensional perovskite structure, enabling a direct comparison with the pristine $MAPbBr_3$. Finally, *AC* and *DC* conductivity methods were employed to understand the distinct variation in the electronic properties of each of the three compounds.

Keywords: Passivator, heterocyclic, photo-response, A-site

Highly Efficient Degradation of Toxic Congo Red Dye under Sunshine Using Mesoporous $BiZnO_3/g\text{-}C_3N_4$ Nanocomposite

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Abstract

The presence of toxic Congo red (CR) dye in water has significant impacts on human health and the environment. The development of a cost-effective and efficient technique for CR degradation is essential. In this study, mesoporous $BiZnO_3/g\text{-}C_3N_4$ nanocomposites were synthesized via thermal decomposition for the degradation of CR dye under sunshine. Powder X-ray diffraction analysis revealed the formation of pure phases of the materials, with the average crystallite size of $BiZnO_3$ being 20.89 nm. FT-IR spectrum shows presence of different functional group such as Bi–O, Zn–O, C–N, and C=N. The surface morphology of the sample showed $BiZnO_3$ nanorods (100 nm – 300 nm) embedded in $g\text{-}C_3N_4$ sheets. HRTEM image showed the formation of lattice fringes with an interplanar spacing of 0.200 nm, corresponding to the (431) plane of $BiZnO_3$. The specific surface areas of mesoporous $BiZnO_3$, g-C N , and BiZnO /g-C_3N were 14.02, 17.30, and 45.82 m^2/g, respectively. The direct band gaps of $BiZnO_3$, $g\text{-}C_3N_4$ and $BiZnO_3/g\text{-}C_3N_4$ were found to be 3.37 eV, 2.90 eV and 3.43 eV respectively. The $BiZnO_3/g\text{-}C_3N_4$ nanocomposite exhibited 99.79% removal of CR dye within one hour and followed a first-order reaction kinetic model, with a rate constant of 0.0470 min ^{1}. Degradation efficiency decreased with an increase in the pH of the solution, with the maximum efficiency observed at pH 2. The presence of co-existing anions affected degradation efficiency in the following order: IO_3 > Cl > Br > NO_3 > PO_4^{3-}. Scavenger experiments indicated that •OH and h are the active species involved in CR degradation. Furthermore, after six recycling runs, the catalyst performance showed only a 6% decrease, indicating the stability of the $BiZnO_3/g\text{-}C_3N_4$ nanocomposite. This study demonstrates that the synthesized $BiZnO_3/g\text{-}C_3N_4$ nanocomposite holds significant potential for the effectively removal of toxic CR dye from wastewater.

Keywords: $BiZnO_3/g\text{-}C_3N_4$, Perovskite, Photocatalyst, Degradation, Congo Red dye

References

1. Najafian, H., Manteghi, F., Beshkar, F., and Salavati-Niasari, M. Efficient degradation of azo dye pollutants on ZnBi38O58 nanostructures under visible-light irradiation. *Separation and Purification Technology*, 2018, *195*, 30-36.

2. Dustgeer, M. R.; Jilani, A.; Ansari, M. O.; Shakoor, M. B.; Ali, S.; Imtiaz, A.; Zakria, H. S.; Othman, M. H. D. Reduced Graphene Oxide Supported Polyaniline/Copper (II) Oxide Nanostructures for Enhanced Photocatalytic Degradation of Congo Red and Hydrogen Production from Water. *Journal of Water Process Engineering* **2024**, *59*, 105053.

Synergistic interface: Enhancement of device performance of rare earth metal oxide decorated Ni-MOF pseudo-supercapacitors

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ABSTRACT

Porous nickel-based metal-organic frameworks (Ni-MOFs) are interesting candidates for electrode applications in high-performance supercapacitors. The tunable structure combined with extensive surface area enable Ni-MOFs to be highly effective in such application. The electrochemical properties of the synthesized Ni-MOF are thoroughly analysed using galvanostatic charge-discharge (GCD) (Figure 1a) and cyclic voltammetry (CV). The Ni-MOF produced with 2-aminoterephthalic acid is polycrystalline in nature, which is confirmed by X-ray diffraction (XRD) as shown in Fig. 1b. Cyclic voltammetry experiments, performed between 0 and 0.8 V at scan rates ranging from 5 to 100 mV/s, exhibit different redox peaks and analogous loop profiles; thereby affirming the electrochemical reversibility of the material. In a three-electrode setup utilizing a 3M KOH electrolyte, the pristine Ni-MOF exhibited a specific capacitance of roughly 377 F/g at a current density of 1 A/g. Nonetheless, a notable disadvantage of pristine Ni-MOFs is their intrinsic low electrical conductivity and restricted long-term stability. A mixture of Ni-MOF and cerium oxide (CeO_2) was created to overcome these constraints, and was validated via XRD analysis (Fig. 1b). The addition of cerium oxide resulted in significant enhancement of electrochemical performance of composite material. This improvement is presumably due to the combined impact of CeO_2's elevated redox activity and its capacity to boost charge transfer kinetics. As a result, the Ni-MOF/CeO_2 composite attained a significant enhancement in specific capacitance to around 600 F/g at a current density of 1 A/g from GCD.

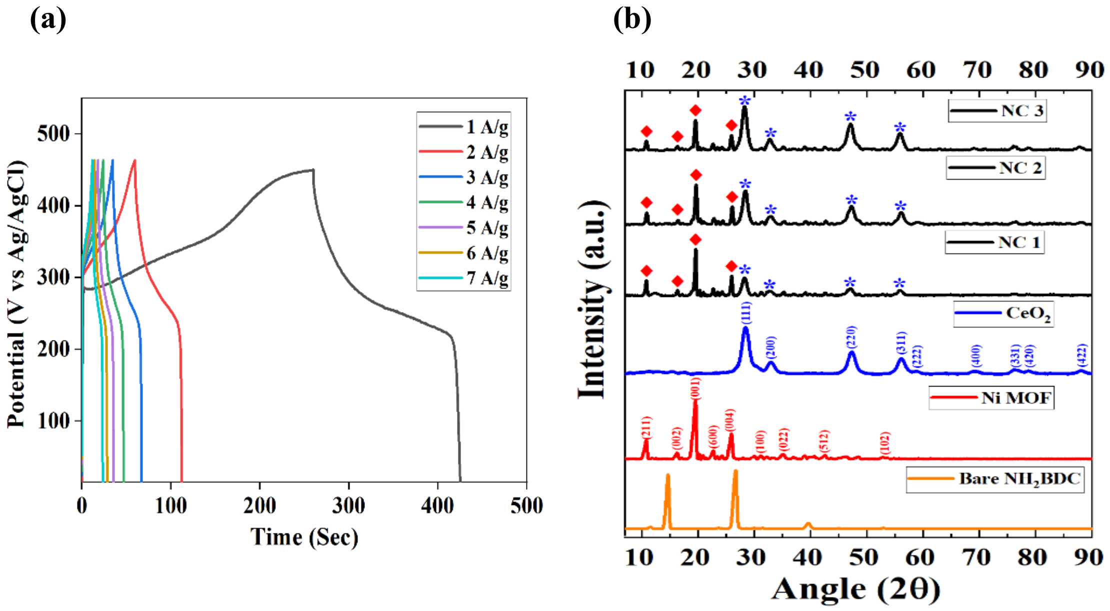

Figure 1: **(a)** Typical charge-discharge cycle obtained from the Ni-MOF, **(b)** XRD patterns of Ni-based MOF and their respective composite materials.

References:

1. Du, J., Zhang, C., Cheng, S., Zhang, H., Wu, X., Du, S., & Zhao, Z. (2018). Fabrication of hierarchical porous nickel-based metal-organic framework (Ni-MOF) constructed with nanosheets as novel pseudocapacitive electrode materials for supercapacitors. Journal of Alloys and Compounds, 740, 269-276.J. Yang, P. Xiong, C. Zheng, H. Qiu, M. Wei, Metal-organic frameworks: a new promising class of materials for a high-performance supercapacitor electrode, J. Mater. Chem. A 2 (2014) 16640–16644.

2. Wu, J., Zhou, J., Liu, G., Li, Q., Lu, Z., Cao, J., & Yang, B. (2020). Construction of metal-organic framework-derived CeO$_2$/C integrated MoS$_2$ hybrid for high-performance asymmetric supercapacitor. Electrochimica Acta, 353, 136502.

CuCo MOF/Ni(OH)$_2$ Composite for High-Performance Supercapacitor Electrodes

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ABSTRACT

This study details the synthesis and comprehensive electrochemical investigation of a novel Copper-Cobalt Metal-Organic Framework (Cu-Co MOF) and Nickel Hydroxide (Ni (OH)$_2$) composite designed as an advanced supercapacitor electrode material. The architectural strategy leverages the high porosity and expansive surface area of the Cu-Co MOF as a scaffold, complemented by the superior pseudocapacitive charge storage capability of Ni(OH)$_2$. The MOF component effectively provides numerous active sites and facilitates rapid ion-transport pathways, while the embedded Ni(OH)$_2$ contributes a high theoretical capacity via reversible redox reactions. The Cu-Co MOF/Ni(OH)2 composite was fabricated via a hydrothermal method, ensuring intimate interfacial contact between the constituents. Structural and morphological characterization, including X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM), confirmed the successful integration, demonstrating that Ni(OH)$_2$ nanoparticles are uniformly dispersed and securely anchored within the Cu-Co MOF matrix. Electrochemical performance, assessed using cyclic voltammetry, galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) in a concentrated aqueous electrolyte, revealed significant synergistic enhancement compared to the individual components. The CuCo MOF/Ni(OH)$_2$ electrode exhibited a high specific capacitance, exceeding 450 F/g at a current density of 1 A/g. This superior capacity is directly attributed to the combined structural benefits of the MOF, which optimizes ion diffusion kinetics, and the inherent high charge storage capability of the Ni(OH)$_2$. Moreover, the composite demonstrated excellent rate capability and robust long-term cycling stability, retaining a high percentage of its initial capacitance over thousands of cycles, validating its structural integrity and electrochemical reversibility. These promising results establish the CuCo MOF/Ni(OH)$_2$ composite as a highly effective and robust electrode material with significant potential for developing next-generation, high-energy-density supercapacitors.

(Abstract Domain : Thin films/Nano-materials Growth, Novel techniques, and concepts)

Next-Generation Nanocomposites: Emerging Photocatalysts for Energy and Environmental Applications

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ABSTRACT

The necessity of sustainable energy solutions and effective environmental remediation technologies has intensified research on solar/light-driven harvesting applications like photocatalytic degradation of pollutants, Hydrogen production (solar water splitting), CO_2 Reduction and carbon capture (artificial photosynthesis), solar desalination, photo-rechargeable devices etc. The performance of traditional photocatalysts is constrained by factors such as limited visible-light absorption, rapid electron–hole recombination, and low quantum efficiency. To achieve versatile and high-performance photocatalytic systems, next-generation binary and ternary nanocomposites are being designed rationally by coupling metal oxides with two-dimensional (2D) layered materials. By synergistic integration of different materials, their structural, optical, and electronic properties can enhance their potential in energy conversion and environmental purification.

Binary nanocomposites, such as $MoSe_2$/g-C_3N_4, Ag_2WO_4/h-BN, ZnO/h-BN, TiO_2/ SnSe-SnO_2 based hybrids, have demonstrated remarkable improvements in charge separation and light-harvesting capability. The interfacial heterojunctions created in these nanocomposites enhance electron transfer pathways, suppress recombination rate and expand the light absorption across both ultraviolet and visible regions of the spectrum. For example, $MoSe_2$ combined with g-C_3N_4 or TiO_2 with SnSe-SnO_2 hybrid not only extends solar absorption but also enables efficient degradation of organic pollutants [1,2]. Similarly, Ag_2WO_4 coupled with 2D h-BN offers excellent stability, high surface area, and superior adsorption–photodegradation synergy [3]. Beyond this, ternary nanocomposites with multiple heterojunctions, offer more efficient charge migration networks. The prospective nanocomposites include TiO_2/MoS_2/h-BN and $MoSe_2$/g-C_3N_4/h-BN, which integrate the benefits of layered semiconductors, narrow bandgap absorbers, and high-surface-area supports. The hierarchical structures, coupled with tailored band alignments, not only ensure efficient photogenerated carrier separation but also improve the durability and recyclability of the photocatalysts.

We have reviewed the most efficient binary and ternary photocatalysts with enhanced degradation rates and explored the underlying factors responsible for their high performance based on their bandgap, BET surface area, heterojunction type (type-II, Z-scheme, and S-scheme), lifetime of photogenerated carriers, free radical or charge carriers involved in degradation of pollutant molecules along with type, concentration of pollutant molecules and catalyst dosage.

Keywords: Nanocomposites, Photocatalysis, heterojunctions, layered semiconducting material

References

1. L. Sarma, G. Mann, A. Datta, M. Thirumal, New J. Chem. 46, 5137 (2022).
2. B.Y. Balarabe, P. Maity, A.C.S.C. Teixeira, S.A. Iwarere, Inorg. Chem. Commun. 158, 111560 (2023).
3. V. Bagga, N. Singh, M. Khanuja, M. Rani, D. Kaur, Mater. Res. Bull. 159, 112109 (2023).

σ-Aromatic Envelope Geometry in Penta Coordinated Group 13-Bridged Transition Metal Carbonyl Clusters

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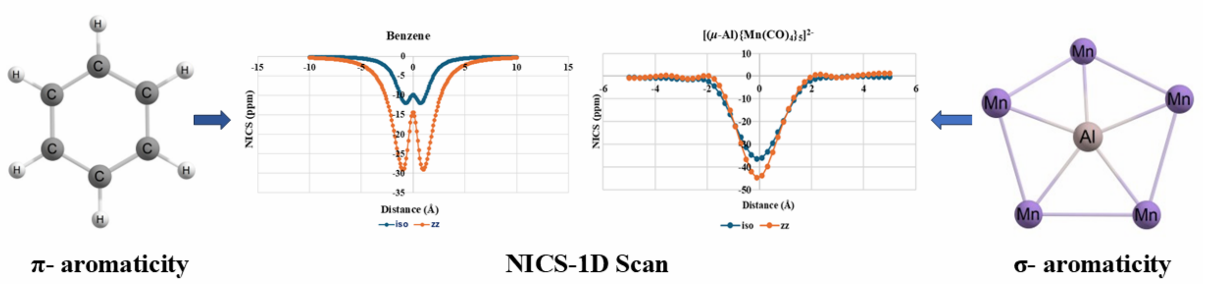
Abstract:
Metal carbonyl complexes and clusters gain stability through aromaticity.[1,2] In this study, five-membered ring containing penta-coordinated group 13 metal carbonyl clusters of the type $[(\mu\text{-E})\{M(CO)_4\}_5]^{2-}$, where E = B, Al, Ga, In, Tl, and M = Mn, Tc, Re are considered. DFT was employed for geometry optimization, revealing unusual but stable envelope-like structures, while aromatic character was evaluated using magnetic criteria, including Nucleus Independent Chemical Shifts (NICS), Gauge-Including Magnetically Induced Currents (GIMIC). All the carbonyl clusters show σ-aromaticity. These studies reveal notable diatropic ring currents and highly negative NICS values in selected clusters of $[(\mu\text{-E})\{M(CO)_4\}_5]^{2-}$ species, indicative of strong σ-aromaticity. The σ-aromaticity is confirmed by NICS scan, NICS decomposition, and Natural Orbitals for Chemical Valence (EDA-NOCV). The trends in aromaticity are NICS: B > Al > Ga > In (Mn), and B > In ≥ Ga > Al (Tc, Re); GIMIC: B > Ga > In > Al (Mn), and B > In ≥ Ga > Al (Tc, Re).



Scheme 1: Comparison of the NICS-1D scan of benzene and penta-coordinated group 13 metal carbonyl cluster.

Keywords: *Aromaticity; metal carbonyls; envelope geometry; ring current; EDA-NOCV.*

Reference:

(1) Patra, S. G. Craig-Möbius Type Antiaromatic Chelate Ring. *Chem. Phys. Lett.* **2020**, *741* (December 2019), 137093. https://doi.org/10.1016/j.cplett.2020.137093.

(2) Patra, S. G.; Mondal, T. Interplay of Hückel and Möbius Aromaticity in Metal-Metal Quintuple Bonded Complexes of Cr, Mo, and W with Amidinate Ligand: Ab Initio DFT and Multireference Analysis. *ChemPhysChem* **2021**, *22* (3), 298–311. https://doi.org/10.1002/cphc.202000923.

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(Abstract Domain: Computational modelling & simulations)

Computational Desiging of Resonant Modes in Defect-Engineered One-Dimensional TiO_2/SiO_2 Photonic Crystals for Enhanced Optical Sensing

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ABSTRACT

Photonic crystals (PCs) with engineered defect modes present a highly promising platform for advanced optical sensing applications. This study conducts a computational investigation into one-dimensional (1D) TiO_2/SiO_2 photonic crystal structures, modified by the introduction of a central defect layer. Using the Transfer Matrix Method (TMM), this work presents simulations of the photonic bandgap (PBG) and systematically vary the defect layer's thickness and refractive index to analyse their impact on resonant transmission characteristics. The introduction of the defect layer generates sharp, high-quality (high-Q) resonant peaks within the PBG, whose spectral positions exhibit strong sensitivity to changes in the defect layer's optical properties. Results of the study demonstrate that the resonant wavelength shifts significantly with variations in the ambient refractive index, underscoring the potential of these structures for label-free optical, chemical, and biological sensing. The findings suggest that defect-engineered 1D TiO_2/SiO_2 photonic crystals offer a robust, cost-effective, and highly sensitive platform for next-generation sensing technologies.

Keywords: Photonic Crystals, Photonic Bandgap, Transfer Matrix Method, Optical Sensing

Influence of Film Thickness on the Performance of CuS-Based Resistive Switching Devices

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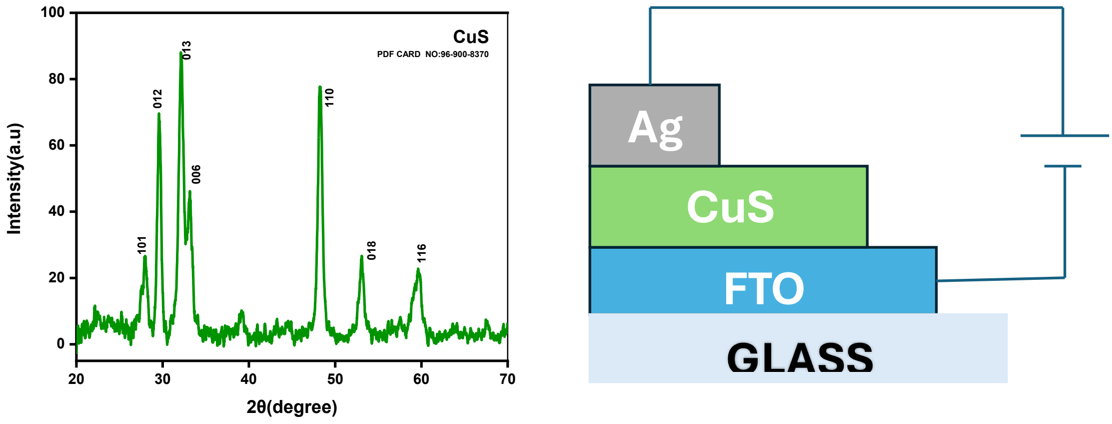
ABSTRACT

We investigate the influence of film thickness on the structural, optical, and electrical properties of Copper Sulfide (CuS) thin films and their application in memristive devices. CuS thin films with varying thicknesses were deposited on Fluorine-doped Tin Oxide (FTO) glass substrates at a temperature of 523 K using a co-evaporation method. Structural and compositional analysis confirmed the successful synthesis of the material. X-ray Diffraction (XRD) measurements verified the formation of the covellite phase of CuS, which is in good agreement with PDF card number 96-900-8370. Furthermore, Energy-Dispersive Spectroscopy (EDS) confirmed the presence of the constituent elements, copper (Cu) and sulfur (S), in the deposited films. Optical and electrical characterization revealed thickness-dependent properties. Optical studies showed that the direct optical band gap decreases from 2.18 eV to 1.6 eV with the decrease in film thickness. Electrical measurements confirmed the p-type conductivity of the CuS films, and analysis of parameters such as charge carrier mobility and electrical conductivity demonstrated a clear dependence on film thickness. Two-terminal memristor devices with structure of <FTO/CuS/Ag> are fabricated and evaluated their resistive switching characteristics. The highest on/off ratio of 96 was observed for devices fabricated with lowest CuS film thickness.

Keywords: copper sulfide; co-evaporation; memristor



(a) (b)

Fig. (a) XRD pattern of CuS thin film (b) schematic diagram of <FTO/CuS/Ag> device

Investigation of optical property of titanium-tungsten oxide doped borosilicate glasses synthesised via microwave-assisted heating and conventional heating method: A comparative study

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ABSTRACT

Energy saving glasses (Near infrared shielding glasses) aim at bridging the gap between global energy consumption and promoting environmental sustainability. The energy-saving glass windows accord an advantage of selective shielding of Near infrared (NIR) radiations while remaining transparent to visible light. The titanium-tungsten oxide doped borosilicate glasses with composition WO_3-SiO_2-B_2O_3-Na_2O-CaO-K_2O-TiO_2 were synthesised via microwave-assisted heating method at temperature 1200 °C, 2 hr. The identical batch was synthesised by conventional heating method. UV-Vis-NIR spectroscopy was employed to study the NIR shielding ability and visible transmittance in the doped borosilicate glasses. The NIR shielding ability was found higher in doped borosilicate glasses synthesised via microwave-assisted heating method. XPS spectroscopy demonstrated formation of W^{4+} ions (WO_{3-x}) as reduced state in synthesised glasses via microwave-assisted heating method, owing to strong NIR shielding ability. The total glass melting time was found to be less in microwave-assisted heating in comparison to conventional heating method. Hence, energy consumption was lesser in microwave-assisted heating as compared to conventional heating. Thus, microwave-assisted heating favours more stabilization of W^{4+} ions in titanium-tungsten oxide doped borosilicate glasses, which is unlike in conventional heating method. Therefore, cost-effective doped borosilicate glasses can be utilized for NIR-shielding application at industrial scale in buildings and infrastructures.

Keywords: Microwave-assisted heating; NIR shielding ability; visible transmittance; non-stochiometric tungsten oxide.

(Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts)

Exploring the memristive behaviour in spray pyrolyzed Cerium Oxide thin film.

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Abstract

The rapid development of information technology has led to the efficient use of energy storage device. ReRAM is a non-volatile memory device which stores data in the form of resistance. Cerium oxide becomes the material of choice because of it has the ability to switch back and forth between two oxidation states +3, +4. When a voltage is applied, cerium switches between these two states either by undergoing oxidation or reduction. Cerium Oxide is not much explored material. Cerium is a rare earth metal. This work aims to the development of FTO/CeO_2/Ag thin film memristor device using spray pyrolysis. Ag and FTO are used as top and bottom electrode. CeO_2 thin film of three different concentrations of 0.01M, 0.03M, 0.05M of precursor solution was coated on FTO. Structural studies were carried out using X ray diffraction. The peaks corresponding to the (111), (200), (220) and (311) plane confirms the presence of Cerium Oxide. Morphological studies were carried out using scanning electron microscopy. Optical properties were analysed using UV-Visible spectroscopy and photoluminescence. The band gap is found to be decreasing with increase in concentration from 3.05eV to 2.91eV. The absorbance peak is found to be around 300 nm. Photoluminescence, reveals a peak formed around 350nm that corresponds to cerium oxide and a peak at 470 nm shows the formation of oxygen vacancy. I-V characteristics were studied using Keysight B2901A. It shows memristor property of the deposited material. The On/Off ratio is 4 for the device fabricated with thin films deposited using 0.03M concentration precursor.

Keywords: Cerium Oxide; Spray Pyrolysis; Memristor

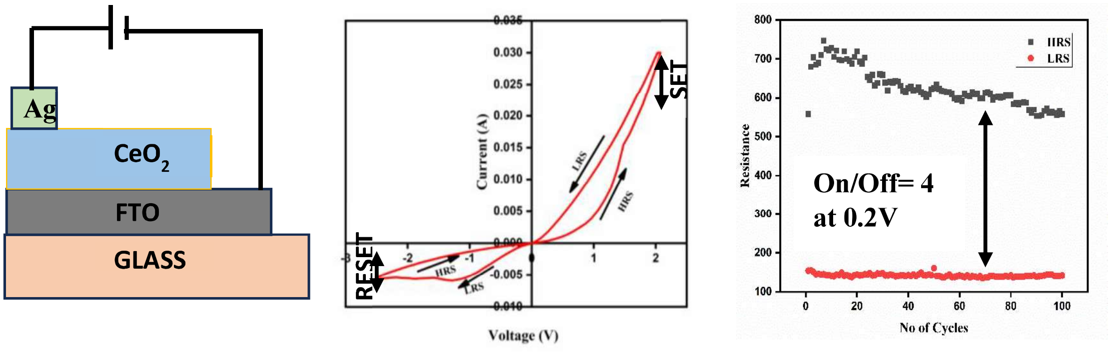

Fig:(a) **Fig: (b)** **Fig:(c)**

Fig:(a) Schematic of <FTO/CeO_2/Ag> Memristor, Fig:(b) I-V curve characteristics of thin film deposited using 0.03M concentration precursor, Fig:(c) endurance cycle of the former graph

Design and development of organic hole transport materials for n-i-p structure perovskite solar cells

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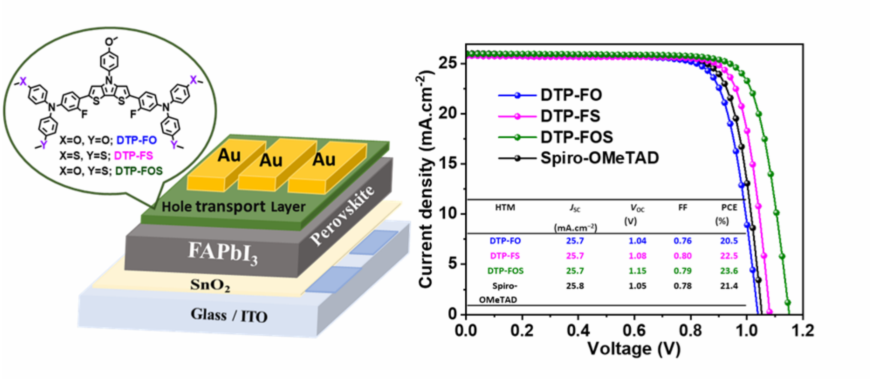
ABSTRACT:

Organic hole-transport materials (HTMs) play complementary and crucial roles in high-performance perovskite solar cells by controlling charge extraction, interfacial energetics, and device stability. Moreover, HTMs (small molecules and polymers) provide the contiguous transport network that selectively extracts and transports photogenerated holes to the anode while blocking electrons. Herein, we introduce novel HTMs featuring a D-π-D molecular structure. These HTMs have 3-fluoro-*N,N*-bis(4-(methylthio)phenyl)aniline (TPASF) peripheral terminal groups, which are linked with various π-core moieties. Our investigation reveals that altering the π-linkers affects the film morphology of the HTMs, significantly influencing device performance. HTMs. In the similar molecular architecture (D-π-D), incorporating a dithieno[3,2-*b*:2',3'-*d*]pyrrole (DTP) core functionalized with various *ortho*-fluorinated triarylamine donor units. Through systematic modification of the terminal groups, we designed three distinct HTMs: DTP-FO (methoxy terminal group), DTP-FS (methylthio), and DTP-FOS, a hybrid structure incorporating both methoxy and methylthio substituents [4,4'-(4-(4-methoxyphenyl)-4*H*-dithieno[3,2-*b*:2',3'-*d*]pyrrole-2,6-diyl)bis(3-fluoro-*N*-(4-methoxyphenyl)-*N*-(4-(methylthio)phenyl)aniline)]. These tailored structural modifications induce intramolecular noncovalent interactions that effectively regulate the optoelectronic properties, crystallinity, and charge transport characteristics of the HTMs. PSCs fabricated with DTP-FO, DTP-FS, and DTP-FOS achieved average power conversion efficiencies (PCEs) of 20.5%, 22.5%, and 23.6%, respectively. Remarkably, the DTP-FOS-based device retained 75% of its initial efficiency after 2500 hours of continuous illumination under maximum power point tracking at 25°C. Furthermore, both DTP-FS and DTP-FOS outperformed the benchmark 2,2',7,7'-tetrakis-(*N*,*N*-di-4-methoxyphenylamino)-9,9'-spirobifluorene (spiro-OMeTAD) (PCE of 21.4%) not only in terms of PCE, but also in thermal and photostability, indicating their considerable potential for realizing stable and scalable PSC technologies.



HTM	J_{SC} (mA.cm^{-2})	V_{OC} (V)	FF	PCE (%)
DTP-FO	25.7	1.04	0.76	20.5
DTP-FS	25.7	1.08	0.80	22.5
DTP-FOS	25.7	1.15	0.79	23.6
Spiro-OMeTAD	25.8	1.05	0.78	21.4

Fig. 1 Chemical structures of the newly developed HTMs.

Keywords: perovskite; hole transport material; stability; efficiency.

References:

1. T. B. Raju, C. A. M. Senevirathne, M. Watanabe, Y. Fujita, D. Senba and T. Matsushima, *J. Mater. Chem. C,* 2025,**13**, 15082-15090.
2. T. Wu, T. B. Raju, J. Shang, L. Wu, J. T. Song, C. A. M. Senevirathne, A. Staykov, S. Wang, S. Ida, N. Shibayama, T. Miyasaka, T. Matsushima and Z. Guo, *Adv. Mater.*, 2025, **37**, 2414576.

3. M. Zhai, N. Shibayama, T. B. Raju, T. Wu, C. Chen, Z. Guo, T. Matsushima, T. Miyasaka and M. Cheng, *Small,* 2025, 2505961.

Yttrium-Doped Molybdenum Oxide Artificial Synapses for Cognitive Learning and Image Denoising

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Energy-efficient neuromorphic devices are essential for future big data administration, as they enable high-performance computing with reduced power consumption, mimicking the brain's energy-efficient processing capabilities. This is essential to support emerging technologies like artificial intelligence, robotics, and the Internet of Things (IoT). In this work, we report on the successful fabrication of yttrium doped molybdenum oxide thin films using RF magnetron sputtering. These films were utilized as active layers in the fabrication of two-terminal synaptic devices, Au/Y-Mo_xO_y/FTO, which demonstrate pronounced neuromorphic behavior, as compared to pure Mo_xO_y devices. The structural properties were studied by XRD, and the elemental composition was analyzed, and stoichiometry was confirmed through XPS analysis. Synaptic behavior such as potentiation/depression, spike-timing dependent plasticity (STDP), spike-number dependent plasticity (SNDP), paired-pulse facilitation (PPF) and spike-frequency dependent plasticity (SFDP) are successfully demonstrated in these synaptic devices. The fabricated devices demonstrate significant improvement in energy efficiency, being approximately 1000 times more efficient than devices with pure molybdenum oxide. A cognitive model based on the Ebbinghaus memory curve was successfully emulated, showcasing the device's potential in mimicking human memory behavior. Pattern recognition of the artificial synapse on the MNIST dataset was performed using an Artificial Neural Network (ANN) model. These devices demonstrated an accuracy of over 90%, which showcases effectiveness of the fabricated device in accurately classifying handwritten digits. In addition, we also have done a CNN-based denoising of scanning tunnelling microscope (STM) images of carbon atoms on a highly oriented pyrolytic graphite (HOPG) surface. This is done by adding Gaussian noise and comparing the denoised images with the original ones by calculating quantitative metrices such as peak-signal-to-noise ratio (PSNR) and structural similarity index measure (SSIM) values. The resulting metrices were sufficiently high, proving the effectiveness of the Au/Y-Mo_xO_y/FTO artificial synapse-based model in image-processing tasks.

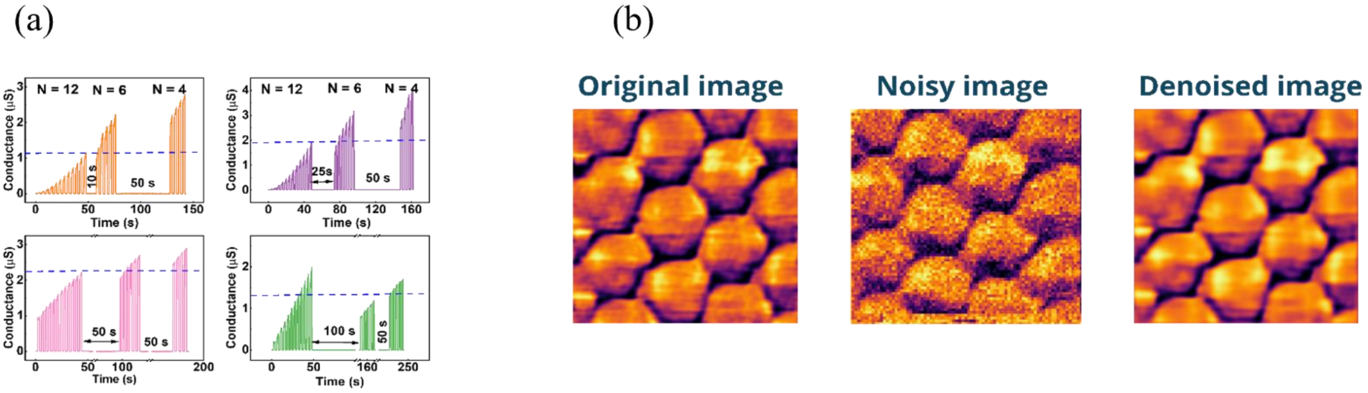

Figure 1 (a) Conductance change following a learning-relearning cycle resembling the Ebbinghaus memory curve, by varying the decay time interval, (b) Original STM image (80 × 80 pixel) with added gaussian noise and its denoised version

References

[1] Rajesh, V. M.; et al. From Hebbian Learning to Pattern Recognition: The Role of Oxygen Vacancies in the Synaptic Responses of Magnetron Sputtered MoxOy Devices. *Mater. Sci. Semicond. Process.*, *188*, 109194 2025.

[2] Zhe Liu; Liu, et al, M. L. Image Denoising Based on a CNN Model. *2018 4th Int. Conf. Control Autom. Robot. ICCAR*, 389–393,2018.

Keywords: Artificial Synapse, Cognitive Learning, Image denoising

Polymer–MXene–Viologen-Based Suprahybrid Electrochromic Device: Flexible Smart Window with Visible and Near-Infrared Switchability

Abstract

Saumya Srivastava

Developing efficient generic electrochromic devices yet capable of demonstrating specialized applications is desired for designing smart (opto)electronic gadgets. An approach of combining material from three different families of (conducting) polymer, organic functional molecules, and modern 2D MXenes has been adopted here to develop a solid-state electrochromic device with improved performance. Such a suprahybrid device is developed where an all-organic polythiophene–viologen-based smart devices have been doped with 2D vanadium carbide (V_2C) MXene not only to enhance the electrochromic performances but also to demonstrate a specialized application in designing multipurpose goggles. The doping of 2D V_2C MXene increases the color contrast and switching speed, which shows switching in the visible as well as near-infrared range so that it can cut heat up to 12%. A high cyclic stability and coloration efficiency was demonstrated in two different wavelength regions. By utilization of the device's flexible nature, a prototype pair of goggles has been prepared that changes the color of one or more frames by selectively giving bias for specialized application in making 3D vision goggles.

A Study on Magnetostrictive and Mechanical Properties Variation in Si-Based Micro-Cantilever with SiO_2 and FeGaCr Thin Films

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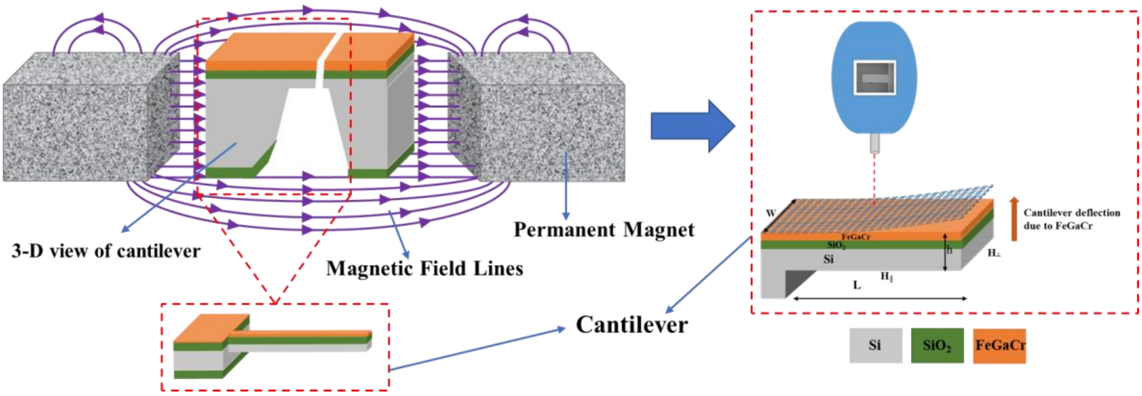
ABSTRACT

Microcantilevers serve as a key component in MEMS devices due to their high sensitivity, low power consumption, and compact form factor. They are extensively used in resonant sensors, bio/chemical detection, energy harvesters, and micro actuator. The mechanical performance of microcantilevers can be significantly tailored through nanoscale material engineering. The ability to tune their mechanical behaviour through magnetostrictive coatings like FeGaCr enables active modulation of device performance under external magnetic fields. Magnetostrictive FeGaCr thin films are very promising for magnetic micro-electro-mechanical systems (magMEMS) due to their exceptional magnetostrictive properties. This study investigates the dynamic and magnetostrictive behaviour of silicon-based microcantilevers modified with SiO_2 and FeGaCr thin films, with a key novelty being the experimental determination of the Young's modulus of the FeGaCr. A cantilever with 578 µm length was fabricated on 8.2 µm thick silicon substrates and coated with a 1 µm SiO_2 layer. The fundamental resonance frequency of the cantilever is 32.175 kHz. The SiO_2 deposited layer showed an effective Young's modulus of 122.60 GPa and a residual stress of -38.946MPa. Subsequent deposition of a 0.7 µm FeGaCr magnetostrictive film led to a reduction in resonance frequency to 31.99 kHz, due to the decrease in effective young modulus to 119.11 GPa. The residual stress decreased to 33.312MPa. The Young's modulus of FeGaCr was found to be 81.46 GPa, while its magnetostriction was measured at 440 ppm. The results highlight the role of magnetostrictive thin films in tuning mechanical and vibrational properties of microcantilever, offering potential for smart MEMS-based applications.

Keywords: Cantilever, Magnetostriction, Young's Modulus, Deflection



Realization and Comparative Performance of MEMS U-Tube Fluid Density Sensor

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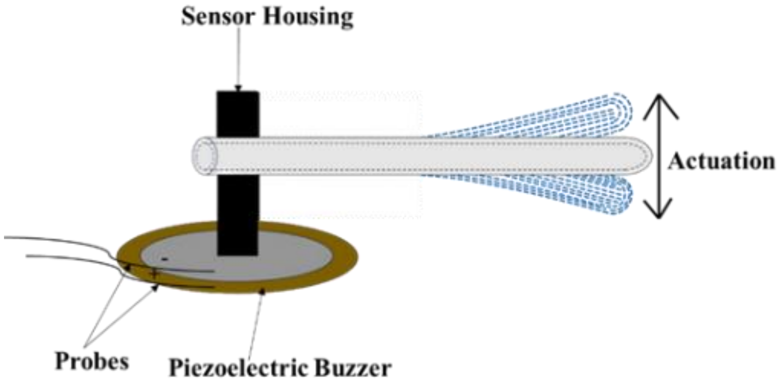
ABSTRACT

A highly sensitive liquid density sensor has been realized using the MEMS-based oscillating U-tube method. Moreover, it is established that high frequency operating U-tube offer enhanced sensitivity and resolution compared to those operating at the lower frequencies. The findings suggest that miniaturized, high-frequency tubes are more efficient and better suited for liquid density sensing applications, especially where small sample volumes and high precision are required. Two different frequency operating devices name as Device-1 (0.898 kHz) and Device-2 (2.269 kHz) are investigated. The devices are fabricated and analysed for their fluid density sensing performance. The experimental setup consists of an oscillating U-tube system incorporating a piezoelectric actuator for mechanical excitation, a micro-pump for accurate fluid delivery, and a compact housing unit to control fluid inlet and outlet. The vibrational behaviour of both U-tubes was studied under different fluid-loading conditions within a density range of 786 to 1000 kg/m³. The Device-1, operating at 0.898 kHz, demonstrated a quality factor in 10.01 - 24.28 range, and deflection amplitudes varies in 8.73 - 40.66 nm range, and a fluid sensitivity of 18.798 ppm $(kgm^{-3})^{-1}$ is experimentally measured. Further, Device-2, operating at 2.269 kHz, with a reduced length of 24.8 mm showed superior performance, including a higher quality factor 51.59 – 98.82 and increased deflection amplitudes 19.32–43.18 nm with improved fluid sensitivity of 26.734 ppm $(kgm^{-3})^{-1}$. These results indicate that high operating frequency U-tube shows enhanced sensitivity and more suitable for high-precision density measurements requiring minimal fluid volume. A key outcome of this study is the demonstrated proportional relationship between resonance frequency and sensitivity, highlighted through a sensitivity–frequency correlation plot.

Keywords: MEMS, piezoelectric excitation, resonance frequency.

Graphical Abstract:



Thin films/Nano-materials Growth, Novel techniques and concepts

Growth and Characterization of CuMnS Thin Films by SILAR for Heterojunction Applications

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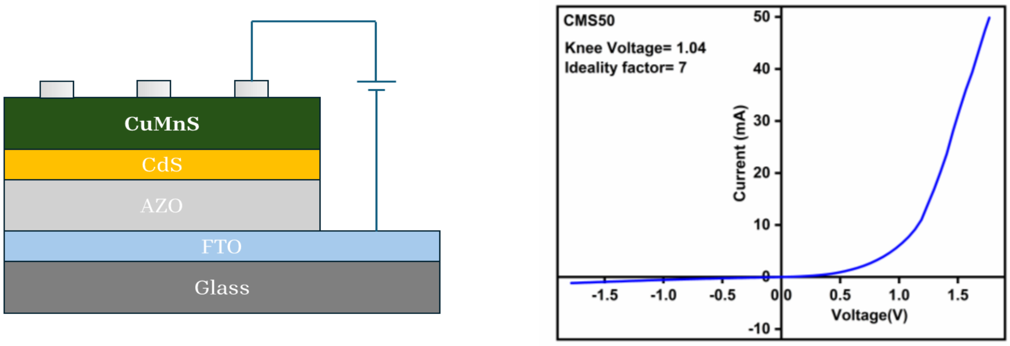
ABSTRACT

Copper manganese sulfide (CuMnS) is an emerging semiconductor that has recently attracted interest owing to its versatile optical and electrical properties. However, reports on its thin-film synthesis and device applications remain limited, making it a largely unexplored material. In this work, CuMnS thin films were successfully deposited on glass substrates using the cost-effective and simple Successive Ionic Layer Adsorption and Reaction (SILAR) technique. Structural, morphological, optical, and electrical properties of the films were systematically investigated as a function of deposition cycles of 50, 65, and 80. X-ray diffraction analysis revealed the formation of hybrid phases with distinct peaks corresponding to MnS, along with additional features indicative of CuMnS. Scanning electron microscopy confirmed a granular surface morphology, while energy-dispersive spectroscopy verified the stoichiometric presence of Cu, Mn, and S in a composition consistent with Cu_2MnS_2. Film thickness increased with deposition cycles, ranging from 60 nm to 140 nm. Correspondingly, optical transmittance decreased with thickness, while all samples exhibited band gaps between 2.0–2.4 eV. Electrical measurements established the p-type nature of the films. A decrease in conductivity with increase in deposition cycles was observed. Heterojunction structures of the form FTO/AZO/CdS/CuMnS/Ag were fabricated. Current-voltage (*I-V*) characterization showed rectifying behaviour, with the device incorporating CuMnS deposited over 50 cycles yielding an ideality factor of 7.

Keywords: Copper Manganese Sulfide; Thin films; Heterojunction devices; SILAR;



(a) (b)

Fig.1 (a) Schematic diagram of <FTO/AZO/CdS/CuMnS/Ag> (b) *I-V* plot of CMS50 device

Early Detection of Lung Cancer Using Vacancy-Ordered Perovskite

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Cancer cases are rapidly increasing worldwide, with lung cancer being one of the leading causes of cancer-related deaths. Cancer detection at an early stage benefits in factors like better survival rate, faster prognosis, etc. There are various lung cancer biomarkers present in saliva, feces, urine, and breath of human beings that can help in the prediction of cancer.[1] One of the biomarkers is Ethyl Acetate present in human urine, whose detection leads to the early detection of lung cancer.[2] For the sensing application, we investigated Vacancy-ordered double perovskite, which is one of the highly potential materials with its optoelectronic and redox properties. In our work, we synthesised Cs_2PdBr_6 using the chemical precipitation method and further explored it for sensing Ethyl Acetate (EA). Moreover, the material characteristics have been investigated using XRD, UV, XPS, and Raman spectroscopy. Due to its low bandgap, the material efficiently absorbs visible light, enabling the generation of electrical power, thus enhancing its feature for self-powered sensors. Additionally, with ample Pd-based vacancies, it shows excellent electrochemical sensing properties. Cs_2PdBr_6 facilitated both electrochemical and photoelectrochemical EA sensing that was inspected in potentiometric and amperometric modes. The sensing material showed interesting results in both dark and light at -0.2 V. In the wide linear concentration range from 1 nM to 1000 nM. The Limit of Detection is 1.72 pM. This sensor exhibits excellent selectivity towards interfering species, including urea, uric acid, glucose, sucrose, and ions such as Na^+, K^+, Cl^-, etc. The LSV approach demonstrates efficient real-time detection capabilities in simulated urine samples. Moreover, the self-powered sensor showed high selectivity, high sensitivity, low response, and low recovery time.

Keywords: Double Halide Perovskite, lung Cancer, Biomarker, Electrochemical detection

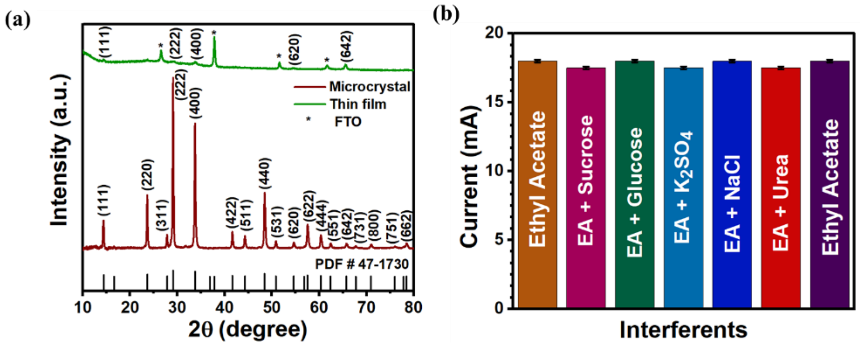

Figure: (a) XRD analysis of Cs_2PdBr_6, (b) Interference testing towards EA

References:

1. Subawickrama Mallika Widanaarachchige, N. R. *et al.* Advancements in Breathomics: Special Focus on Electrochemical Sensing and AI for Chronic Disease Diagnosis and Monitoring. *ACS Omega* **10**, 4187–4196 (2025).
2. da Costa, B. R. B. & De Martinis, B. S. Analysis of urinary VOCs using mass spectrometric methods to diagnose cancer: A review. *Clin. Mass Spectrom.* **18**, 27–37 (2020).

Homoepitaxial Growth of Titanium Dioxide Using Plasma-Enhanced Atomic Layer Deposition

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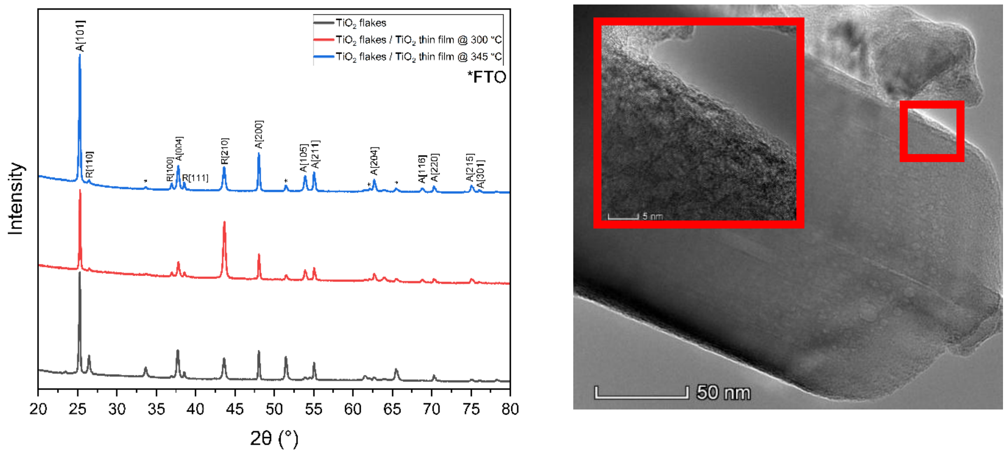
Titanium dioxide (TiO_2) is a well-established wide band-gap semiconductor valued for its electrical and optical properties, including low work function, its high dielectric constant, elevated refractive index, and minimal absorption in the visible range. These characteristics make TiO_2 highly relevant for applications such as solar energy harvesting and photocatalysis. Among the polymorphs, anatase, rutile, and brookite, the anatase phase is particularly appealing due to its superior electron mobility, longer diffusion lengths, and extended carrier lifetimes. While bulk single crystals typically exhibit the best material parameters, thin films are essential for device integration. Achieving epitaxial thin films remains a challenge, as it requires precise control over crystallinity and microstructural quality.

In this abstract, we present the development of a plasma-enhanced atomic layer deposition (PEALD) process tailored for the epitaxial growth of anatase TiO_2 films on hydrothermally grown single-crystal TiO_2 flakes (~2 µm × 2 µm). The flakes, confirmed to be highly crystalline anatase by X-ray diffraction (XRD) (Fig. 1a) and Raman spectroscopy, serve as substrates. Titanium tetraisopropoxide (TTIP) was used as the metal precursor, while oxygen plasma as a coreactant in PEALD. Depositions were carried out under ultra-high vacuum conditions at substrate temperatures in a range around 300 °C. Films deposited below 300 °C exhibited an amorphous structure, while those grown at higher temperatures were polycrystalline. Raman spectroscopy validated the anatase phase of the deposited films. Atomic force microscopy (AFM) revealed smooth surfaces, with roughness values of ~7 Å for the flakes and ~4 Å for the deposited TiO_2 films. High-resolution transmission electron microscopy (HR-TEM), in conjunction with XRD, confirmed the successful epitaxial alignment of the anatase TiO_2 films with the underlying single-crystal flakes, as shown in Fig. 1b



a) b)

Fig. 1a) XRD spectra of bare TiO_2 flakes and with deposition of TiO_2 thin film on TiO_2 flake at different temperatures, b) HR-TEM image of TiO_2 thin film on TiO_2 flake (higher magnification image in inset).

Keywords: PEALD, hydrothermal, homoepitaxial growth

Delevepment of Biomass-derived Activated Carbon/Impregnated with NMC111 composites for Supercapacitor Applications

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Abstract

In this study the porous structure of activated carbon enables swift ion diffusion and adsorption, resulting in elevated power density and energy density. Moreover, the affordability and eco-friendliness of activated carbon position it as a sustainable and economical choice for energy storage applications. At present, the preparation of highly porous biomass activated carbon using the usual physical and chemical activation methods. In this study we are going to investigate results obtained from the production of low-cost and highly porous activated carbon by impregnating NMC111 nanoparticle. Electrochemical characterization reveals that the composite electrode delivers a high specific capacitance (~412 F/g at 1 A/g), excellent rate capability (~70% capacitance retention at 20 A/g), and long-term cycling stability (~95% capacitance retention after 10,000 cycles). The NMC111 nanoparticle impregnation enhances the electrical conductivity and pseudocapacitive behaviour of the biomass-activated carbon, resulting in improved supercapacitor performance.

Keywords: biomass-activated carbon; graphite nanoparticles; supercapacitor; electrode material; sustainable energy storage.

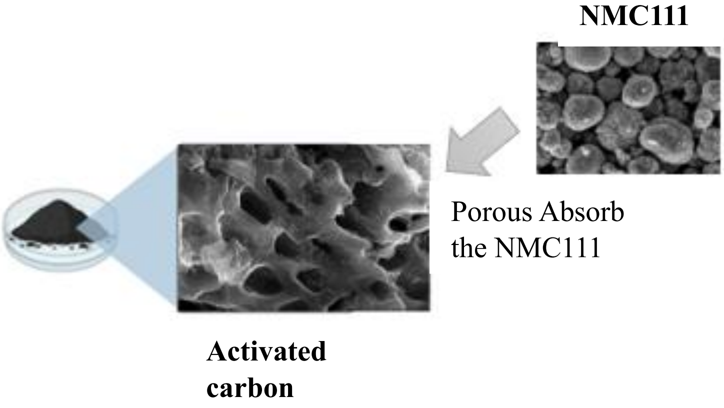

FIG: 1 ACTIVATED CARBON POROUS IMPREGNATED WITH NMC111.

References:

1. Shrestha, Rajesh, and Narendra Phulara. "Review on Activated Carbon for Supercapacitors." *Semiconductor Science and Information Devices* 5.2 (2023): 11-18.

2.Deng, Dingfei, et al. "A novel layered activated carbon with rapid ion transport through chemical activation of chestnut inner shell for capacitive deionization." *Desalination* 531 (2022): 115685.

3. Sevilla, Marta, and Robert Mokaya. "Energy storage applications of activated carbons: supercapacitors and hydrogen storage." *Energy & Environmental Science* 7.4 (2014): 1250-1280.

(Abstract Domain: 2)

UNVEILING THE ROLE OF FILM THICKNESS IN SEMICONDUCTOR-BASED PHOTOELECTROCHEMICAL WATER SPLITTING

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In this work, we report the systematic growth of vanadium pentoxide (V_2O_5) thin films with controlled thicknesses at 500 °C to investigate their influence on photoelectrochemical (PEC) water-splitting performance. The working electrodes were fabricated using pulsed laser deposition (PLD), where the number of laser shots was varied to tune the film thickness. Three representative films were employed: 2000, 6000, and 10,000 laser shots, resulting in average thicknesses of approximately 600 nm, 200 nm, and 50 nm, respectively. PEC measurements demonstrated a strong dependence of photocurrent density on film thickness. Among all samples, the electrode deposited with a thickness of 600nm delivered the highest photocurrent density of 1.8 mA cm^{-2} at 1.0 V versus Ag/AgCl, which was considerably higher than that of the thinner films. Electrochemical impedance spectroscopy further confirmed that the third electrode exhibited the lowest charge-transfer resistance at the semiconductor–electrolyte interface, for efficient interfacial charge separation and transport. Optimal thickness ensures full surface coverage and maximizes light absorption. Optimized thin-film thickness is crucial for maximizing PEC efficiency, as overly thick layers limit carrier diffusion, while ultrathin layers enhance charge extraction. Tailoring electrode dimensions improves solar-to-hydrogen conversion in V_2O_5 photoanodes.

Keywords: Photoelectrochemical water splitting, Pulsed laser deposition, Electrochemical impedance spectroscopy, film thickness optimization.

Fabrication of Surface immobilized High-Entropy Alloy Nano Particles by Laser Dewetting and Characterization

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Abstract.

High-entropy alloy nanoparticles (HEA-NPs) exhibit excellent properties such as multifunctional catalytic activity, physiochemical, and tunable optical properties with a large span of applications. Surface-immobilized nanoparticles exhibit improvement in catalytic activity compared to that in a solution and are most suitable for various industrial applications. However, phase separation and aggregation due to immiscible elements are a challenge in the fabrication of HEA-NPs. Herein, we present a scalable Synthesis of Surface-immobilized (AgAuCrPtTi) HEA-NPs on a silicon substrate by the laser dewetting process. The laser dewetting method ensures the atomic-level mixing of immiscible elemental metal precursors rapidly, thus avoiding the aforementioned challenges. All elemental metal coatings of(each coating thickness ~5 nm) were deposited on a silicon wafer (100) by using the sputter coating process in the order of high melting point to low melting point. Followed by laser dewetting with optimal process parameters. Field-emission electron microscopy and a non-contact mode atomic force microscope were used to analyze the size, morphologies and areal density. an energy-dispersive x-ray spectra analysis reveals that all alloy constituent elements in the nanoparticles are homogeneously dispersed at an atomic level. We believe that this approach offers a saleable, low cost, rapid synthesis technique that will produce large scale surface-immobilized HEA-NPs for various applications.

Keywords: High Entropy alloys, Nano-structured Surfaces, Dewetting.

New insight on the effect of 2D spacer (4FPEAI) treatment on 3D perovskites for the development of stable 2D/3D perovskite solar cells

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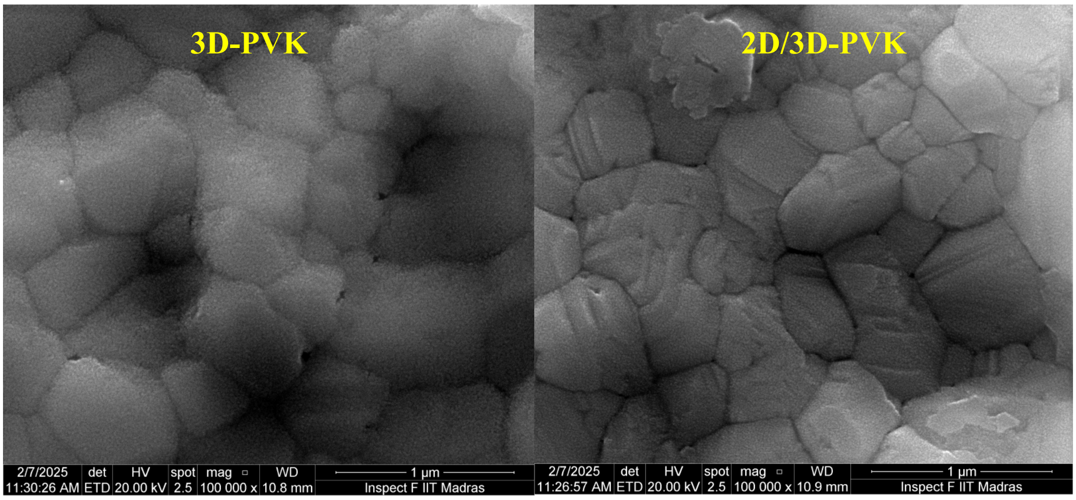
ABSTRACT

Development of 2D/3D perovskite solar cells receives greater attention due to their superior stability against moisture and device performance. In the present work, a 2D-spacer cation, 4-fluorophenethylammonium iodide (4FPEAI) is prepared from solutions with various concentrations (3, 5 and 10M) of the precursor in isopropyl alcohol solvent. The prepared solution is used to form a thin 2D perovskite layer on top of a 3D triple-cation perovskite by a spin-coating deposition method. Both 2D/3D and 3D layers are subjected to powder X-ray diffraction analysis to understand their structural differences. The XRD data show an improved crystalline nature of 3D perovskites by the 2D treatment, however, without any fundamental change of 3D perovskite structure. Scanning Electron Microscopy study revealed that the 2D spacer increases the grain size of 3D perovkside film from 0.5 μm^2 to 1 μm^2. The surface topography study by Atomic Force Microscopy revealed that the average roughness (Ra) value of 3D perovskites decreased from 120 nm to 47 nm with 2D treatment. The contact angle measurement analysis was carried out on the perovskite layers using water as a liquid drop. The wettability angle value of single 3D perovskite layer is 63.86°, whereas it increased to 72.13° on top of the 2D treated perovskite layers. It infers that the 2D spacer supress the surface wettability of water drop on 3D perovskites, ensuring protection the perovskite from moisture attack. However, the 2D ink on 3D layer show very small angle, 10.21°, which confirms conformal growth of 2D on 3D layer due to the high wettability. This is an important feature for the formation of stable 2D/3D interface. The current research work provides new insights into the formation of 2D/3D perovskite heterostructures, which can be easily implemented as absorber in solar cell device architecture.

Keywords: 2D spacer; 2D/3D perovskites; Roughness; Wettability.



Temporal Decay and Cognitive Image Denoising in Yttrium-Doped Molybdenum Oxide Artificial Synapses

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Energy-efficient neuromorphic devices are essential for advanced applications, as they enable high-performance computing with reduced power consumption, mimicking the brain's energy-efficient processing capabilities. This is essential to support emerging technologies like artificial intelligence, robotics, and the Internet of Things (IoT). In this work we report on the successful fabrication of yttrium doped molybdenum oxide thin films using RF magnetron sputtering. These films were utilized as active layers in the fabrication of two-terminal synaptic devices, Au/Y-Mo_xO_y/FTO, which demonstrate pronounced neuromorphic behavior, as compared to pure Mo_xO_y devices. The structural properties were studied by XRD, and the elemental composition was analyzed, and stoichiometry was confirmed through XPS analysis. Synaptic behavior such as potentiation/depression, spike-timing dependent plasticity (STDP), spike-number dependent plasticity (SNDP), paired-pulse facilitation (PPF) and spike-frequency dependent plasticity (SFDP) are successfully demonstrated in these synaptic devices. The fabricated devices demonstrate significant improvement in energy efficiency, being approximately 1000 times more efficient than devices with pure molybdenum oxide. A cognitive model based on the Ebbinghaus memory curve was successfully emulated, showcasing the device's potential in mimicking human memory behavior. Pattern recognition of the artificial synapse on the MNIST dataset was performed using an Artificial Neural Network (ANN) model. These devices demonstrated an accuracy of over 90%, which showcases effectiveness of the fabricated device in accurately classifying handwritten digits. In addition, we also have done a CNN-based denoising of scanning tunnelling microscope (STM) images of carbon atoms on a highly oriented pyrolytic graphite (HOPG) surface. This is done by adding Gaussian noise and comparing the denoised images with the original ones by calculating quantitative metrices such as peak-signal-to-noise ratio (PSNR) and structural similarity index measure (SSIM) values. The resulting metrices were sufficiently high, proving the effectiveness of the Au/Y-Mo_xO_y/FTO artificial synapse-based model in image-processing tasks.

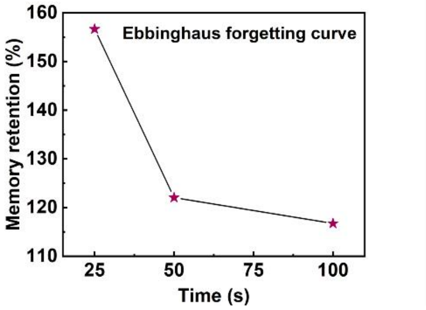

Figure 1. Ebbinghaus forgetting curve illustrating the decline in memory retention (%) over time (s) after stimulus pulses, indicating temporal decay with increasing pulse intervals.

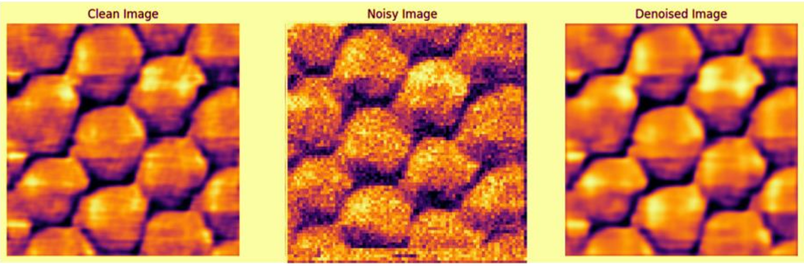

Figure 2 Original STM image (80 × 80 pixel) with added gaussian noise and its denoised version

References

[1] Rajesh, V. M.; et al. From Hebbian Learning to Pattern Recognition: The Role of Oxygen Vacancies in the Synaptic Responses of Magnetron Sputtered MoxOy Devices. *Mater. Sci. Semicond. Process.*, *188*, 109194 2025.

[2] Zhe Liu; Liu, et al, M. L. Image Denoising Based on a CNN Model. *2018 4th Int. Conf. Control Autom. Robot. ICCAR*, 389–393,2018.

Nano-Nest Type Porous NiCo2S4@polyindole Core–Shell Array: Efficient Energy Storage Supercapacitor Device

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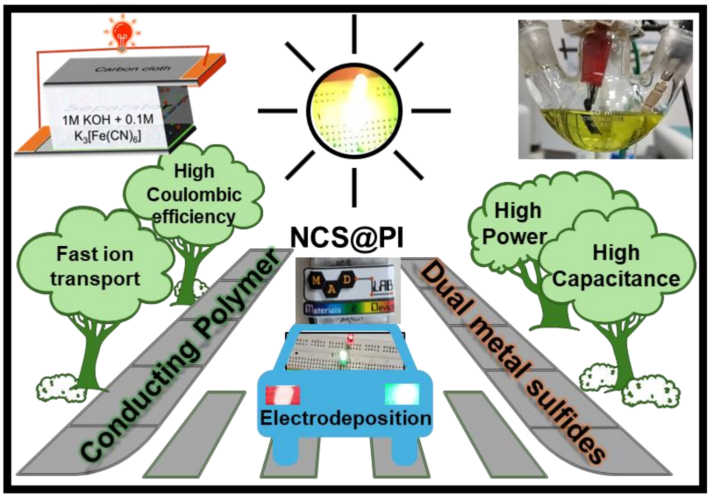
Abstract

Designing materials in appropriate nanoarchitectures can improve several electrochemical properties to yield power storage devices. Here, an inorganic–organic core–shell nanostructure in an appropriate morphology has been designed to improve ion-transportation as well as the ion diffusion mechanism for possible application in supercapacitor materials and eventually in a solid-state supercapacitor.[1] The NiCo2S4@PI core/shell electrode material shows high specific capacitance with approximately 1800 mF/cm² at 1 mA/cm², with a remarkable 92% contribution from surface-controlled processes at 10 mV/s due to the presence of dual active metal sites for ion adsorption. When incorporated into a solid-state asymmetric supercapacitor, the device delivers a specific capacitance of 217 mF/cm² at 4 mA/cm², along with high energy and power density of 0.06 mWh/cm² and 2.8 mW/cm², respectively. Notably, the device maintains 100% capacitance retention after 2000 continuous charge-discharge cycles at a high current density of 18 mA/cm². Furthermore, a prototype device successfully powered two LEDs simultaneously for several minutes, demonstrating its potential for real-life applications. This work underscores the effectiveness of core–shell nanoarchitectures in enhancing ion transport and overall electrochemical energy storage performance, paving the way for next-generation supercapacitors.[2]



[1] Thadathil, A.; Ismail, Y. A.; Periyat, P. Ternary 3D Reduced Graphene Oxide/Ni0.5Zn0.5Fe2O4/Polyindole Nanocomposite for Supercapacitor Electrode Application. RSC Adv. 2021, 11, 35828−35841.

[2] Guan, B.; Li, Y.; Yin, B.; Liu, K.; Wang, D.; Zhang, H.; Cheng, C. Synthesis of Hierarchical NiS Microflowers for High Performance Asymmetric Supercapacitor. Chemical Engineering Journal 2017, 308, 1165−1173.

Mixed Chalcogenides Nanoflakes' Infrared Cutting Effect: Utilization in Thermal Soothing Electrochromic Goggles

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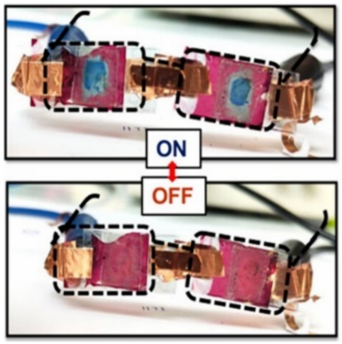
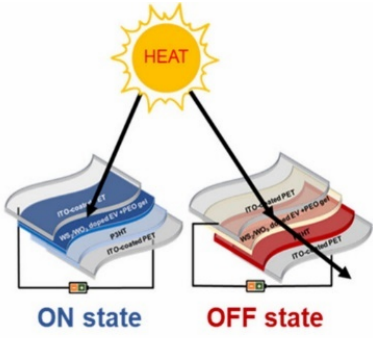
The development of multifunctional electrochromic devices minimizes energy consumption by offering multiple applications. A highly flexible electrochromic device (*f-ECD*) prototype goggle with heat filtering capabilities has been designed and demonstrated to have a heat soothing effect by the optical modulation in the near-infrared (NIR) region[1]. A *f-ECD* has been developed by the doping of metal oxide/chalcogenide mixture[2] (WO_3/WS_2), in thiophene-viologen based electrochromic materials[3]. The *f-ECD* switches in ∿1s, making it one of the fastest devices in the family. The highly flexible NIR-cutting ECD shows high NIR shielding by maintaining a temperature difference of up to 6 °C and cuts more than 15% of the heat when in the ON state. Also, the high optical modulation of up to 60% in visible region and high coloration efficiency of 260 cm^2/C with a cyclic stability of more than 100 toggles was achieved in the visible region. The real-world applicability has been demonstrated by making mini-goggles which change color between blue and magenta and cut heat making a way for a heat-calming eye-care gadget with bendable and twistable properties.





Keywords: *flexible electrochromic devices, NIR shielding, coloration efficiency, optical modulation.*

References

[1] B. Sahu, L. Bansal, N. Ahlawat, A. Ghanghass, D.K. Rath, S. Kaladi Chondath, S. Kandpal, R. Bhatia, I. Sameera, R. Kumar, ACS Appl. Opt. Mater. (2024).

[2] S. Kandpal, L. Bansal, A. Ghanghass, T. Ghosh, C. Rani, B. Sahu, D. Kumar Rath, R. Bhatia, I. Sameera, R. Kumar, Journal of Materials Chemistry C 11 (2023) 12590–12598.

[3] A. Chaudhary, D.K. Pathak, S. Mishra, P. Yogi, P.R. Sagdeo, R. Kumar, Solar Energy Materials and Solar Cells 188 (2018) 249–254.

A novel architectured BiCe metal organic framework-integrated MoS2 nanosheet: An intriguing strategy for deriving synergistic effects in high-performance symmetric supercapacitors

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Abstract

Metal-organic framework (MOF) based supercapacitors have attracted enormous attention nowadays due to their unique physiochemical properties. In this study, we are addressing the synergistic effect of MoS_2 when intercalated with redox-active bimetallic MOF-2 to enhance the efficiency of the electrode material. Herein, bimetal MOF incorporating bismuth and cerium has been synthesized and MoS_2 is introduced to increase the electron transport potentially. All the samples underwent experimental characterization techniques to procure their crystal structure, morphology, surface area, and electrochemical properties. Electrochemical measurement demonstrates that the MOF-2@MoS_2 electrode presents a significant specific capacitance of 510 F g^{-1} at a current density of 1 A g^{1} corresponding to a capacity of 255 C g^{-1}, while its initial capacitance remains at over 94 % even after 4500 cycles, with outstanding cycling stability. The MOF-2 rod-like structure is uniformly distributed on the surface and within the pores of the MoS_2 nanosheet, maintaining structural integrity throughout repeated cycles. Subsequently, a symmetric supercapacitor has been constructed using MOF-2@MoS_2 electrodes which delivers an energy density of 20.12 Wh kg 1 at a power density of 799.47 W kg^{-1}, with excellent cycling stability of 92 % over 4500 cycles at 10 A g^{1}. These findings suggest intercalating 2D material with bimetal MOF shows great promise for further practical application.

3rd International Conference on Thin Films and Nanomaterial Growth, Novel techniques and concepts

High-Performance PVA-Ni-Carbon Composite Coatings for Aerospace and Automotive Applications: Experimental and Theoretical Investigations

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Abstract

A well-known and cost-effective synthetic polymer, polyvinyl alcohol (PVA) has a wide range of uses in the food, automotive, aerospace, medical, and material industries for building structures. Polyvinyl alcohol (PVA) coatings are often limited in their practical applications due to their relatively poor mechanical properties, weak interfacial adhesion, and low wear resistance. To overcome these drawbacks, the polymeric matrix was reinforced through metallization and the incorporation of carbonaceous allotropes. Among the developed composites, the nickel and diamond reinforced PVA coating (PVA-Ni-D) demonstrated superior performance, exhibiting the lowest wear rate (7.34×10^{-3} mm^3), minimal penetration depth (19.2 µm), and highest scratch hardness (4.92 GPa) compared to coatings reinforced with carbon nanotubes (PVA-Ni-CNT) and graphene (PVA-Ni-Gr). The significant enhancement in wear resistance was attributed to factors such as contact depth, contact radius, and shear stress, as predicted by several theoretical models. Unlike CNTs and graphene, which possess high surface areas leading to stronger inter-particle interaction and easier detachment from the matrix, thereby compromising mechanical strength and tribological performance diamond particles exhibited superior interfacial bonding with the PVA matrix due to stronger particle-matrix interactions. Furthermore, density functional theory (DFT) based electronic structure analyses were conducted using two metallized polymer composite configurations, which provided valuable insights into the enhanced stability of the PVA-Ni-D system. Overall, the improved mechanical integrity and interfacial bonding of the PVA-Ni-D coating highlight its potential as a durable and multifunctional composite coating for advanced material applications.

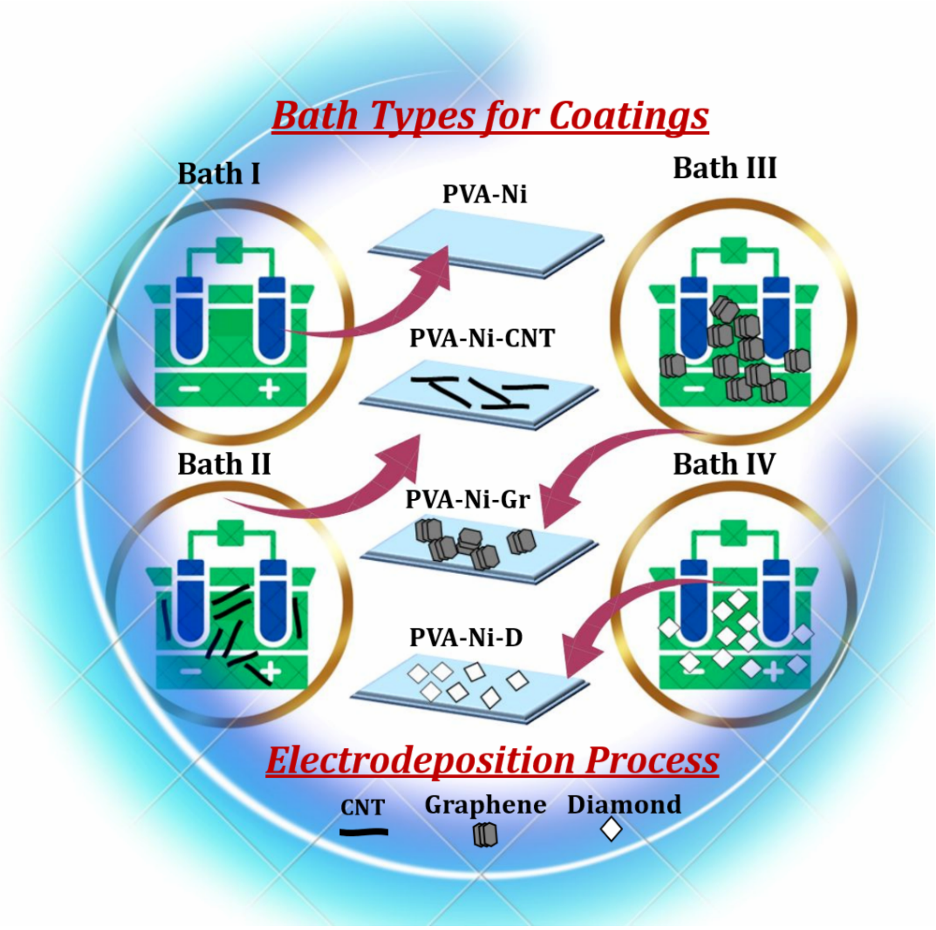

Figure 1: Schematic representation of bath types used in the electrodeposition process of PVA-Ni, PVA-Ni-CNT, PVA-Ni-Gr, and PVA-Ni-D composite coatings.

Keywords: Coatings, Electrodeposition, Nanocomposites

Multi-pollutant degradation from 2D MoO_3 /g-C_3N_4 /functional carbon nanomaterial based composite utilizing Z-scheme photocatalysis

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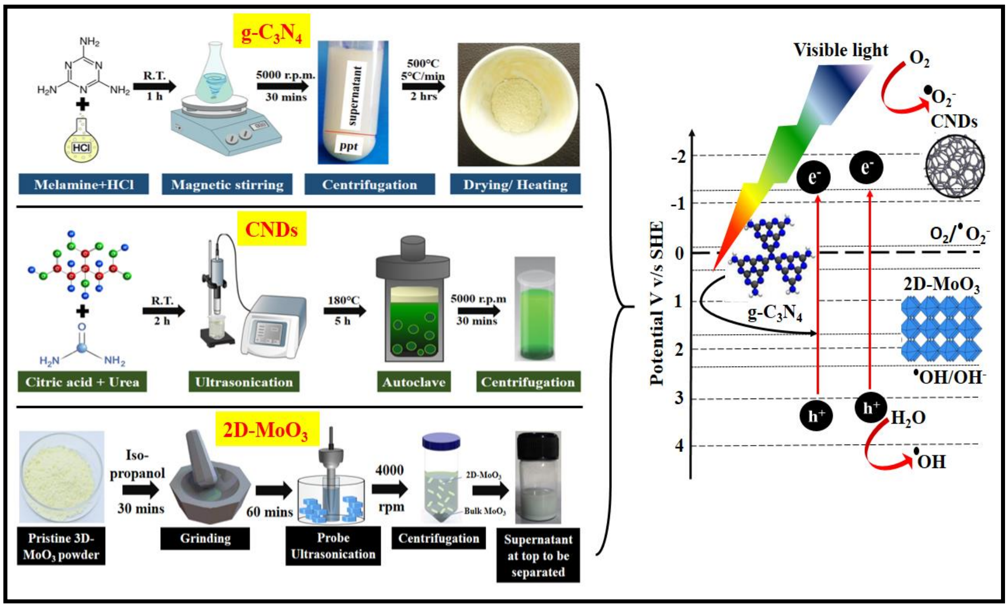
Abstract: Utilising the inexhaustible and costless solar energy for the remediation of crucially important resource water is the need of the time. Photocatalysis amongst various Advance Oxidation Process (AOPs) prove to be the most suitable for degrading customary dye pollutant like textile Methylene Blue (MB) and pharmaceutical Acriflavine Red (AF) [1]. Current vivid study converges the consideration towards the superior photocatalytic property of the synthesised Z-scheme photocatalyst composed of 2D MoO_3/g-C_3N_4 modified with functional carbonaceous material (FCM). The biocompatibility, reusability, chemical, thermal and hydrothermal stability of g-C_3N_4 when complemented with better charge transport and enhanced surface area of 2D-MoO_3 results in a stable and an abundant reactive species photocatalyst [2]. Utilising this Z-scheme construct to cover a broad spectrum range, especially the visible spectrum range, CNDs which exhibits up-conversion photoluminescence are used to modify them and form the composite [3].The morphological, structural and optical features of the synthesised composite were revealed by techniques like XRD, FESEM, EDX, FTIR, UV-VIS, Raman spectroscopy and its photocatalytic activity was assessed by the degradation of MB and AF dye. The biocompatibility, reusability, chemical, thermal and hydrothermal stability of g-C_3N_4 and FCM when complemented with 2D-MoO_3 for improved charge transport and enhanced surface area including Z-scheme catalysis, results in a stable and an abundant reaction for nearly 100 % degradation of AF dye in just 60 min and 94 % degradation of MB dye in 100 min under visible light. Further, the demonstration of efficient visible range utilization (from 300 to 500 nm) by the composite that exhibits up-conversion as well as broad photoluminescence from FCMs in its nano-dimension form, is observed. Possible effect of internal electric field which reduces the electron-hole recombination, the suitable band positions for Z-scheme charge transfer, ease of production and scaling up, cost effectiveness and multi-dye degradation study suggest that the proposed composite is highly suitable in the family of photocatalysis for environmental cleaning of multiple cationic dyes.

[1] N.A. Barakat, G.M. Tolba, K. Khalil, Methylene blue dye as photosensitizer for scavenger-less water photo splitting: New insight in green hydrogen technology, 14 (2022) 523.
[2] S. Singh, K. Verma, Advanced Applications of 2D Nanostructures, IGI Global2020.
[3] Z. Ji, Z. Yin, Z. Jia, J.J.L. Wei, Carbon nanodots derived from urea and citric acid in living cells: Cellular uptake and antioxidation effect, 36 (2020) 8632-8640.



Thin films/Nano-materials Growth, Novel techniques and concepts

Addressing the Charge Transport Bottlenecks in Flexible Organic Electrochemical Transistors Through Structural Ordering

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Organic electrochemical transistors (OECTs) are promising biocompatible devices for ionic–electronic signal transduction, amplification, and biochemical sensing. Their low-voltage operation and the mechanical flexibility make them a strong contender for next-generation wearable bioelectronics. To enable these applications, high-performance flexible OECTs with optimized charge transport are highly desired. In OECTs, gate-driven ion injection induces electrochemical doping of the channel, with ions compensating electronic charges. As device performance depends on the efficiency of this coupled ion–electron transport, enhancing in-plane charge transport within the channel is a key strategy to boost the charge carrier mobility and overall OECT functionality.

This work focuses on enhancing the in-plane charge transport by improving structural ordering using the unidirectional floating film transfer method (UFTM). This fabrication approach enables the formation of highly ordered, anisotropic, edge-on oriented thin films, which significantly boost in-plane electronic charge transport in OECTs. The fabrication conditions for poly(3,3‴-didodecyl-quaterthiophene) (PQT) were first optimized, and the dichroic ratio (DR) of the oriented films was measured across polymer solution concentrations ranging from 1 to 6% (w/v) to identify the concentration yielding the highest DR. The fabricated films exhibited DR values between 5.4 and 17.6, with the highest value at 5% concentration, which was subsequently used for device fabrication.

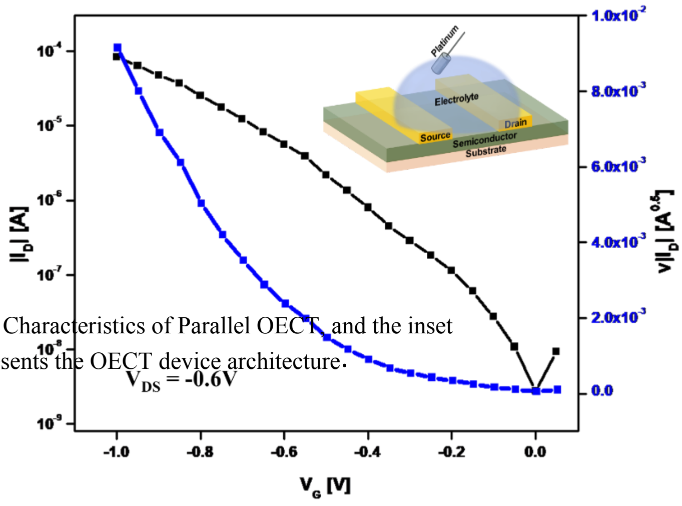

Fig. 1. Transfer Characteristics of Parallel OECT, and the inset represents the OECT device architecture.

For device fabrication, flexible PEN substrates were cleaned, and gold electrodes were deposited using physical vapour deposition. Parallel and perpendicular thin films were then cast using the UFTM method, and an additional spin-coated OECT device was prepared for comparison. The electrolyte used was 1-ethyl-3-methylimidazolium tetrafluoroborate (EMIM-BF), with a platinum (Pt) gate electrode employed for output and transfer characteristic measurements (**Fig. 1, inset**). Upon measuring, the parallel OECT transfer curve as shown in **Fig.1** has the highest mobility-volumetric capacitance product (μC*) of 6.82 $F\cdot V^{-1}\cdot cm^{-1}\cdot s^{-1}$, which is an order of magnitude greater than the perpendicular and spin-coated devices. Furthermore, the fabricated devices maintained nearly stable performance for up to 10,000 bending cycles.

Keywords: Conjugated Polymers, thin film, organic electrochemical transistors

Navigating Marine Corrosion: The Synergistic Effects of Nitrogen in TiMoN Coatings

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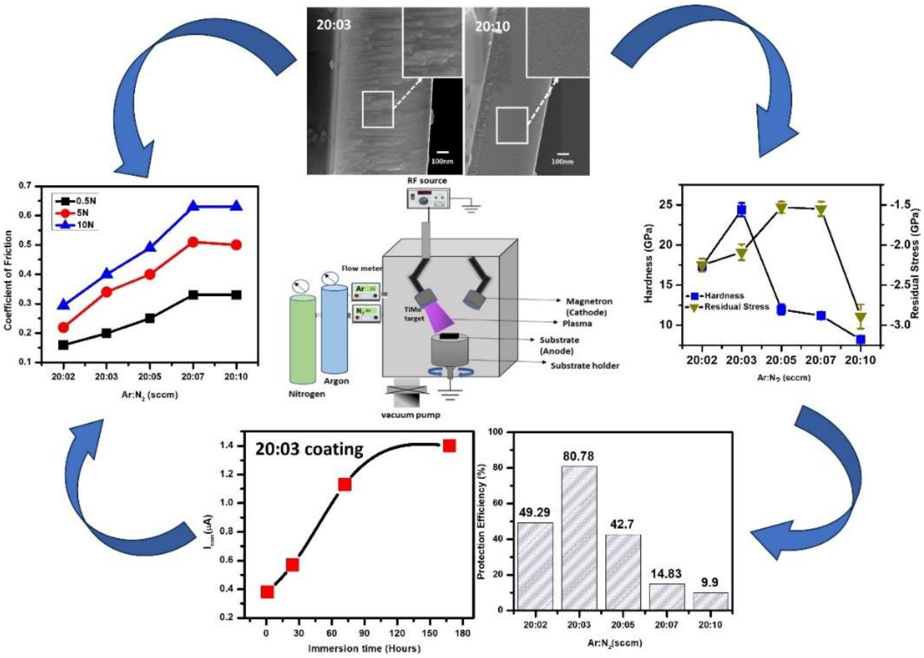
Abstract

Advanced coating technologies are key enablers for extending component lifetimes in marine, microelectronic, and energy systems. Developing coatings that combine mechanical robustness with long-term corrosion resistance is crucial for translating thin-film research into industrial and commercial solutions. In this context, TiMoN coatings were deposited via RF magnetron sputtering to achieve superior protection in aggressive environments. Deposition was carried out under constant argon flow with systematically varied nitrogen flow to tailor phase composition and film density. Structural analysis (XRD, FESEM) revealed that nitrogen incorporation significantly influenced crystallite refinement and surface morphology. The coating grown at an Ar:N_2 ratio of 20:03 exhibited outstanding mechanical properties — hardness of 24.40 ± 0.84 GPa, elastic modulus of 213.71 ± 8.74 GPa, and high elastic recovery — along with remarkable corrosion resistance in simulated seawater, as confirmed by polarization and EIS analyses. This optimized composition demonstrates a synergistic balance of hardness, adhesion, and electrochemical stability. The findings not only advance understanding of nitride coating behaviour but also highlight the potential of TiMoN as a scalable, high-value surface solution for next-generation marine and energy technologies.



References

[1] Jin, R. Cao, J. Zhang, Y. Tao, X. Tian, X. Kou, Study on Corrosion Resistance and Conductivity of TiMoN Coatings with Different Mo Contents under Simulated PEMFC Cathode Environment, Materials (Basel). 15 (2022).

[2] F. Regent, J. Musil, Magnetron sputtered Cr-Ni-N and Ti-Mo-N films: Comparison of mechanical properties, Surf. Coatings Technol. 142–144 (2001) 146–151.

(Computational Modeling & Simulations)

Computational investigations on oligomeric charge transport materials having $(D_1)_n$–π–D_2 (n = 1, 2, … 5) type of molecular architecture for perovskite solar cell applications

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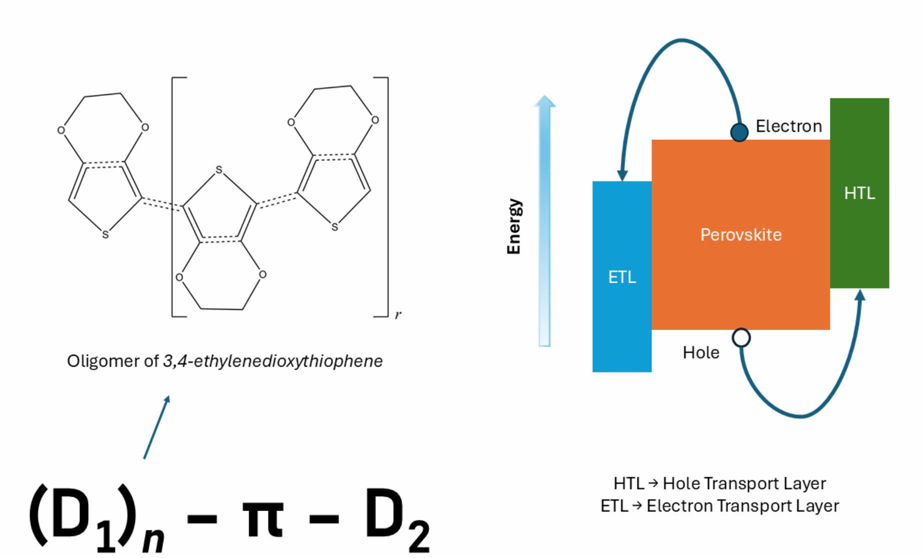
ABSTRACT



Charge transport layers facilitate extraction and movement of electrons and holes (generated by photovoltaic effect) from the active material to their respective electrodes. The corresponding materials used for transportation of electrons and holes are known as electron transport material (ETM) and hole transport material (HTM) respectively. Organic compounds based on the D–π–D structure have been widely investigated for development of HTM. In current investigation, charge transport materials based on a modified structure $(D_1)_n$–π–D_2 (n = 1, 2, … 5) have been simulated and analyzed. Here, D_1 and D_2 represent electron donor moieties which are connected together through π-conjugated bridge. The D_1 unit is composed of increasing monomers of *3,4 ethylenedioxythiophene* (EDOT) forming oligomers. *Gaussian 16W* quantum chemical software was used for simulating reorganization energies, frontier molecular orbitals and other relevant properties of title compounds. All calculations were performed using the density functional theory along with B3LYP functional and 6-31G(d,p) basis set. The properties were used to predict whether the subject molecules will behave as ETM or HTM. A theoretical perovskite based solar cell containing selected title compounds as charge transport layer was constructed. The results obtained from DFT calculations were used in the solar cell simulator SCAPS-1D to determine the output characteristics.

Keywords: Charge Transport Material; Oligomer; Electron Donor; Perovskite.

RF-Sputtered Al_2O_3/SiC Bilayer Thin Films on Si Substrates: Tailoring for Extreme Environments

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Abstract

Al_2O_3/SiC bilayer thin films were deposited on Si substrates using radio-frequency (RF) magnetron sputtering to develop thermally stable coatings for extreme environments. Sequential deposition of a SiC base layer and an Al_2O_3 top layer under optimized Ar–O_2 plasma produced dense, adherent, and stoichiometric films. Raman and XRD confirmed polycrystalline SiC (770–970 cm^{-1}) and an amorphous Al_2O_3 layer with smooth morphology (RMS < 10 nm). Strong interfacial bonding and chemical compatibility were achieved through interlayer mixing. The bilayer combines the thermal conductivity and chemical inertness of SiC with the protective barrier of Al_2O_3, demonstrating a robust route for high-temperature, radiation, and corrosion-resistant applications.

Study of Multifunctional Characterization of Titanium Dioxide Nanoparticles Synthesized via Sol–Gel Method

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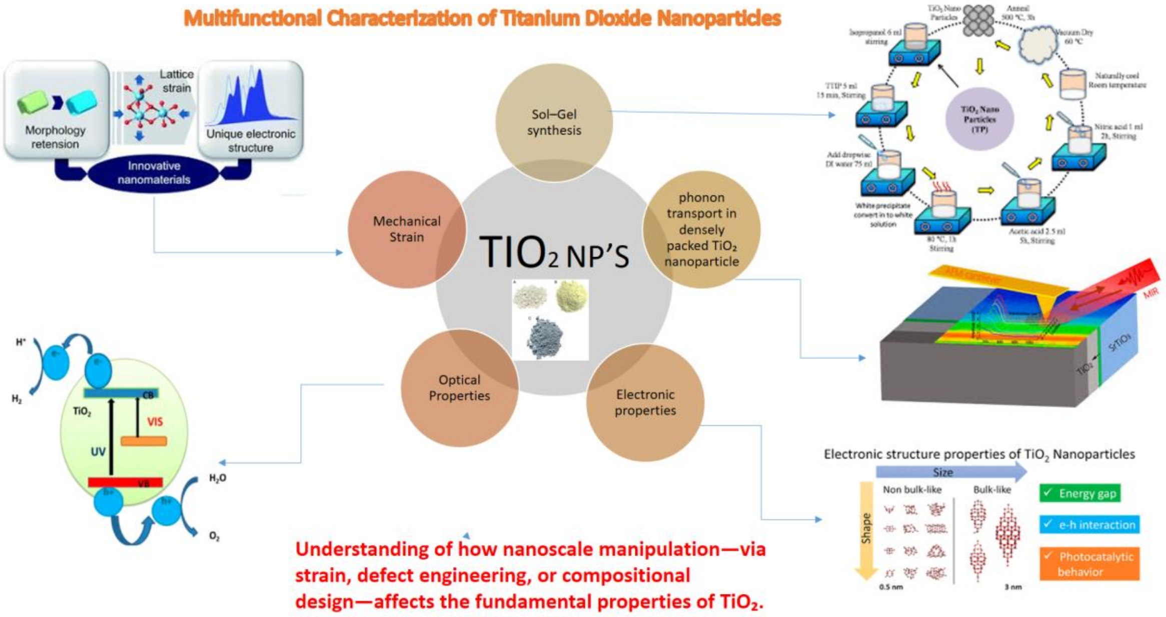
Abstract

Titanium dioxide (TiO_2) nanoparticles have emerged as multifunctional materials with exceptional physical, optical, and electronic properties, making them integral to advanced technologies in energy harvesting, catalysis, and optoelectronic systems. The present research investigates TiO_2 nanoparticles from a multifunctional perspective, exploring how structural, mechanical, and electronic factors influence their performance at the nanoscale. Study of X-ray diffraction (XRD) confirmed the formation of anatase phase TiO_2 with high crystallinity and average particle size in the nanometer range. The study encompasses several experimental approaches aimed at uncovering the interplay between structure and properties. In one direction, TiO_2 nanoparticles were embedded in a flexible polymer (PDMS) matrix to study the effect of mechanical strain on optical and electronic properties. Systematic strain application revealed measurable band gap shifts, confirmed through optical absorption and photoluminescence spectroscopy, demonstrating the feasibility of strain-engineering band structures in oxide nanomaterials. In a complementary study, core–shell TiO_2 nanoparticles with varying amorphous shell thicknesses were fabricated to explore carrier recombination dynamics using ultrafast time-resolved spectroscopy. Results indicated that the shell morphology significantly affects trap density and carrier lifetime, providing a route to control charge dynamics in photocatalytic and photovoltaic systems. Collectively, these investigations offer a comprehensive understanding of how nanoscale manipulation—via strain, defect engineering, or compositional design—affects the fundamental properties of TiO_2. The combination of sol–gel synthesis, strain modulation, ultrafast spectroscopy, and thermal-optical analysis presents a practical and scalable framework for designing multifunctional nanomaterials. This research highlights the potential of TiO_2-based systems for flexible electronics, energy-efficient devices, and next-generation quantum and optical technologies.

Keywords
Titanium dioxide, Nanoparticles, Sol–Gel synthesis, Optical, Electronic

Graphical Abstract:


Multifunctional Characterization of Titanium Dioxide Nanoparticles

Understanding of how nanoscale manipulation—via strain, defect engineering, or compositional design—affects the fundamental properties of TiO₂.

Investigation of Optical and ctrical Properties of ZnO Thin Film for Optoelectronics Application

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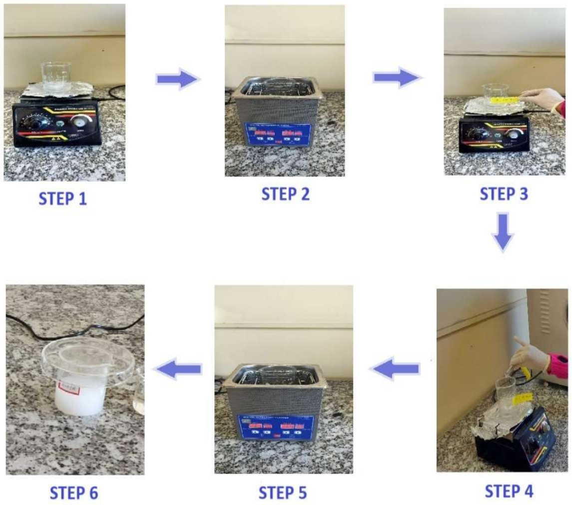
Abstract

Zinc oxide (ZnO) thin films were successfully synthesized via a sol-gel spin coating technique-a simple, cost-effective, and scalable approach suitable for large-area deposition. This investigation aims to assess the suitability of the prepared ZnO thin films for efficient optoelectronic applications. Structural analysis revealed well-defined peaks corresponding to the hexagonal wurtzite structure of ZnO, confirming phase purity and crystalline nature. The calculated average crystallite size was found to be approximately 133 nm. The SEM micrographs showed a uniform surface morphology composed of densely packed, nearly spherical grains with particle sizes ranging from 2 µm to 8 µm, suggesting good surface coverage and reduced porosity, which are favorable for enhancing carrier transport and optical uniformity. Optical studies showed that high optical transparency in the visible region, exceeding 85 %, with a sharp absorption edge near 420 nm and the optical band in the range of 1.66 eV indicating excellent optical transparency suitable for optoelectronic devices. The electrical conductivity of ZnO solution is obtained in the range of 0.20to 3.9 S/cm.The results demonstrated semiconducting behavior with enhanced electrical conductivity at elevated temperatures, consistent with thermally activated carrier transport. These electrical findings, coupled with the optical transparency, highlight the potential of the sol–gel derived ZnO thin films for multifunctional optoelectronic device integration.The results suggested that spin-coated ZnO thin films exhibit desirable optical clarity and electrical performance. The obtained results establish ZnO thin films as a robust platform for future transparent and flexible optoelectronic technologies.



Prepared Solution of ZnO

Deposition of Thin film

(Abstract Domain:Perovskite, Silicon and CdTe thin films solar cells)

Design and Simulation of a Two-Terminal Perovskite–Chalcogenide Tandem Solar Cell

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ABSTRACT

Tandem perovskite solar cells offer an effective way to surpass the single-junction Shockley-Queisser (SQ) efficiency limit by splitting the AM1.5G spectrum between two subcells with optimal band gaps. In this work, we propose and numerically evaluate a two-terminal (2T) monolithic perovskite-chalcogenide tandem comprising a wide-bandgap (WBG) top subcell and a narrow-bandgap (NBG) bottom subcell. The WBG top absorber (1.6–1.9 eV) selectively harvests high-energy photons in the visible region, minimizing thermalization losses, while the NBG bottom absorber (0.97–1.3 eV) captures the transmitted low-energy photons extending into the near-infrared, thereby reducing transmission losses. This spectrally complementary absorption, coupled with series electrical connection, enables voltage addition across the two subcells with a common, current-matched operating point, thus raising the tandem's power conversion efficiency beyond that achievable by either subcell alone.

Each subcell is engineered with carrier-selective contacts to ensure efficient charge extraction and suppressed interfacial recombination. Specifically, electron-transport layers (ETLs) with suitably aligned conduction bands and high transparency are paired with hole-transport layers (HTLs) possessing high work function and robust valence-band alignment to the respective perovskite absorbers. The interconnecting recombination layer is optimized to minimize optical and electrical losses while maintaining mechanical and thermal compatibility for monolithic integration.

Beyond baseline J–V characteristics, operational robustness is examined through (i) light-intensity-dependent measurements, (ii) temperature-dependent analyses, and (iii) parasitic resistance sensitivity studies for both series and shunt components, providing insights into device reliability and fabrication tolerance critical for real-world photovoltaic operation. Current-matching strategies, including absorber thickness tuning, optical management, and transport-layer optimization, are employed to maintain the tandem at its maximum-power point across these perturbations.

The anticipated outcome is a perovskite-chalcogenide 2T tandem that combines broadened spectral utilization with voltage stacking and low interfacial recombination to deliver high stabilized PCE under AM1.5G illumination, while demonstrating resilience to realistic variations in irradiance, temperature, and parasitics. The study provides a generalizable design and evaluation framework applicable to emerging perovskite chemistries and scalable thin-film manufacturing for next-generation photovoltaics.

Keywords: Tandem solar cell; Perovskite; Wide-bandgap top cell; Narrow-bandgap bottom cell.

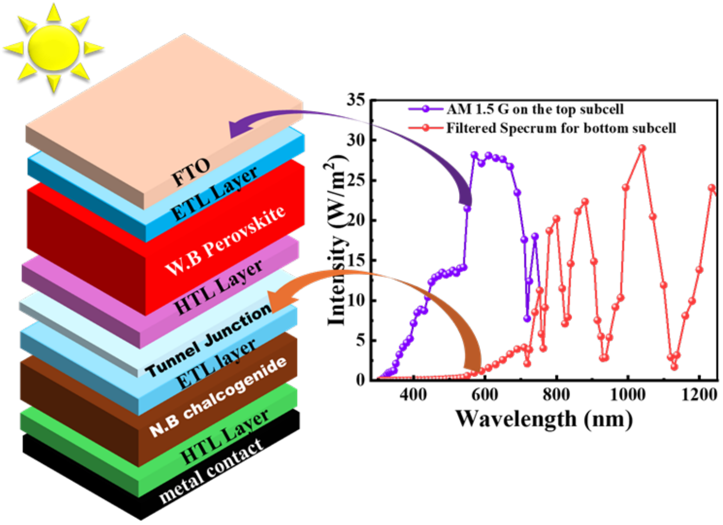

Fig. 1: Perovskite-chalcogenide tandem solar-cell architecture with solar-spectrum splitting.

Electrochemical Characterization of Nickel–Cobalt Oxide Nanoparticles Synthesized by the Sol–Gel Method

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The growing global energy demand and the urgency to mitigate climate change have intensified the pursuit of renewable and sustainable energy storage technologies. Solar-integrated batteries have recently gained attention as next-generation systems that unify photovoltaic energy harvesting and electrochemical storage in a single device. In this study, nickel cobalt oxide (NiCo O) nanocomposites were synthesized via the sol–gel method and evaluated for their suitability as photoactive electrodes. Electrochemical performance, which determines the efficiency of charge storage and transfer, is a key factor in advancing batteries, supercapacitors, and related energy devices. The fabricated solar-integrated battery directly converts sunlight into stored electrochemical energy, eliminating the need for separate solar panels or external wiring. Upon illumination, the NiCo O electrode absorbs photons, generating electron–ion pairs that drive simultaneous charge separation and storage. The stored energy can later power small electronic devices such as LED bulbs and mobile phones, ensuring reliable operation even in the absence of sunlight. This integrated design minimizes energy losses, reduces cost, and saves space compared to conventional solar panel–battery systems while utilizing eco-friendly electrode materials. The structural properties of NiCo O were confirmed using X-ray diffraction (XRD). Electrochemical studies, including cyclic voltammetry (CV) and galvanostatic charge–discharge (GCD), demonstrated a high specific capacitance of 456 Fg ^{1} at at 1 A g^{1}, highlighting its potential as an efficient electrode material. These results establish NiCo O -based solar-integrated batteries as compact, sustainable, and environment-friendly technologies for future applications in portable electronics, self-powered sensors, and off-grid energy systems.

Engineered Interfaces Drive Superior Charge Dynamics in $NiCoSe_4$@NiCoLDH Electrodes for High Performance Supercapacitors

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Achieving high capacitance together with long cycling stability in supercapacitors requires electrode materials that combine rapid charge transport with strong interfacial integrity. Transition-metal layered double hydroxides (LDHs) have emerged as promising candidates owing to their rich redox activity, yet their performance is often limited by insufficient conductivity and weak coupling with the current collector. To address these challenges, a NiCo-based hybrid electrode was constructed through a rational interfacial design strategy integrating LDH and metal selenide phases.

The engineered $NiCoSe_4$@NiCoLDH heterostructure forms a coherent and strongly coupled interface that facilitates efficient electron transport and balanced ion diffusion. The conductive $NiCoSe_4$ domains accelerate charge transfer, while the NiCoLDH framework supplies abundant redox-active sites and structural robustness. This hierarchical configuration ensures high active-material utilization, low interfacial resistance, and stable operation during extended charge-discharge cycling.

When combined with activated carbon in an asymmetric device, the hybrid electrode demonstrates fast kinetics, superior energy-storage capability, and outstanding long-term reliability.

This work highlights interfacial engineering as a core design principle for enhancing electrochemical performance in hybrid electrodes. The $NiCoSe_4$@NiCoLDH architecture provides valuable insights into constructing strongly coupled heterostructures capable of delivering high energy density, excellent rate response, and durable stability for next-generation supercapacitor systems.

Keywords: $NiCoSe_4$@NiCoLDH; interfacial engineering; supercapacitors; electrochemical energy storage

Solid Polymer Electrolyte with COF-Induced Li-ion Pathways for Solid-State Lithium Batteries

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Abstract: The development of solid polymer electrolytes is critical for advancing safe and flexible lithium batteries, yet their limited ionic conductivity and poor mechanical robustness remain major obstacles to practical deployment. In this work, we explore a strategy of incorporating covalent organic framework nanofillers into a polymer matrix to simultaneously enhance ion transport pathways and mechanical integrity. The tailored porous structure and abundant functional groups of the framework promote segmental mobility and efficient ion conduction, while also contributing to structural reinforcement of the polymer host. The resulting composite electrolytes exhibit improved flexibility, electrochemical stability, and cycling durability compared to pristine polymer systems. Furthermore, their integration into flexible lithium-based devices demonstrates reliable performance under various mechanical deformations, underscoring their potential for next-generation wearable and portable electronics. This study highlights the promise of framework–polymer hybrid electrolytes as a route to combine safety, flexibility, and high performance in solid-state lithium energy storage systems.

(3. Microelectronics and optoelectronics devices)

Mn_3O_4-based Bipolar Resistive Switching Memory Devices

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ABSTRACT

Resistive switching phenomenon-based memory devices (RRAMs) are considered to be the memory of the future era due to their simple structure, ultrafast switching, low fabrication cost, and less power consumption, etc. In this study, Two Mn_3O_4 nanostructures-based Al/Mn_3O_4/FTO RRAM devices were fabricated using Aluminum and FTO as top and bottom electrodes, respectively. The XRD and Raman spectroscopy have been performed to characterize the semiconducting layers, which confirmed the presence of pure phase of tetragonal Mn_3O_4 in both devices. The first RRAM device was fabricated using sol-gel synthesized Mn_3O_4 nanoparticles as a semiconducting layer and shows a forming-free feature. Another RRAM device is based on spin-coated Mn_3O_4 thin film, which exhibits a gradual RESET feature. This gradual RESET feature offers the multi-level resistance states. The current-voltage characteristics confirm the presence of stable bipolar restive switching in both cases. Both devices show ohmic behaviour in low resistance state, while non-ohmic conduction mechanisms govern the devices in high resistance state. Al/Mn_3O_4/FTO devices may be used in numerous applications including physical unclonable function (PUF) hardware security systems, true or random number generators (TNG/RNG), neuromorphic engineering, and logic gates.

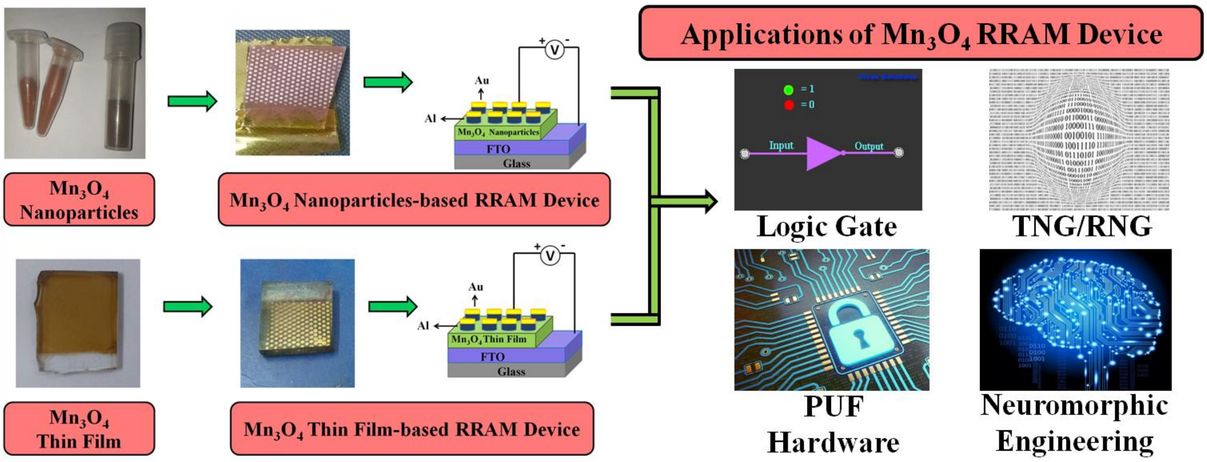

Fig. Mn_3O_4 nanoparticles and thin film on FTO, deposition of top electrodes, Mn_3O_4-based RRAM devices and their applications.

Keywords: Mn_3O_4; Forming Free; Gradual Reset; Multilevel Switching.

Engineering Charge Transport in $CsPbBr_3$ Nanoparticles via Controlled Temporal Surface Treatments for Thin-Film Transistor Applications

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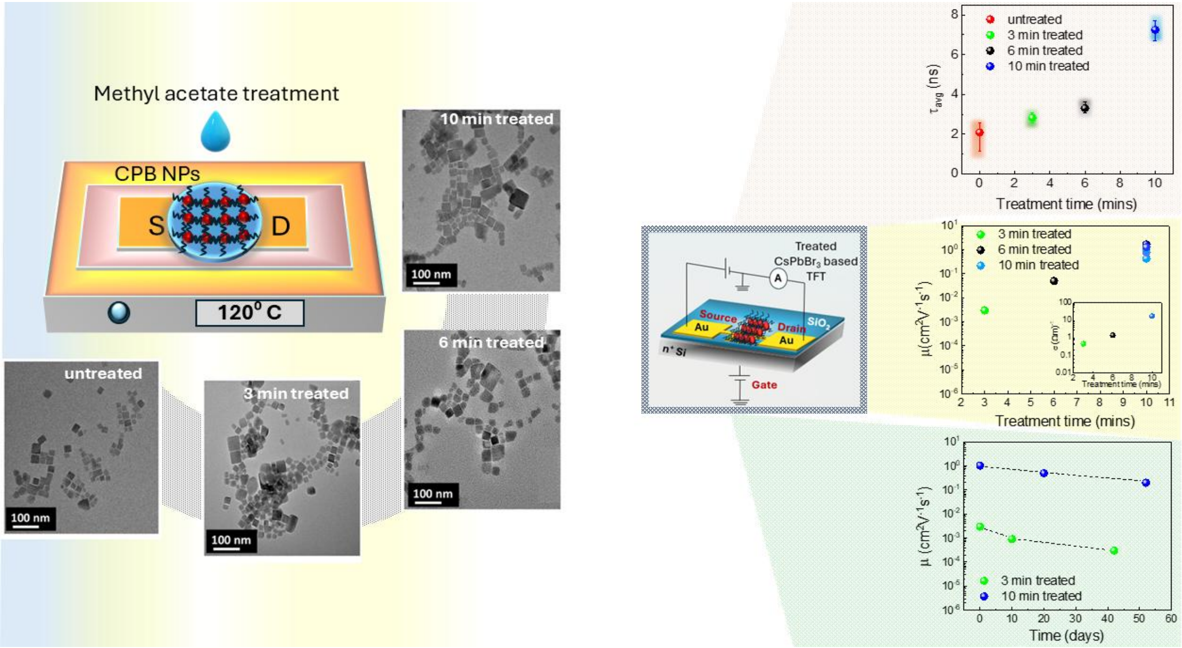
Inorganic halide perovskites of $CsPbX_3$ (X = Cl, Br, I) family have showcased remarkable optoelectronic properties as a virtue of bandgap tunability achievable via compositional engineering. Although extensive studies have been conducted on these perovskite nanoparticles (NPs) illustrating their robust luminescence abilities, high quantum efficiencies and long-term stabilities, charge transport in these materials has been less explored. A vital concern stems from the organic capping ligands enveloping NPs which impede the charge carrier mobility due to their insulating nature and limited transport cross-section, resulting in low conductivity across nanoparticles. To improve the overall charge transport across NPs, various ligand engineering strategies have been adopted which result in reduced trap densities resulting from ligand exchange processes. Treatment with methylamine gas has been used to enhance the crystallinity and reduce defect density in perovskite films [1]. More recently, methyl acetate soaks have been shown to result in large carrier lifetimes and high electron mobilities, presumably due to Ostwald ripening in conjunction with efficient ligand removal [2]. However, the modification in the conduction mechanism due to these treatments has not yet been explored.

In this work, we employ temporal surface engineering of $CsPbBr_3$ nanoparticles resulting in an exceptional field effect mobility (μ_h) of 1.336 $cm^2V^{-1}s^{-1}$ in thin film transistors (TFTs). By optimizing the post-annealing duration following antisolvent surface treatment, we achieve considerable enhancement in the steady-state current and field-effect mobility in $CsPbBr_3$-based thin-film transistors, while maintaining device stability. FTIR spectroscopy evidences the progressive removal of insulating long-chain organic ligands with increasing annealing time, whereas KPFM measurements show a steady rise in surface work function, signifying Fermi-level shifts that promote improved hole injection. Structural characterization reveals that extended thermal treatment induces Ostwald ripening and stabilizes the cubic perovskite phase, thereby enhancing grain connectivity and film uniformity. The observed enhancement in photoluminescence lifetimes confirms effective defect passivation at the nanoparticle surface. Furthermore, temperature-dependent charge transport measurements indicate that the mobility enhancement arises from increased electronic coupling and extended carrier localization lengths, consistent with three-dimensional Mott variable-range hopping behaviour. Collectively, these findings establish temporal surface engineering as a controllable and scalable strategy to concurrently enhance charge transport, defect tolerance, and operational stability in halide perovskite-based thin-film transistors and related optoelectronic systems.



Keywords: perovskite nanoparticles, thin-film transistors, charge transport, surface passivation

References:

1. Hao, Lianzheng, et al. "Methylamine gas healing of perovskite films: a short review and perspective." *Journal of Materials Chemistry C* 10.7 (2022): 2390-2399.
2. Kim, Jiyun, et al. "P-type charge transport and selective gas sensing of all-inorganic perovskite nanocrystals." *ACS Materials Letters* 2.11 (2020): 1368-1374.

(Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts)

Fabrication of TiO_2 Nanoparticle-Based Thin Films via Dracaena trifasciata Extract for Enhanced DSSC Performance

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ABSTRACT

Nanomaterial-based thin films have emerged as a promising strategy to improve dye-sensitized solar cell (DSSC) performance by enhancing light absorption, electron transport, and dye adsorption. In this study, TiO_2 nanoparticles were synthesized through a green hydrothermal route using varying concentrations of *Dracaena trifasciata* (snake plant) leaf extract as a natural reducing and stabilizing agent. The bioactive phytochemicals in the extract played a crucial role in modulating the crystallinity, morphology, and surface properties of the TiO_2 nanoparticles, directly impacting their photovoltaic efficiency. The resulting nanoparticles were characterized by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), UV–Visible Spectroscopy (UV–Vis), and Fourier Transform Infrared Spectroscopy (FTIR) to evaluate structural, morphological, and optical characteristics. Thin films were fabricated using controlled deposition techniques to optimize porosity, film thickness, and surface area—key parameters influencing dye loading and electron mobility. This bio-inspired approach offers a sustainable alternative to conventional chemical synthesis, reducing environmental impact while improving DSSC performance through better nanoparticle control and photoelectrode efficiency.

Keywords: TiO_2 Nanomaterials, DSSCs, Green synthesis, Thin films

Thin films/Nano-materials Growth, Novel techniques and concepts

Novel Z-W and W^2 solar module architecture – pathway towards utilization of the 3 orthogonal axes for electron flow

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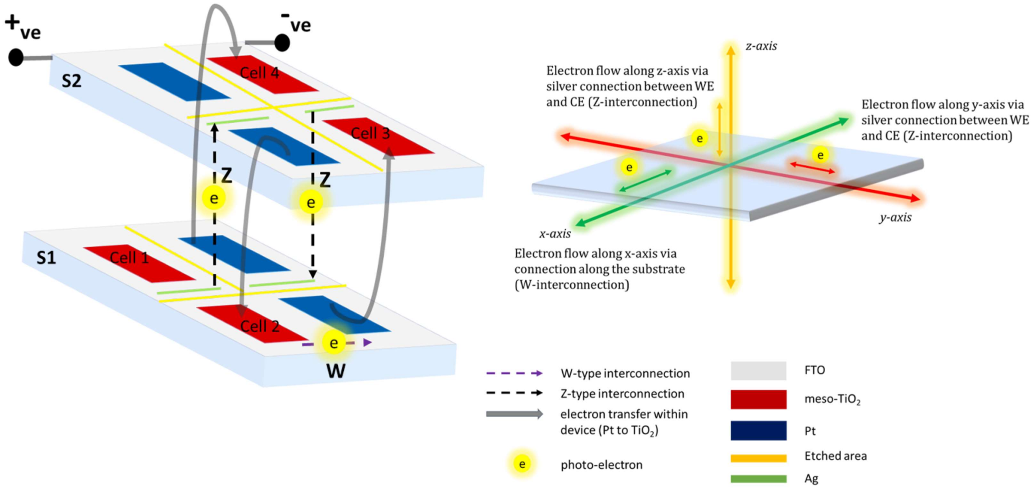
ABSTRACT

The fourth industrial revolution coupled with the rise of Internet of Things (IoTs) has intensified the global demand for new and innovative, clean and sustainable energy resources. With ~ 41 billion IoT devices projected,[1] and with the current utilization of solar energy stagnated at ~ 8%, improvisation, development and implementation of solar technology is the need of the hour. Among the various generations of photovoltaics, 3rd generation and more specifically, dye sensitized solar cells (DSCs) has made a major contribution in providing a clean and environmentally benign energy source with efficiencies touching 15% under full sun irradiation (AM 1.5G) and above 35% under indoor conditions.[2–5] Herein we propose two novel dye-sensitized solar module (DSM) based series architectures: 'Z-W' and 'W^2' configuration which can deliver higher voltage (higher series interconnections) for the same substrate footprint as that of the existing Z-type and W-type architectures. The proposed module architectures realize electron flow along all 3 orthogonal axes (as provided in the schematic below) and hence provide the possibility of expanding 'n' number of series interconnections two-dimensionally i.e. series interconnection via both the x-axis and y-axis, unlike the traditional unidirectional 'Z' and 'W' type DSMs, paving the way for efficient and smart engineered solar modules. The newly developed DSMs reproduced an output voltage of ~ 'x 3 times' and 'x 2 times' w.r.t Z-type and W-type DSMs with similar substrate foot print while delivering an identical power conversion efficiency under standard 1 sun condition.



Scheme 1: Working principle of a 'Z-W' DSM

Keywords: Solar Modules; DSMs; Z-W architecture; W^2 architecture.

References

1. The Top Growth Opportunities for IoT in **2023**, https://www.frost.com/frost-perspectives/the-top-growth-opportunities-for-iot-in-2023/.
2. Muñoz-García, A. B. et al., *Chem. Soc. Rev*. **2021**, 50, 12450–12550.
3. Freitag, M. et al., *Nat. Photonics*. **2017**, 116, 11, 372–378.
4. Meethal, S.M. et al., *J. Mater. Chem. A*. **2024**, 12, 1081–1093.
5. Jebin, P.R. et al*., J. Mater. Chem. A*, **2024**, 12, 32721–32734.

C–C Linked Porphyrin-Based COFs for High-Performance Aqueous Zn-Ion Hybrid Supercapacitor

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ABSTRACT

The growing demand for scalable and high-performance energy storage technologies is driving innovation in both electrode materials and device architectures. In this work, we present a new class of nitrogen-rich covalent organic frameworks (COFs) synthesized via Suzuki miyaura coupling strategy [1], enabling precise control over framework architecture and electronic properties. These COFs, featuring extended π-conjugation and tailored porosity, are deployed as efficient cathodes in dual-cation water-in-salt aqueous Zn-ion supercapacitors [2]. By integrating these frameworks with an advanced, specially engineered electrolyte system, we achieve a remarkable synergy that suppresses parasitic side reactions, stabilizes interfacial processes and delivers superior electrochemical performance. The optimized BPy-COF cathode exhibited high performance with a specific capacitance of 217 F g^{-1}, excellent energy density of 120.7 Wh kg^{-1}, and 92.7% capacity retention over 25,000 cycles at 10 A g^{-1}. This study demonstrates the untapped potential of C-C coupled porphyrin-COFs in energy storage while addressing interfacial instability in aqueous systems through innovative electrolyte engineering, paving the way for next-generation, durable and high-rate energy storage systems [3].

Keywords: Covalent Organic Frameworks (COFs), Suzuki Coupling, Aqueous Zn-ion Supercapacitors, Electrolyte Engineering

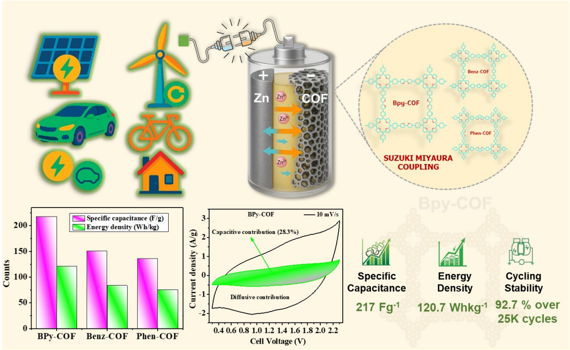

Figure: Suzuki-coupled porphyrin COFs enable efficient energy storage as cathodes in hybrid aqueous zinc-ion supercapacitors with dual-cation water-in-salt electrolyte.

References

1. R. Deka, K. Prakash and S. M. Mobin, *ACS Appl. Mater.* Interfaces, 2024, **16**, 68487.
2. X. Hou and Y. Wu, *ACS Appl. Energy Mater.*, 2019, **2**, 5835.
3. S. Halder and C. Chakraborty, *ACS Appl. Eng. Mater.*, 2023, **1**, 1799.
4. A. K. Deval, I. Ahmad, M. Sankar, manuscript submitted.

Computational modelling & simulations

Simulation-Based Optimization and Current Matching Strategy for High-Performance Perovskite/Silicon Tandem Solar Cells

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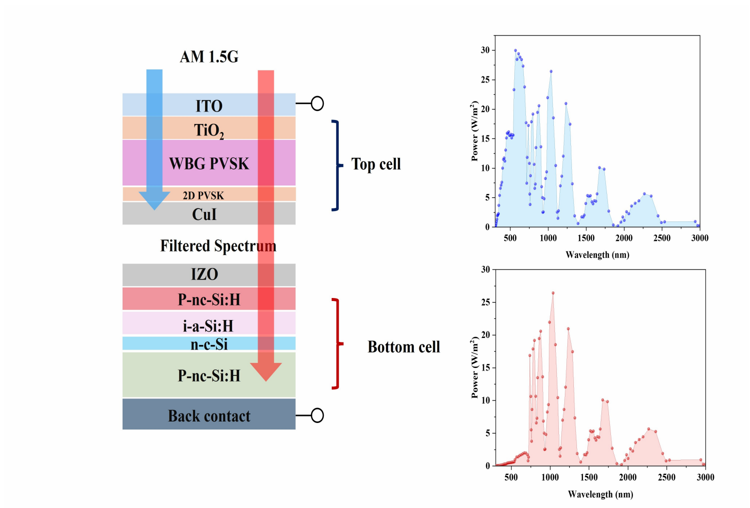
ABSTRACT

Perovskite/silicon tandem solar cells (PSTSCs) represent a promising pathway to exceed the Shockley–Queisser efficiency limit of single-junction silicon photovoltaics by effectively utilizing a broader portion of the solar spectrum. This research designs and simulates a high-efficiency tandem solar cell (TSC) using SCAPS-1D, exploiting tandem perovskite technology to enhance photovoltaic performance. The central aim of this work is to minimize two dominant loss mechanisms inherent to single-junction solar cells thermalization and transmission losses by employing a complementary bandgap configuration that allows efficient photon absorption across the visible to near-infrared region. The proposed simulation framework first calibrates both the top and bottom sub cells using available experimental data, ensuring that the simulated results accurately replicate experimentally observed trends. The simulation investigates the influence of the wide-bandgap perovskite top sub cell (E_g ~1.68 eV) integrated with a crystalline silicon bottom sub cell (E_g~1.12 eV). The top cell exhibited a peak J_{SC} of 21.64 mA/cm², while the silicon bottom cell generated up to 43.58 mA/cm² under AM 1.5G illumination. To achieve current matching a stringent requirement in 2T tandems the perovskite layer thickness was optimized, where both sub cells produced nearly balanced current densities (~21 mA/cm²). The resulting tandem configuration demonstrated improved open-circuit voltage (V_{OC}) and enhanced overall power conversion efficiency compared to the standalone sub cells. Furthermore, band alignment and interface quality were examined to minimize recombination losses and optimize carrier transport pathways across the perovskite/Si interface. The results underline the importance of simultaneous optical-electrical optimization and interface engineering in realizing stable, low-cost, and high-efficiency perovskite/silicon tandem devices.

Keywords: Perovskite/Silicon Tandem; SCAPS-1D Simulation; Current Matching; Optical–Electrical Optimization; Efficiency Enhancement



Abstract Domain: Thin films/ Nano-materials growth, Novel techniques and concepts

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 $CsPbBr_3$ 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 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 presents 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.

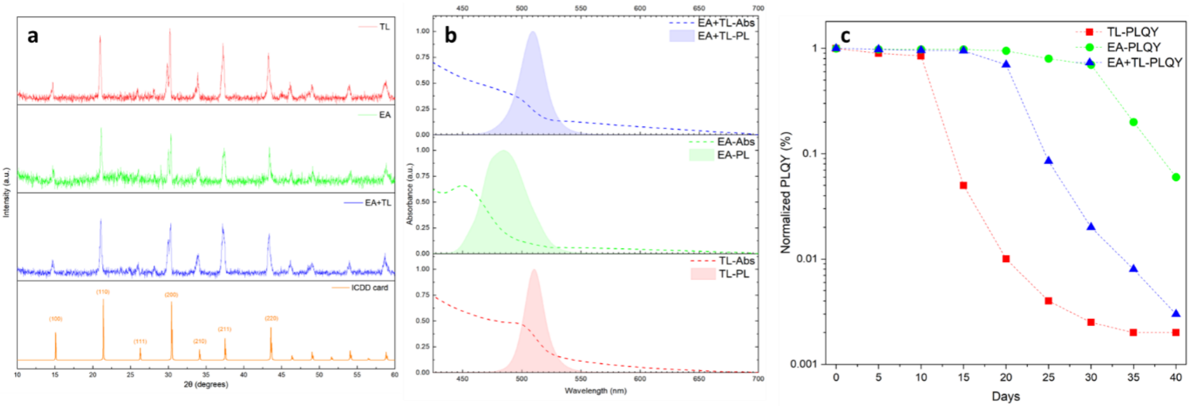

Figure 1: (a) X-Ray diffraction pattern of the synthesized PNCs under different polar environments show a consistent cubic structure. (b) UV-visible absorption spectra and respective PL curves excited at 400 nm at 300 K. (c) Stability studies portraying rate of decrease in the PL quantum yield of the PNC under different environments.

(Abstract Domain : Thin films/Nano-materials growth, Novel techniques and concepts)

Optical and Scintillation Properties of Record-Efficiency CdTe Nanoplatelets toward Radiation Detection Applications

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ABSTRACT

Colloidal CdTe nanoplatelets featuring a large absorption coefficient and ultrafast tunable luminescence coupled with heavy-metal-based composition present themselves as highly desirable candidates for radiation detection technologies. Historically, however, these nanoplatelets have suffered from poor emission efficiency, hindering progress in exploring their technological potential. Here, we report the synthesis of CdTe nanoplatelets possessing a record emission efficiency of 9%. This enables us to investigate their fundamental photophysics using ultrafast transient absorption, temperature-controlled photoluminescence, and radioluminescence measurements, elucidating the origins of exciton and defect related phenomena under both optical and ionizing excitation. For the first time in CdTe nanoplatelets, we report the cumulative effects of a giant oscillator strength transition and exciton fine structure. Simultaneously, thermally stimulated luminescence measurements reveal the presence of both shallow and deep trap states and allow us to disclose the trapping and detrapping dynamics and their influence on the scintillation properties.

Keywords: CdTe nanoplatelets, GOST, exciton fine structure, scintillation

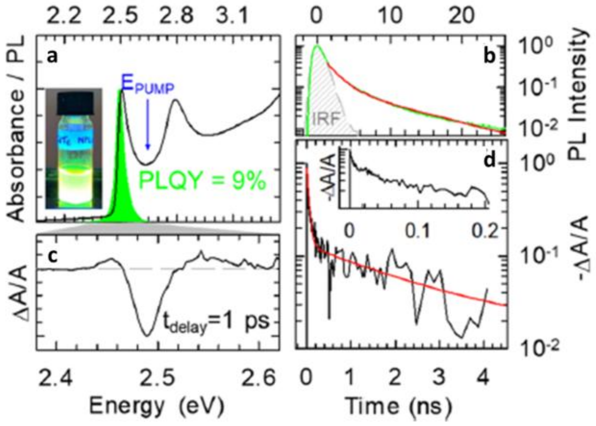

Figure 1: (a) Optical absorption and PL spectra (E_{EXC} = 3.54 eV, 300 K). Inset: photograph of a hexane NPL solution under UV light. (b) Normalized PL decay curve. (c) Normalized TA spectrum collected at 1 ps after pumping at 2.69 eV. (d) Normalized TA kinetics for the HH-1S_e transition at 2.49 eV.

Tailored Band Alignment and Enhanced Interface Engineering in SnS based Thin Film Solar Cell Heterostructure"

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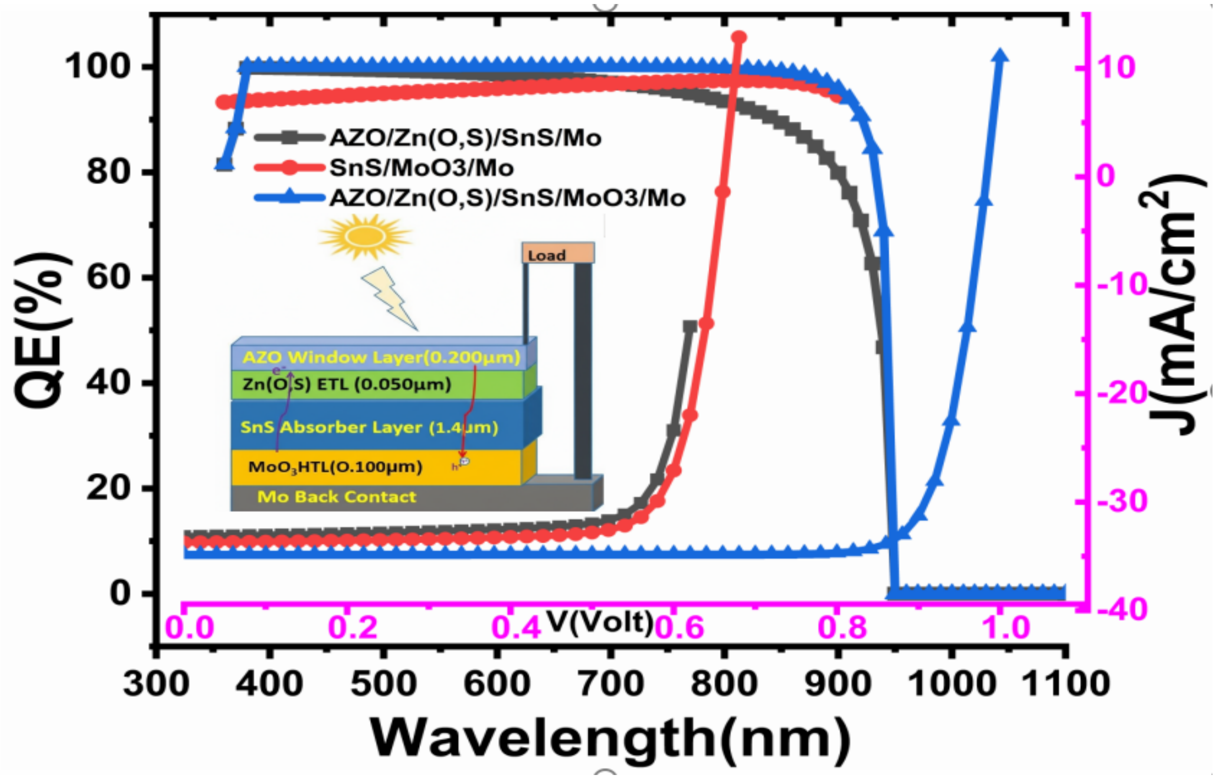

Figure 1. Quantum Efficiency(Q.E.) and J–V Characteristics of Optimized SnS-Based Solar Cells

Abstract

The global turnaround from fossil fuels towards clean and renewable energy sources continues to spur innovation in the field of thin-film solar cells as lightweight, cheap, and scalable replacements for conventional silicon photovoltaics. Among the absorber materials, tin sulfide (SnS) has attracted research interest due to its earth abundance, environmental friendliness, and favourable optical absorption capabilities in both the visible and near-infrared wavelengths. In this work, we simulate the novel

AZO/Zn(O,S)/SnS/MoO /Mo heterojunction solar cell using the SCAPS-1D simulator, aiming to provide a clear scientific roadmap for maximizing performance through layer and defect engineering.

These simulations explore the in-depth optimization of all layers in the proposed structure for efficient charge transport, selective carrier extractions, and beneficial band alignment. The AZO layer works as a transparent and conductive front contact, while Zn(O,S) serves as a tunable buffer layer with suitable alignment with the SnS absorber. The MoO interfacial layer enhances hole extraction and suppresses recombination losses at the Mo back contact, leading to improved charge collection efficiency and stability of the device. Under optimal conditions, the simulated solar cell structure has shown extraordinary power conversion efficiency (PCE) of nearly 32% with the open circuit voltage (Voc) of 1.05 V, short circuit current density (Jsc) of 34.7 mA/cm², and fill factor (FF) of over 87%. Increasing the bulk and interfacial defect densities starts to deteriorate the J–V behavior and external quantum efficiency (QE) which highlights the importance of defect passivation in achieving the superior performance and stability. Capacitance-voltage (C–V) and capacitance-frequency (C–F) studies assess the effects of the trap states on charge storage, recombination, and transient responses. The losses and improvements in electrical behavior have also been explored systematically by varying the series and shunt resistances, layer thickness, and other recombination mechanisms such as radiative and Auger. Thus, this work provides a comprehensive simulation perspective on the efficiency enhancement of SnS-based thin-film solar cell. Present theoretical modelling results provide a concept of high efficiency solar cell structure for the experimentalists to work in the near future.

Keywords: Thin-film photovoltaics, SCAPS-1D, SnS absorber, Zn(O,S) buffer layer, defect passivation, heterojunction solar cell

Perovskite, Silicon and CdTe thin films solar cells

Hysteresis-Free Carbon-Based Perovskite Solar Cells with Enhanced Open-Circuit Voltage for Indoor Photovoltaics

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ABSTRACT

Hysteresis in perovskite solar cells (PSCs) compromises their stability, and hysteresis-free PSCs are crucial for commercialization of PSC technology.[1,2] Carbon-based perovskite solar cells (C-PSCs) offer a cost-effective solution for PSC commercialization; however, higher recombination lower the open circuit voltage (V_{OC}) in C-PSCs.[3,4] The present study demonstrates the incorporation of a self-assembled monolayer (SAM), between the hole transport layer (P3HT) and the perovskite layer in C-PSCs. By optimizing the SAM layer thickness, we achieved hysteresis-free devices, with a low hysteresis index of 0.4%. Incorporating SAM, also enhanced the V_{OC}, which we attribute to an improved built-in potential in the newly developed device architecture. Our investigations revealed an ideality factor of 1.07 in SAM/P3HT bilayer devices, indicating reduced recombination compared to SAM-only and P3HT-only configurations, which normally exhibit higher ideality factors. This finding was further confirmed through open-circuit voltage decay (OCVD) measurements, transient photovoltage decay, electrochemical impedance spectroscopy (EIS), and intensity-modulated photovoltage spectroscopy (IMVS). Photovoltage decay analysis showed that carrier lifetimes were approximately 30 µs in SAM-only and P3HT-only devices, while the SAM/P3HT bilayer extended the lifetime to 99.8 µs. The enhanced carrier lifetime in the bilayer devices makes them suitable for low-intensity indoor applications, achieving a record high efficiency of 27.8% under a realistic light intensity of 50 lux using warm white LED illumination.

Keywords: Perovskite Solar Cells; Carbon electrode; Indoor Performance; Self Assembled Monolayers

References

1 R. Singh and M. Parashar, in *Soft-Matter Thin Film Solar Cells*, AIP Publishing LLCMelville, New York, 2021, pp. 1–42.
2 B. Chen, M. Yang, S. Priya and K. Zhu, *J. Phys. Chem. Lett.*, 2016, **7**, 905–917.
3 C. K. Vipin, S. Chandra Pradhan, K. N. N. Unni and S. Soman, *Sol. Energy*, 2024, **276**, 112705.
4 Y. Song, B. Xu, Y. Deng, M. Yao, J. Tong, Q. Wang, W. Wang, G. Yue, W. Zhang, C. Dong and F. Tan, *J. Mater. Chem. C*, 2024, **12**, 6628–6636.

(Computational modelling & simulations)

Design and Simulation of Gate-field-Plated β-Ga_2O_3 MOSFET having high PFOM of 106.9MW/cm^2

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ABSTRACT

In this work, we have designed and simulated Gallium oxide-based MOSFET having structure Metal field plate/Al_2O_3/Ga_2O_3.Gallium Oxide is used in Channel, buffer as well as in substrate layers, whereas Al_2O_3 is taken as gate di-electric. Design and simulation of this device is carried out using SILVACO TCAD Atlas tool. The source/drain contacts are assumed to be ohmic, whereas the gate contact is considered as Schottky. Throughout the simulation L_{GS}, L_G and L_{GD} layer is taken as 2µm, 2µm and 12µm respectively. At lower gate Voltage, the drain current increases linearly indicating Ohmic behaviour. While increases further, the device enters saturation (active) region, where current becomes nearly constant for a fixed gate voltage signifying the channel pinch-off. Moreover, the breakdown analysis of the device has been studied using Selberherr's model of impact ionization and is found to be **1.02kV**. Furthermore, we have increased the channel doping to observe its effect which resulted in a shift of the device operation toward the depletion mode and on the other hand when the channel doping is decreased the device moves towards enhancement mode with the cost of reduced drain current. Additionally, a lower specific on-Resistance ($R_{ON,SP}$) of **9.729mΩ.cm²** with breakdown voltage as **1.02kV** gives a Power figure of Merit (PFOM=$V_{br}^2/R_{ON,SP}$) of around **106.95MW/cm²**.

Keywords: Field-Plated; Gallium Oxide (Ga_2O_3) Mosfet; Power Mosfet; Breakdown Voltage

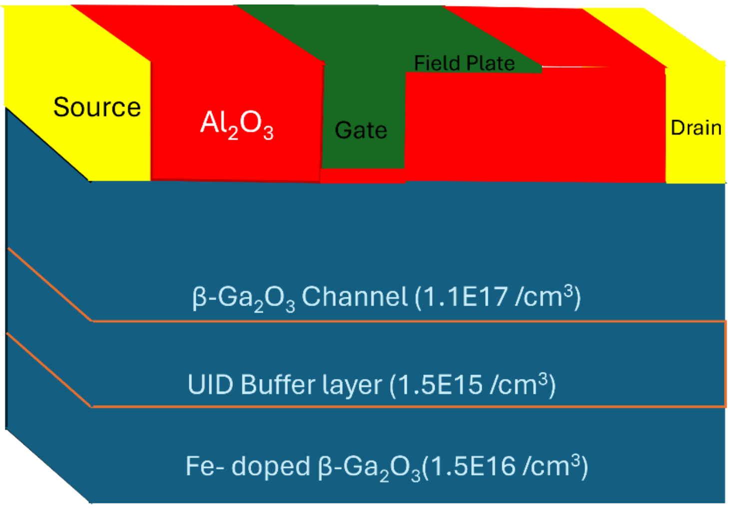

Figure 1 Schematic of Gate-Field-Plated β-Ga_2O_3 MOSFET

(Abstract Domain: 2)

Understanding the Role of Pendant Chain and Cationic Head Groups in Perfluorinated Anion Exchange Membranes

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ABSTRACT

Anion Exchange Membrane Fuel Cells (AEMFCs) represent a promising advancement in renewable energy technologies, offering efficient and environmentally sustainable power generation while enabling the use of non-precious metal catalysts. In the pursuit of developing durable and high-performance anion exchange membranes (AEMs) for such systems, understanding how molecular architecture governs ion transport and morphology is crucial[1,2]. In this study, four perfluorinated AEM systems were systematically designed to investigate the role of pendant chain chemistry specifically variations in alkyl chain length and cationic head group structure. Classical molecular dynamics (MD) simulations employed to explore the impact of these structural modifications on microphase separation, hydroxide ion transport, and overall membrane morphology at 300 K and 353 K. A comprehensive analysis involving the radial distribution function (RDF), mean square displacement (MSD), radius of gyration (Rg), and average end-to-end distance was performed to elucidate ion mobility, chain flexibility, and polymer conformation. Furthermore, spatial distribution function (SDF) analysis was conducted to visualize the preferential organization of hydroxide ions and water around cationic sites, providing detailed insight into the ion–polymer interactions at the molecular level. The results reveal that subtle variations in pendant chain architecture significantly influence nanoscale morphology, ion aggregation, and diffusion behavior. These findings offer a rational framework for tailoring the structural features of perfluorinated AEMs to enhance hydroxide ion conductivity and thermal stability in next-generation AEMFCs.

Keywords: Fuel Cell, Anion Exchange Membrane.

Reference: 1. Sharma, P., & Sunda, A. P. (2025). Molecular insights of hydrated perfluoro quaternary ammonium anion-exchange membranes: ionomer structure and hydroxide ion transport. *ACS Applied Polymer Materials*, *7*(3), 1886-189.

2. Tomasino, E., Scardi, P., & Ataollahi, N. (2025). Experimental and computational strategies for the enhancement of anion exchange membranes for electrochemical applications: A review. *MRS Energy & Sustainability*, 1-20.

The synthesis and characterization of dual doped (Al and Nb) $Li_7La_3Zr_2O_{12}$ electrolyte ceramic by citrate precursor gel method

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Lithium containing garnet type cubic phase $Li_7La_3Zr_2O_{12}$ (LLZO) are considered as good solid state electrolyte for Li-ion batteries. For stabilizing the cubic phase of LLZO for high conductivity with structural correlation, the doping of one or two cations are studies extensively in recent years. Highly dense (~ 94%) LLZO based garnet type electrolyte $Li_6Al_{0.25}La_3Zr_{1.75}Nb_{0.25}O_{12}$ (LALZNO) were prepared. The LLZO and LALZNO powders were synthesized by modified Sol-gel method. The citrate precursor gel was fired at 800°C for 4 hours. The calcinated powders show cubic crystallographic structures. The pellets sintered at 1300°C shows high ionic conductivity (~ 5.0×10^{-4} S cm^{-1}) at room temperature. The Scanning electron microscopy (SEM) were carried out for microstructural evolution and energy-dispersive X-ray spectroscopy (EDX) was done for elemental distribution. The doping of Al and Nb is found synergistic in stabilizing the cubic phase and reducing the calcination temperature.

Keywords: LLZO; LALZNO; SEM; EDX.

(Perovskite, Silicon and CdTe thin films solar cell)

Interface and Energy Band Engineering in Perovskite Solar Cells

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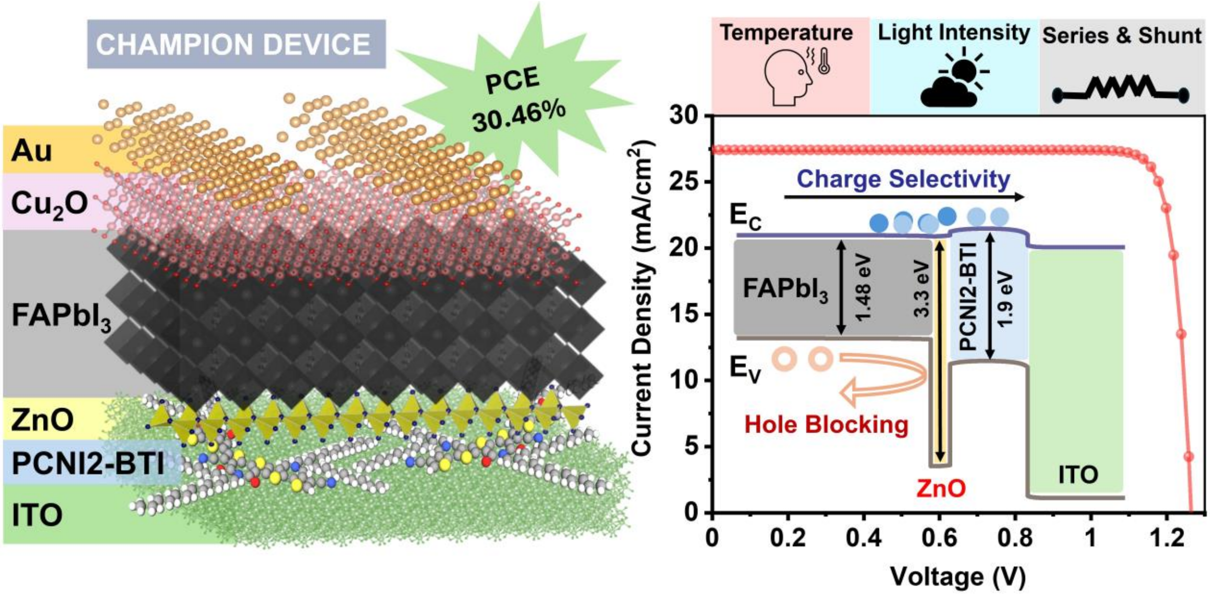
ABSTRACT

This study presents a comprehensive theoretical investigation into enhancing charge transport and energy level alignment in perovskite solar cells (PSCs) using a novel non-fullerene electron transport material (ETM), PCNI2-BTI a cyano-functionalized bithiophene imide copolymer, combined with optimized inorganic interlayers. Utilizing a standard *n-i-p* device architecture, systematic simulations were carried out using SCAPS-1D to evaluate the performance of PCNI2-BTI across various perovskite absorbers ($FAPbI_3$, $MAPbI_3$, $CsPbI_3$, and a triple-cation composition) and ten hole transport layers (HTLs). Among all HTL-absorber combinations, the Cu_2O/$FAPbI_3$ configuration demonstrated superior photovoltaic performance, achieving a baseline efficiency of 25.17%. The superior alignment between the valence band of Cu_2O and $FAPbI_3$ promoted efficient hole extraction and reduced interfacial recombination losses. Subsequent parameter optimization of the $FAPbI_3$ absorber, through fine-tuning of bandgap, doping concentration, and bulk and interface defect densities, further improved the simulated power conversion efficiency (PCE) to 27.47%. To mitigate remaining interface losses, interfacial engineering was introduced by incorporating ultrathin n-type interlayers (IGZO, WS_2, ZnO) between PCNI2-BTI and $FAPbI_3$. Among them, ZnO yielded the most favorable conduction band alignment ($\Delta E_C \approx 0$ eV) and strong hole-blocking capability, leading to an impressive simulated efficiency of 30.46% with $V_{OC} = 1.26$ V, $J_{SC} = 27.4$ mA cm^{-2}, and FF = 84.13%. The ZnO interlayer effectively enhanced quasi-Fermi level splitting, reduced interfacial trap-mediated recombination, and provided excellent thermal and operational stability under variable illumination and resistive losses. Mechanistically, the synergy between PCNI2-BTI and ZnO stems from enhanced *pi-pi* stacking induced out-of-plane conductivity and interfacial chemical interactions (Pb-O, Pb-N, and hydrogen bonding), which promote efficient electron extraction and energy-level alignment. Analytical modeling further confirmed that the increased selectivity at the ETL/perovskite interface lowers reverse saturation current (J_0) and enhances V_{OC} via suppression of non-radiative recombination pathways. Extending this strategy to lead-free perovskites, the PCNI2-BTI ETL also demonstrated excellent compatibility with $FASnI_3$, delivering a notable efficiency of 20.31%, underscoring its potential for sustainable, nontoxic photovoltaic applications. In a nutshell, this work highlights PCNI2-BTI as a versatile, high-performance non-fullerene ETM capable of replacing conventional fullerene-based counterparts. The integrated interfacial engineering approach demonstrates a viable pathway toward next-generation perovskite solar cells exceeding 30% theoretical efficiency while maintaining strong stability and environmental compatibility.

Keywords: perovskite solar cell, interface engineering, band alignment.


CHAMPION DEVICE
PCE 30.46%
Au
Cu$_2$O
FAPbI$_3$
ZnO
PCNI2-BTI
ITO
Temperature
Light Intensity
Series & Shunt
Charge Selectivity
E$_C$
E$_V$
FAPbI$_3$
1.48 eV
3.3 eV
PCNI2-BTI
1.9 eV
Hole Blocking
ZnO
ITO
Current Density (mA/cm^2)
Voltage (V)
0
5
10
15
20
25
30
0
0.2
0.4
0.6
0.8
1
1.2

(Abstract Domain: Computational modelling and simulations)

Self-assembly of Conformationally Asymmetric ABC Linear Triblock Copolymer under Cylindrical Confinement

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Block copolymers (BCPs) can spontaneously self-assemble into ordered nanostructures, making them important materials for tailoring advanced functional materials for applications ranging from high-density data storage and catalytic supports to advanced filtration membranes and targeted drug delivery systems. The morphology and dimensions of these structures are usually determined by intrinsic molecular parameters *viz.* block composition and segregation strength. The size ratio of monomeric segments constituting each of the blocks provides an additional parameter. This conformational asymmetry impacts the phase behaviour, leading to asymmetric phase diagrams, shifting of phase boundaries, and most importantly the introduction of novel exotic Frank-Kasper phases, which are not typically observed in conformationally symmetric systems. Beyond intrinsic molecular parameters, external factors such as geometrical confinement affect the BCP self-assembly. Confinement, whether in thin films, nanopores, or spherical cavities, introduces geometric constraints and surface interactions which break the BCP's natural periodicity that significantly alter the equilibrium phase behavior and induce novel structures absent in the bulk. Self-Consistent Field Theory (SCFT) stands out as a powerful mean-field approach to predict the equilibrium ordered phases of complex BCP systems.

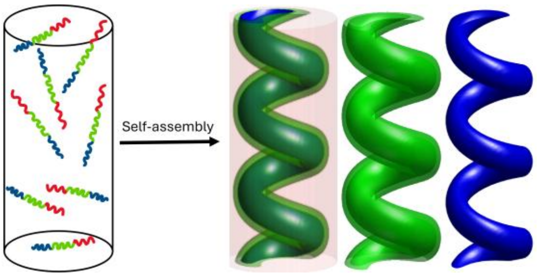

Figure 1. Schematic shows ABC linear triblock copolymer chains inside a cylindrical nanopore which self-assemble into core-shell single-helix nanostructure. Here light red, green and blue colour represents A, B and C-block respectively.

We investigate the self-organization of conformationally asymmetric BCPs constrained by geometric confinement. The phase behaviour of the molten diblock and triblock copolymers is examined under cylindrical and spherical nanopores using SCFT. The interplay of curvature-inducing conformational asymmetry and block fractions of BCPs and the curvature and structural frustration imposed by the confining boundaries of the nanopore results into interesting ordered nanostructures not reported earlier. A rich array of novel ordered morphologies ranging from chiral structures, core-shell ordering, and perforated microstructures are obtained. The degree of conformation asymmetry and curvature of nanopore govern the order-order transition across the wide range of self-assembled phases.

Keywords: Block Copolymers; SCFT; Ordered Nanostructures; Conformationally Asymmetry.

Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts

Design, Fabrication, and Characterization of Wide Bandgap RadHard Semiconductor Detectors for Applications in Particle Colliders and Particle Detectors in High Energy Physics

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ABSTRACT

Wide bandgap (WBG) semiconductor materials have emerged as promising candidates for next-generation radiation-hardened (RadHard) detectors in particle physics, owing to their superior electrical, optical, and thermal properties compared to conventional silicon-based devices. Among them, titanium dioxide (TiO_2), with its high bandgap energy (3.0–3.2 eV), excellent chemical stability, and inherent radiation tolerance, stands out as a cost-effective alternative for high-temperature and high-radiation environments encountered in particle accelerators such as the Large Hadron Collider (LHC) at CERN-Geneva and Nuclotron-based Ion Collider fAcility (NICA) at JINR-Dubna.

In this study, we report the design, fabrication, and multi-modal characterization of TiO_2-based wide bandgap semiconductor detectors for applications in high-energy physics and radiation detection systems. Thin films of titanium (200 nm) were deposited on Si/SiO_2 substrates using the electron beam evaporation technique under high vacuum conditions, followed by controlled thermal oxidation to form TiO_2. The annealing conditions were systematically optimized to achieve the desired crystalline phase—predominantly rutile, given its superior optical coupling and plasmonic response for localized surface plasmon resonance (LSPR) studies.

The structural evolution of the TiO_2 films was examined using X-ray diffraction (XRD) and Raman spectroscopy, confirming phase formation and crystallinity. Field Emission Scanning Electron Microscopy (FESEM) and Atomic Force Microscopy (AFM) provided insights into the surface morphology and nanostructural uniformity, while Energy Dispersive X-ray (EDX) analysis validated stoichiometry and elemental composition. UV–Vis–NIR spectroscopy was employed to estimate the optical bandgap and absorption edge, revealing characteristic features of wide bandgap semiconductors. Cross-sectional SEM images confirmed the film thickness and uniform adhesion to the substrate.

To enhance the optical absorption and plasmonic sensitivity, Localized Surface Plasmon Resonance (LSPR) was introduced by depositing a thin aluminum (10 nm) layer atop the TiO_2 surface. The LSPR coupling between Al nanoparticles and the underlying TiO_2 layer significantly enhanced near-field optical confinement, improving the device's spectral selectivity and potential responsivity in the UV–visible regime. This step represents a novel integration of plasmonic effects into a TiO_2-based RadHard detector platform.

Subsequent metallization using Ti/Au contacts enabled the formation of the detector device architecture. Electrical characterization—including I–V measurements, dark current, sheet resistance, responsivity, and transient response—was conducted to assess the detector's performance. The fabricated detectors were then irradiated with low-energy proton beams at the Inter-University Accelerator Centre (IUAC), New Delhi, to simulate the high-radiation environment of particle colliders. Post-irradiation electrical measurements demonstrated the robustness and stability of the devices under radiation exposure.

Finally, Deep Level Transient Spectroscopy (DLTS) measurements were performed to investigate defect levels and trap states induced by proton irradiation, providing critical insights into defect dynamics and radiation-induced degradation mechanisms in TiO_2-based WBG materials.
This integrated approach, from thin film deposition to post-irradiation defect characterization, demonstrates a comprehensive framework for developing radiation-hard, wide bandgap semiconductor detectors for high-energy physics experiments, nuclear instrumentation, and even industrial applications in railway and construction electronics under harsh operating environments.

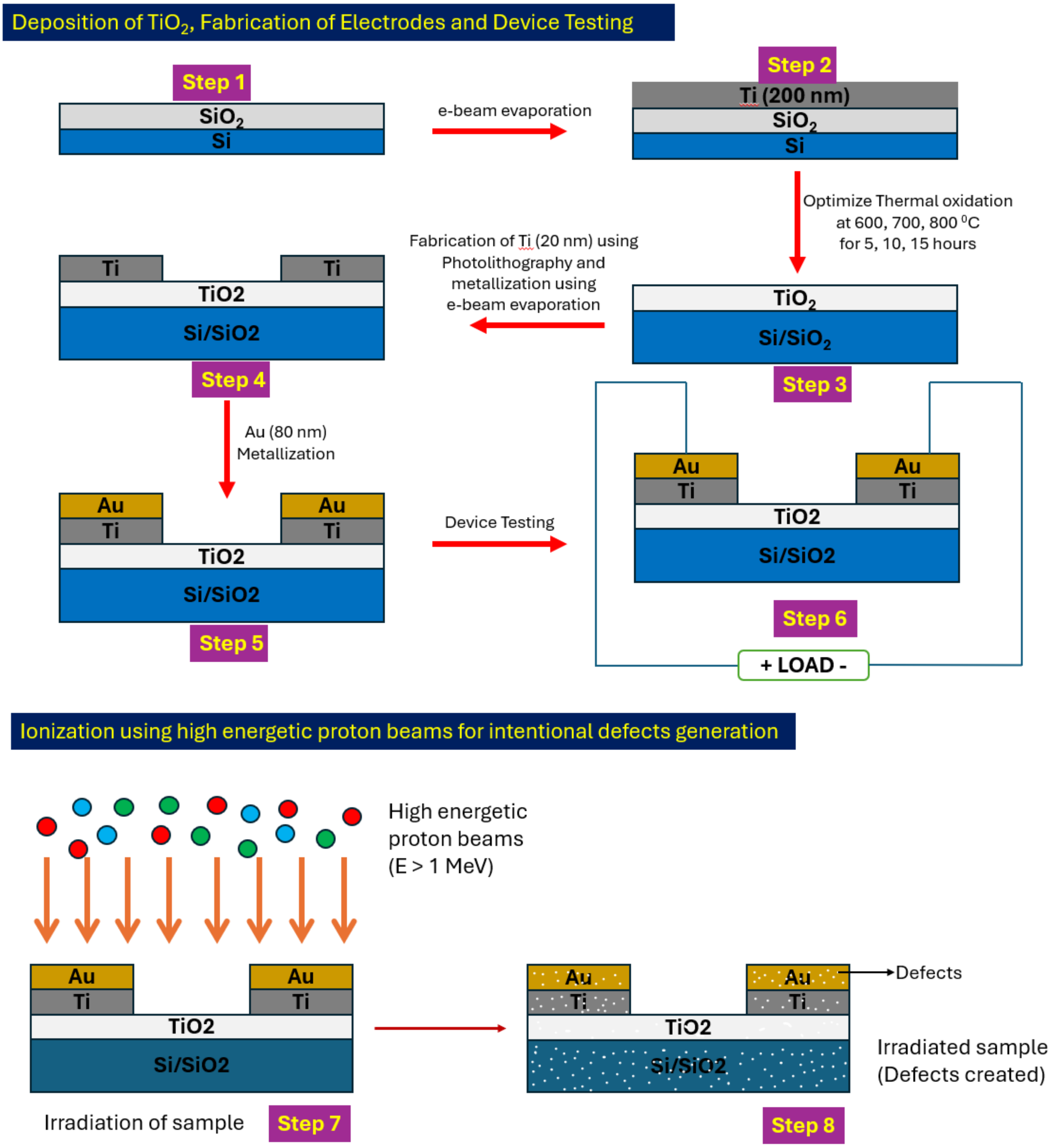

Fig. 1

Keywords: Wide Bandgap Semiconductor; Localized Surface Plasmon Resonance (LSPR); Radiation Hardening; Deep Level Transient Spectroscopy (DLTS).

(Perovskite, Silicon and CdTe thin films Solar cells)

Phase segregation induced hysteresis in mixed halide Perovskite

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ABSTRACT

Mixed halide Perovskite have recently become very attractive in optoelectronic fields, resulting in high performance photoelectric devices like solar cells, photodetectors light-emitting diodes owing to its small excitation binding energy, large carrier diffusion length, tenable bandgap, high defect tolerance and high electron mobility. Mixed halide perovskite owing to its stability is considered as a promising material for next generation solar cells. However, phase segregation in such films is a major bottleneck for achieving high performance. We here investigate phase segregation in mixed halide perovskite $CsPbBr_2I$ using in-plane electrical transport measurements under light. Secondary phase, generated under light irradiation causes significant charge carrier trapping and leads to hysteresis in electrical transport. We observed that the stoichiometry of film has play an dominant role on defects present in the film and therefore have significant impact on phase segregation. This work presents advancements in addressing critical reliability issues in perovskites.

We began our investigation by enhancing the conductivity of $CsPbBr_2I$ thin films. To achieve this we engineer with the ratio of I:Br in the precursor and named Plain CPBI, I-deficient and I-rich. Upon modifying the precursor stoichiometry, we found that the band structure of the thin films did not change significantly (UV and PL data). This suggest that the electronic structure of the films remains largely unaffected while it leads to improves conductivity. From our study it is clear that I-rich films show the largest hysteresis area. This is because of as a monochromatic light source falls upon the plain and I-rich films a $CsPbBr_3$ phase is segregated which is dominant for I-rich film. This secondary phase works as a trap state for the charge carrier which hinder efficient charge transport and hence hysteresis area increases whereas, I-deficient film because of compressive strain doesn’t show secondary phase generation, exhibit the smallest hysteresis area suggesting a relatively smooth charge transport.

Keywords: Phase segregation, Mixed Halide Perovskite, Hysteresis.

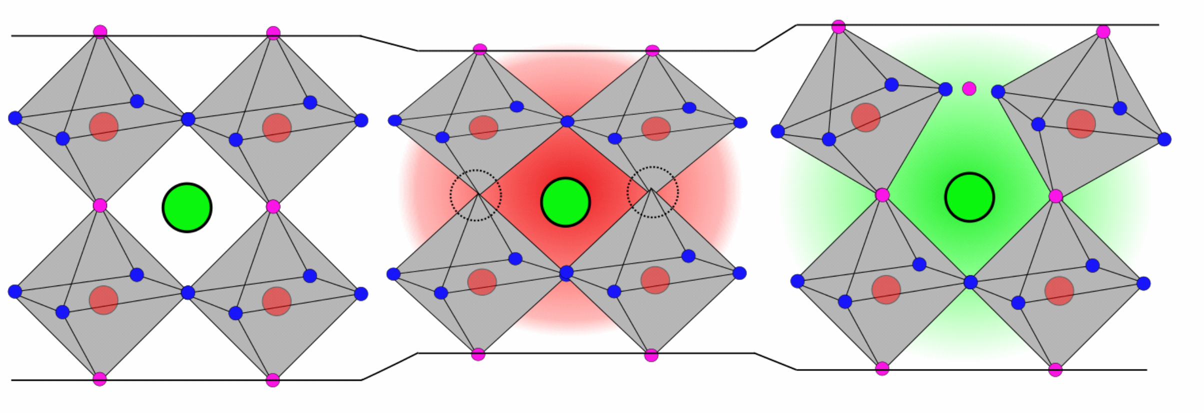

Figure 1. Schematic representation of Plain CPBI, I-deficient, and I-rich thin films.

(1. Thin films/Nano-materials Growth, Novel techniques and concepts)

Growth of Reusable Zinc Ferrite Nanoparticles for White LED-based Photocatalytic Treatment

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ABSTRACT

In this study, normal spinel zinc ferrite ($ZnFe_2O_4$) nanoparticles-based photocatalytic have been grown by hydrothermal method. X-ray diffraction was used to investigate the structural properties of $ZnFe_2O_4$, which confirms the pure phase of $ZnFe_2O_4$ with cubic symmetry having lattice parameter ~ 8.73 Å. The average crystallite size of $ZnFe_2O_4$ nanoparticles has been calculated by Debye-Scherrer formula and linear fit of Williamson-Hall equation, which is found to be ~ 22 nm and ~ 28 nm, respectively. Scanning electron microscopy images confirm the pseudo-spherical morphology of $ZnFe_2O_4$ nanopowder, with average grain size ~ 500 nm. The spectroscopic studies of the synthesized nanoparticles were carried out using Fourier transforms infrared, Raman, photo-luminescence, ultra-violet visible (UV-vis) spectra. The UV-vis spectroscopy has been performed to study the various optical parameters of $ZnFe_2O_4$ nanoparticles and the average value of direct optical band gap was calculated as ~ 2.03 eV, which belongs to visible region. The synthesized nanopowder was employed in the degradation of methylene blue (MB) dye under the low power white LED light at room temperature. Initially, the synthesized nanoparticles decomposed the ~ 70 % dye in the solution. But, after adding hydrogen peroxide (H_2O_2) dye in the dye solution, the degradation efficiency was increased upto 91 % in 60 minutes. The scavenging tests were also performed to check the dominant reactive species in the degradation of dye. Magnetic separable characteristics of $ZnFe_2O_4$ helps to recover the catalysts from degraded MB dye solution for the next photo-degradation cycles. This research paves the path for an eco-friendly, cost-effective, and energy-efficient waste-water management through magnetically separable $ZnFe_2O_4$ photocatalytic with H_2O_2.

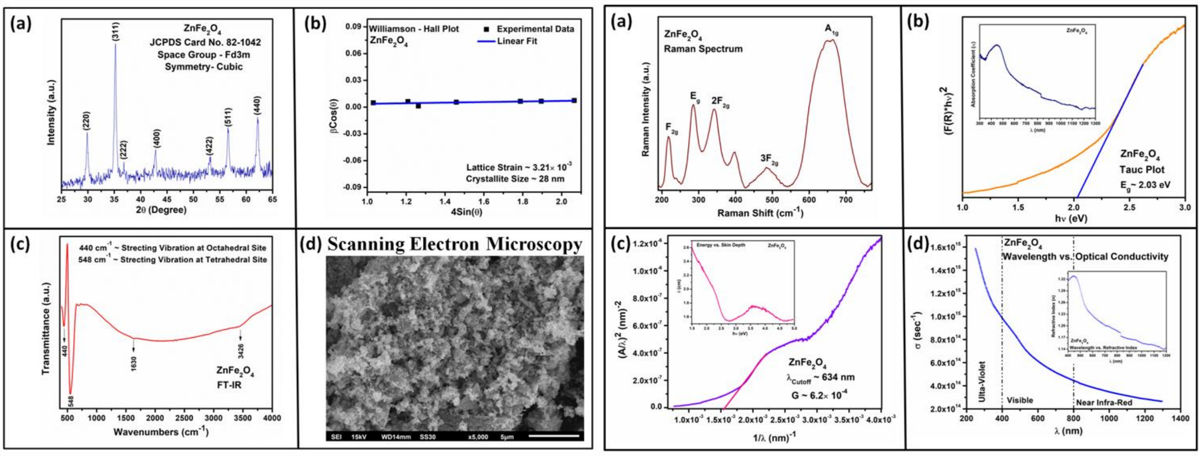

Fig. Structural, morphological, and optical analyses of synthesized $ZnFe_2O_4$ photocatalysis for dye degradation under white LED light.

Keywords: $ZnFe_2O_4$; Hydrothermal Growth; Dye Degradation; White LED Light.

Spin-dependent electronic transport in NiMnSb/MoS_2(001)/NiMnSb magnetic tunnel junction

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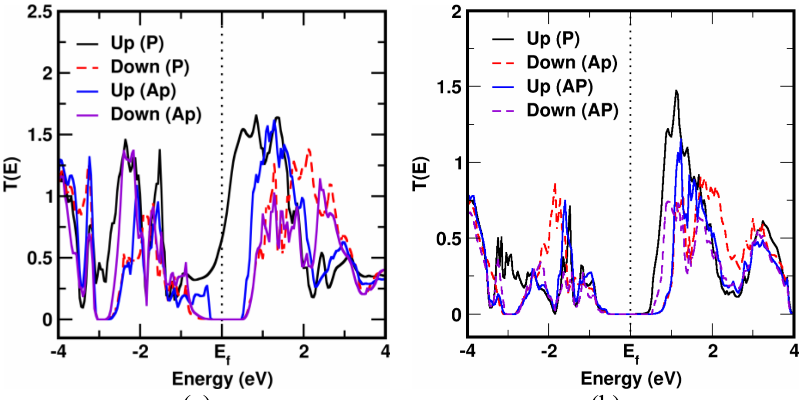
ABSTRACT

Spintronics aims to use 'spin' degrees of freedom of the electron for storage and transportation of information. Significant enhancement with increased data processing speed and low power consumption is possible in spintronics devices over traditional electronic devices. The primary focus in spintronics remains on the injection and transportation of spin-polarised carriers in heterointerface nanoscale devices, optimisation of electron spin lifetime, manipulation, and detection of electron spin in nanoscale devices. Generating large spin-polarised currents requires ferromagnetic material having a large spin-polarised state at the Fermi level. Spintronic devices with normal ferromagnetic material as electrode are inefficient or require large polarising magnetic fields. Half-metallic Heusler alloy compounds with Curie temperatures above room temperature are suitable candidate for electrode materials for injecting large spin-polarised charge carriers into the semiconducting barriers at the ferromagnet semiconductor junction to obtain highly spin-polarised current. Combining the density functional theory and non-equilibrium Green's function method, the electronic structure, and spin-dependent electron transport in NiMnSb/MoS_2(001)/NiMnSb magnetic tunnel junction is studied. The possibilities of injecting 100% spin polarised electron into MoS_2 using half metallic NiMnSb as an electrode, and the effect of the type of interface bonding on electronic structure and spin-transport properties in magnetic tunnel junction devices are studied. We show that the half-metallicity of NiMnSb is preserved at the interface between the half-Heusler alloy NiMnSb and the semiconducting 2H-MoS_2. NiMnSb keeps a fully spin-polarised state in the majority spin channel at the interface between NiMnSb and MoS_2, injecting fully spin-polarised electrons into the semiconductor. The device based on NiMnSb/MoS_2(single-layer)/NiMnSb has a metallic interface. Metal-induced states in the spin-majority channel of MoS_2 are seen after making an interface with half-metallic NiMnSb. In contrast, the NiMnSb/MoS_2(three-layer)/NiMnSb interface with a multilayer of MoS_2 has a band gap region, and electrons can tunnel through the junction.

Keywords: Heusler alloy; heterostructure; spin-transport; Molybdenum disulfide.



(a) (b)

Figure 1: Spin-dependent transmission spectrum for (a) NiMnSb/MoS_2(single-layer)/NiMnSb, and (b) NiMnSb/MoS_2(three-layer)/NiMnSb junction in parallel and anti-parallel orientation of electrodes.

(Abstract Domain: 1. Thin films/Nano-materials Growth, Novel techniques and concepts)

Enhanced NO Gas Detection Using Au and Ag Nanoparticle-Decorated MXene-Based Sensors

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ABSTRACT

MXenes, an emerging class of two-dimensional transition metal carbides, exhibit remarkable electrical conductivity, large surface area, and tunable surface terminations, making them highly suitable for gas-sensing applications. In this study, Ti C T_x MXene was synthesized via a selective etching process and subsequently decorated with metal nanoparticles to enhance its NO sensing performance. The structural and morphological characteristics of the synthesized materials were confirmed using X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR), Transmission Electron Microscopy (TEM), and Raman spectroscopy. Gas sensing evaluations carried out at room temperature and at an elevated temperature of 50 °C demonstrated a sensitivity trend of pristine MXene < Ag@MXene < Au@MXene, with higher responses observed at 50 °C. Among the samples, Au-decorated MXene exhibited the highest sensitivity and excellent repeatability. The improved performance can be attributed to enhanced surface reactivity, catalytic activity, and efficient charge transfer at the MXene–metal nanoparticle interface. These findings underscore the potential of noble metal-functionalized MXenes as highly effective and reliable NO gas sensors for real-world applications.

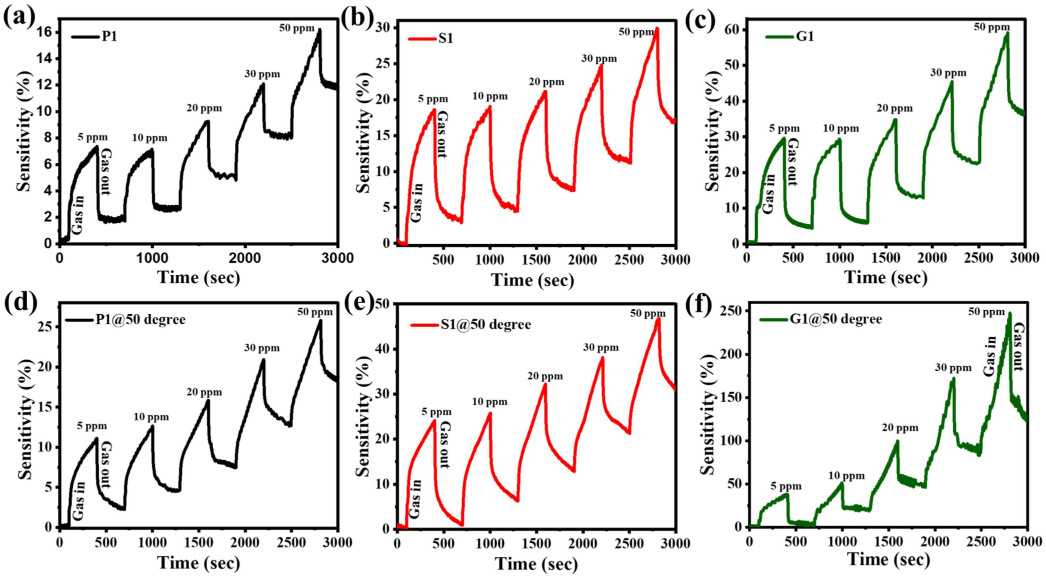

Figure: Gas sensing responses of pristine MXene, Ag-decorated MXene (Ag–MXene), and Au-decorated MXene (Au–MXene) toward NO gas at various concentrations (5, 10, 20, 30, and 50 ppm) measured at room temperature and an elevated temperature of 50 °C.

Keywords: MXene, nanoparticles, Ag, Au, NO_2 Gas Sensing.

(Abstract Domain : Computational modelling & simulations)

Graphene Based Flexible Piezo-resistive Pressure Sensors on PDMS Substrates: A Simulation Study

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ABSTRACT: In this study, we report the design and simulations of flexible piezo-resistive pressure sensors using COMSOL Multiphysics software. Throughout the modelling, Polydimethylsiloxane (PDMS) is used as a flexible substrate, whereas graphene is taken as active sensing layer for the devices with a structure graphene/PDMS. Finite element method is used to model the device containing a thin rectangular shaped PDMS along with a patterned graphene. A thin rectangular shaped PDMS and embedded patterned graphene-based sensors structures are designed. The thicknesses of graphene are taken as 0.3, 0.4 and 0.5 mm, whereas the sensing areas is considered to be 38, 56, and 82 mm^2 throughout device modelling. Type I devices (graphene thickness ~0.3 mm, area 38 mm^2) shows superior performance as compared to Type (II) and Type (III). For Type I(1) devices the sensitivity is determined to be 1.02 kPa^{-1} within a full-scale pressure range of 0–100 Pa. The pressure applied on the thin film is varied to study the change in membrane displacement, stress, terminal voltage, and resistance. It is observed that displacement, stress, terminal voltage, and resistance vary linearly with increasing pressure on the graphene-embedded PDMS substrate. The proposed simple structure having reasonably good sensing characteristics may find its application in the family of flexible piezoresistive pressure sensors. Moreover, the same sensor has been fabricated and used as IoT enabled wearable controller demonstrating forward and reverse motion of presentation slides, speed of motors etc.

Keywords: Flexible, Piezo-resistive, Pressure sensor, Patterned Graphene, Sensitivity.

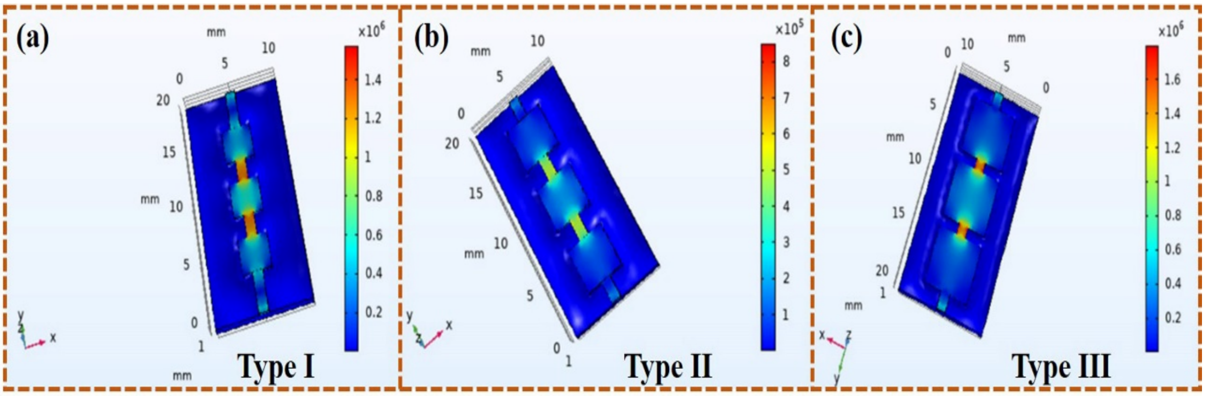

Fig. 1. von Mises stress (N/m^2) plot deformation of graphene embedded PDMS substrate for (a) Type I,(b) Type II (b) and (c)Type III sensors.

Microelectronics and Optoelectronics devices

RF Sputtered Molybdenum Oxide Thin Films for ReRAM Applications

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Abstract

Present day computers use Von-Neuman architecture for computing and data transfer. Which restricts the data transfer speed. Need for next generation computers can be encountered with the resistive memory devices in which the C.P.U and storage on a single device, which mimics the neural network of brain. Which in turn enhances the speed, energy efficiency and scalability of the computer. These devices operate by changing resistance according to the applied voltage which is converted to binary data for computing.

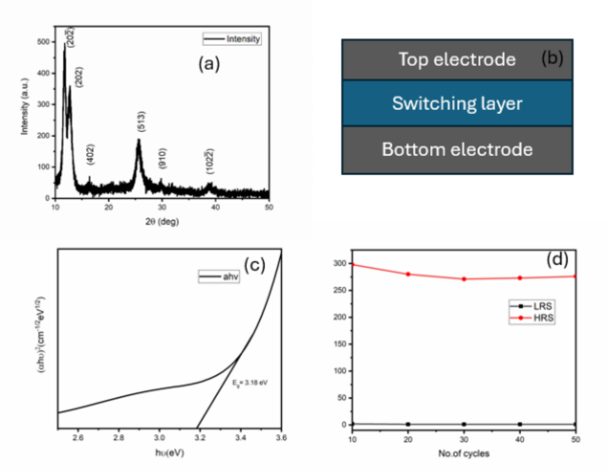

Figure 1. (a) XRD spectra of Molybdenum oxide thin film, (b) device structure (c) Tauc plot of Molybdenum oxide thin film and (d) Endurance characteristics of the device.

In this study the Molybdenum oxide thin films are deposited by RF magnetron reactive sputtering by varying the oxygen partial pressure from 0.002 mbar to 0.005 mbar in the steps of 0.001 mbar at a substrate temperature of 300 °C, over stainless-steel substrates. The study discusses the scope of molybdenum oxide thin films in resistive switching applications. X-ray diffraction pattern confirms the formation of monoclinic Molybdenum oxide (PDF# 98-004-34750). The optical studies were carried out using the UV-VIS-NIR spectrophotometer and the optical bandgap is 3.18 eV, which is obtained from Tauc plots. In order to investigate the Memristor properties, metal semiconductor metal device structure was fabricated. In these devices, stainless-steel substrate act as the bottom electrode, Molybdenum oxide as switching layer and the silver conducting paste as the top conducting electrode. I-V measurements were carried out on the fabricated devices. On/off ratio of 225 was observed for the devices within a voltage range of -1.5 V to +1.5 V with good endurance. The I-V studies of the devices showed promising results for Re-RAM and Neuromorphic computing applications.

Keywords: RF Sputtering; Thin films; Resistive Switching; and Optical Bandgap

Magnetic properties of CoCrFeNi and CoCrFeNiNb$_{.10}$ high entropy alloys

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High entropy alloys (HEAs) represent a class of materials with remarkable structural, mechanical, and functional properties arising from their unique multi-principal-element compositions. This study focuses on the magnetic behavior of two alloys: CoCrFeNi MEA a widely studied single-phase face-centered cubic (FCC) alloy, and CoCrFeNiNb$_{.10}$ HEA a derivative with Nb addition, which introduces structural and magnetic changes. The magnetic properties of equiatomic CoCrFeNi MEA and CoCrFeNiNb$_{.10}$ HEA were systematically investigated using experimental approaches. The alloys were synthesized via arc melting, followed by homogenization, and characterized using X-ray diffraction (XRD) to confirm phase formation and crystal structure. Magnetic measurements were performed using a Physical Property Measurement System (PPMS) in the temperature range of 5 K to 300 K. CoCrFeNi exhibits ferromagnetic contribution at low temperatures. And CoCrFeNi MEA showed paramagnetic behavior at room temperature. The alloy's magnetization is primarily influenced by the Co, Ni and Fe elements, which induce a ferromagnetic phase, while Cr tend to disrupt magnetic ordering. MH measurements present that CoCrFeNiNb$_{.10}$ HEA shows minimum coercivity and high magnetic saturation compare to CoCrFeNi MEA. This is attributed to the Nb-induced lattice distortions and local variations in electronic density. Ferromagnetic materials are used in transformer cores, electric motors, and generators for efficient energy conversion; in electromagnetic devices like inductors and solenoids; and in magnetic shielding to protect sensitive equipment from external magnetic fields.

Key words: HEAs, CoCrFeNi, CoCrFeNiNb

Hybrid mesoporous structure for improving the performance of DSSC

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Abstract

DSSCs are regarded as a possible substitute for traditional silicon-based solar cells and have been widely accepted by both academia and industry because of moderate energy conversion efficiency, cheap production costs, straightforward processing, and less hazardous manufacturing. However, it is still waiting for commercial application due to low power conversion efficiency. In this work, our objective is to modify a new type of cell design to enhance the performance of the DSSC. We designed a new type of cell by using low-density core-shell ZnO-TiO_2 nanorod arrays as the photoanode material. Low-density zinc oxide nanorod arrays were grown on the dewetted polystyrene film of the FTO glass by using zinc nitrate and hexamethylenetetramine (HMTA). Fabricated cells and synthesized materials are characterized by FESEM, HRTEM, XRD, FTIR, UV-DRS spectroscopy, and EIS analysis. All the photovoltaic properties (short circuit current density (Isc), open circuit voltage (Voc), fill factor (FF), and power conversion efficiency (PCE) of the DSSCs have been measured by using different sizes of masks. Masking and edge masking were done for the measurement of aperture area and active area based on DSSCs, respectively. The best performance is obtained as PCE~14.72 % and 5.31 % for 4 mm^2 aperture area based DSSC and 25 mm^2 active area based DSSC, respectively. Again, we have also reported the performance comparison study of TiO_2 nanoparticles-based DSSCs and core-shell ZnO-TiO_2 nanorod arrays-based DSSCs.Modification cell design from bare TiO_2 nanoparticles to core-shell ZnO- TiO_2 nanorod arrays with inserted TiO_2 NPs improves the cell performance 40 % approximately for a 4 mm^2 aperture area-based DSSC and 34 % for a 100 mm^2 active area-based DSSC.

Keywords: Dye sensitized solar cell (DSSC), Short circuit current density (Isc), Open circuit voltage (Voc), fill factor (FF), and power conversion efficiency (PCE)

Abstract Domain 3: Microelectronics and optoelectronic devices

Optically Enhanced Associative Learning and Pavlovian Conditioning in CuPc-based Synapses

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ABSTRACT

Emerging artificial intelligence systems offer advantages over conventional computers in terms of low power consumption, high efficiency, and parallel processing capability. Neuromorphic devices are brain-inspired systems that mimic the functions of biological neurons. The distinguishing feature of human brain is adaptive learning, allowing it to respond more effectively to previously encountered scenarios. Studies have shown that some devices exhibit increased conductance when exposed to light pulses, forming the foundation for optical neuromorphic devices. Recent studies have identified organic materials as prime candidates for fabricating optical neuromorphic devices. In our study, we used Copper Phthalocyanine (CuPc), which exhibited appreciable optical neuromorphic behaviour when subjected to various LEDs and white light.

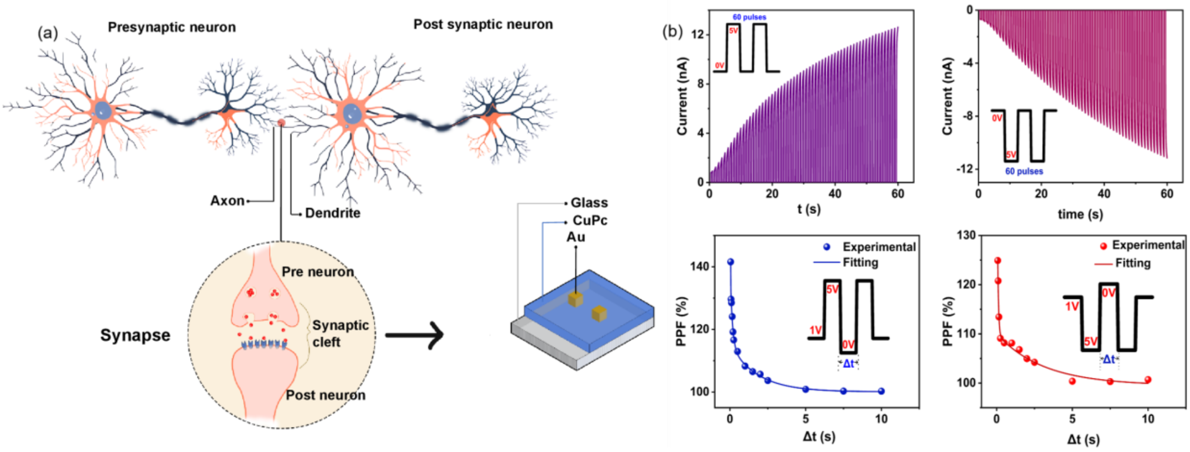

Figure: (a) The schematic of a biological synapse and its artificial counterpart. (b) The demonstration of various synaptic activities.

The Gold/CuPc/Gold (Au/CuPc/Au) surface device (Fig. a) features two Schottky barriers due to the high work function of gold. Theoretically, the conductance of this system varies due to ion flow through the interfaces, facilitated by the presence of light. We observed an enhancement in neuromorphic behaviour when the device was exposed to light. The absorption band centred around red region prompted the use of red LED as optical stimulus. The essential features of a neuromorphic device such as Paired Pulse Facilitation (PPF), Spike Timing Dependent Plasticity (STDP) and Spike Number Dependent Plasticity (SNDP) were realised (Fig. b) and were further facilitated under the influence of light. We were able to observe the associative learning capability of the device by demonstrating the Pavlov conditioning behaviour, where voltage acts as an unconditional stimulus and light as a neutral stimulus. The ability of the Au/CuPc/Au device to associate optical stimuli to voltage stimuli suggests the potential for optical enhancement of neuromorphic behaviour as a new application domain. This adaptive learning capability was implemented for optical enhancement of pattern recognition accuracy of the device when trained to recognize handwritten images.

Keywords: Copper (II) Phthalocyanine; artificial synapses; neuromorphic device; Pattern recognition.

(Abstract Domain : Materials & coating for batteries, super-capacitors and fuel cells)

Dual Ion Conducting Electrolyte Material for Fuel Cell

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ABSTRACT

Fuel cells convert chemical energy directly into electricity, producing water as the only by-product. Solid Oxide Fuel Cells (SOFCs) offer high efficiency but require high operating temperatures (~1000 °C). Combining oxygen ion conductors such as Yttria-Stabilized Zirconia (YSZ) with proton conductors like Barium Cerate (BCO) can enable dual ion conduction at intermediate temperatures[1]. YSZ and BCO were synthesized via solid-state and sol–gel routes, respectively. FESEM showed grain sizes of 0.652 µm (YSZ) and 0.289 µm (BCO). TGA, DSC, and FTIR confirmed thermal stability, thermodynamic behavior, and metallic–oxygen bonding. Impedance spectroscopy revealed conductivities of $\sim 10^{-4}$ S/m with activation energies of 1.13 eV (YSZ) and 0.56 eV (BCO)[2,3]. The composite exhibited multiple stable phases, indicating promise for intermediate temperature SOFC electrolytes.

Keywords: Fuel Cell, SOFC .

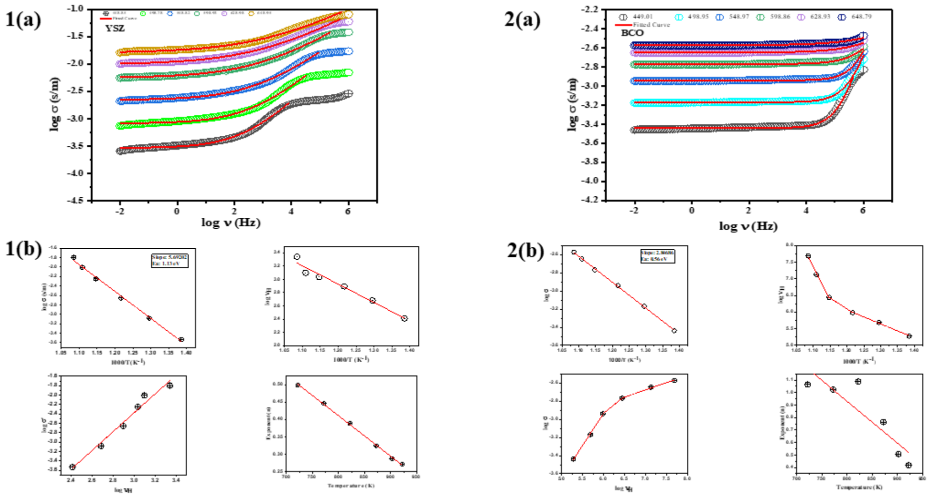

Fig.1(a) Shows the conductivity of YSZ 1(b) Arrhenius plots of YSZ 2(a)Conductivity of BCO 2(b) Arrhenius plots of BCO

References

1. Huangang Shi, Chao Su, Ran Ran, Jiafeng Cao, Zongping Shao, Electrolyte materials for intermediate-temperature solid oxide fuel cells, Progress in Natural Science: Materials International (2020), **30** ,764–774
2. Gilardi, Elisa,Gregori, Giuliano,Maier, Joachim, Epitaxial 8YSZ/Y2Zr2O7 multilayers: a conductivity and strain study, Phys.Chem.Chem.Phys., 2018, **20**, 19995
3. Kannan, R., Singh, K., Gill, S. *et al.* Chemically Stable Proton Conducting Doped $BaCeO_3$ -No More Fear to SOFC Wastes. *Sci Rep* (2013) ,**3**, 2138

An adapted ALD method to fabricate low-resistivity and high-transparency aluminum-doped zinc oxide TCO for silicon heterojunction solar cells

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In this study, aluminum-doped zinc oxide (ZnO:Al or AZO) thin films were developed using different atomic layer deposition (ALD) modes, namely thermal ALD (THALD), plasma-enhanced ALD (PEALD), and a newly proposed hybrid approach termed DTH (DEZ – TMA - H_2O) ALD. The ultimate objective is to fabricate bifacial silicon heterojunction solar cells with carrier-selective contact (CSC), using sequential deposition of multiple functional layers on both sides of the wafer, i.e., passivation, electron transport, and hole transport layers, transparent conductive oxide layers within the same vacuum system, thereby minimizing contamination and simplifying the fabrication of complete CSC devices. We are employing ALD to achieve this objective. The growth per cycle (GPC) values of PEALD-deposited films on c-Si wafer at 200 °C, determined by spectroscopic ellipsometry and X-ray reflectometry, were 1.45 ± 0.12 Å for Al_2O_3 and 1.28 ± 0.08 Å for ZnO, respectively, confirming the self-limiting nature of the ALD growth. The GPC values for these layers, as determined by THALD, were slightly lower at 1.00 ± 0.14 Å and 0.98 ± 0.10 Å, respectively. The effect of this difference, attributed to enhanced surface reactivity and oxidation kinetics under plasma activation, manifests in the more amorphous nature of PEALD ZnO:Al. The Al incorporation in ZnO was tuned by varying the (1:n) pulse ratio of Al_2O_3:ZnO sub-cycles to achieve a ~2 at% Al at a (1:21) pulse ratio, yielding the optimum trade-off between conductivity and optical transmittance for the PEALD process. The THALD AZO showed higher carrier mobility, attributed to the improved film crystallinity. However, the doping efficiency improves by modifying the doping precursor (TMA) dosing and co-reactant exposure (H_2O) in a THALD process. This new approach, we name DTH, resulted in a low resistivity of 2.28×10^{-3} Ω·cm while maintaining an optical transmittance above 85% in the visible region, significantly improved upon both conventional THALD and PEALD modes. By increasing the DTH deposition temperature to 350 °C, a further decrease in resistivity to below 8.0×10^{-4} Ω·cm was achieved, demonstrating performance comparable to that of state-of-the-art TCOs fabricated by sputtering. A model is proposed to explain the doping behaviour under the changed precursor dosing sequence.

Keywords: Aluminum-doped zinc oxide, Atomic layer deposition, Carrier selective contact solar cell,

Field-Assisted Growth of Ferromagnet/Antiferromagnet Thin Films for Spintronic Applications

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The growth of high-quality magnetic thin films with controlled interfacial properties is critical for spintronic device performance. Using ion-beam sputtering, ferromagnet/antiferromagnet bilayers including Ni Fe /Ir Mn , IrMn/Co FeAl, and IrMn/Co FeB are deposited under an *in-situ static in-plane magnetic field of 1 kOe* while the sample holder was continuously rotated to ensure uniform film growth and consistent magnetic anisotropy across the surface. This field-assisted and dynamic growth strategy promotes the alignment of uncompensated spins at the ferromagnet/antiferromagnet interface, inducing robust unidirectional exchange anisotropy and stabilizing both positive and negative exchange bias. Microstructural parameters such as grain size, layer thickness, and interface roughness were systematically controlled, demonstrating their critical role in tuning exchange bias, coercivity, and training effects. Magnetoresistance measurements confirm that films grown under these conditions exhibit enhanced spin alignment, reduced anisotropy dispersion, and improved thermal stability. These engineered thin films are highly suitable for spintronic applications, including magnetic tunnel junctions, spin valves, and MRAM devices. The integration of *in situ* magnetic field, continuous rotation, and microstructure control establishes a reproducible growth methodology for magnetic thin films with deterministic properties. Furthermore, studies show that ion-beam irradiation can be used to intentionally create defects, offering additional control over magnetic anisotropy and interfacial spin structure.

References:

1. S K Kedia, *et al.,* "*Grain diameter-dependent tuning of exchange anisotropy in the ion-beam sputtered Co-based full Heusler alloy coupled with antiferromagnet*", *J. Appl. Phys.* 135 (2024) 053903.
2. S K Kedia, *et al.*, "*Tuning of exchange bias by regulating the microstructural parameters in* $Ni_{81}Fe_{19}$ *(5, 8, 11, 14, 17, and 20 nm)/Ir7Mn93(10 nm) bilayers probed using magnetoresistance*", *J. Appl. Phys.* 134 (2023) 173904.
3. S K Kedia, *et al.*, "*Investigation and tailoring the strengths of positive and negative exchange bias in the ion-beam sputtered* $Ni_{81}Fe_{19}/Ir_7Mn_{93}$ *bilayers by tuning the grain size of the antiferromagnetic Ir7Mn93 layer*", *J. Magn. Magn. Mater.* 584 (2023) 171073.
4. S K Kedia, *et al.*, "*Defect-Induced Modulation of the Exchange Anisotropy by Swift Heavy Ion Irradiation in* $Ni_{81}Fe_{19}/Ir_7Mn_{93}$ *Bilayers*", *Nuclear Inst. and Methods in Physics Research, B* 555 (2024) 165466.

Enhanced Surface Passivation and Interface Quality of Ultrathin HfO_x Films Deposited by PEALD on Silicon

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Ultrathin hafnium oxide (HfO_x) films were deposited on p-type crystalline silicon substrates using plasma-enhanced atomic layer deposition (PEALD) to evaluate their surface passivation performance. The influence of film thickness (10 and 50 ALD cycles, ~3 nm and ~7 nm) before and after annealing on electrical and interfacial properties was systematically investigated. As-deposited films exhibited poor passivation while annealing enhanced the minority carrier lifetime to 465 μs and reduced the surface recombination velocity below 35 cm/s for 50-cycle films. High-frequency (1 MHz) C-V and G-V analyses revealed reduced hysteresis, a positive flat band voltage shift and a lower interface defect density ($D_{it} \approx 10^{10}$ $eV^{-1}cm^{-2}$), indicating improved charge neutrality and interface quality. FTIR spectra confirmed structural densification, partial crystallization and SiO_x interlayer formation, whereas impedance spectroscopy indicated reduced series resistance and enhanced carrier transport. The results demonstrate that PEALD-deposited ultrathin HfO_x films provide excellent passivation and interfacial stability, making them promising candidates for integration in high-efficiency silicon solar cells and advanced MOS-based devices.

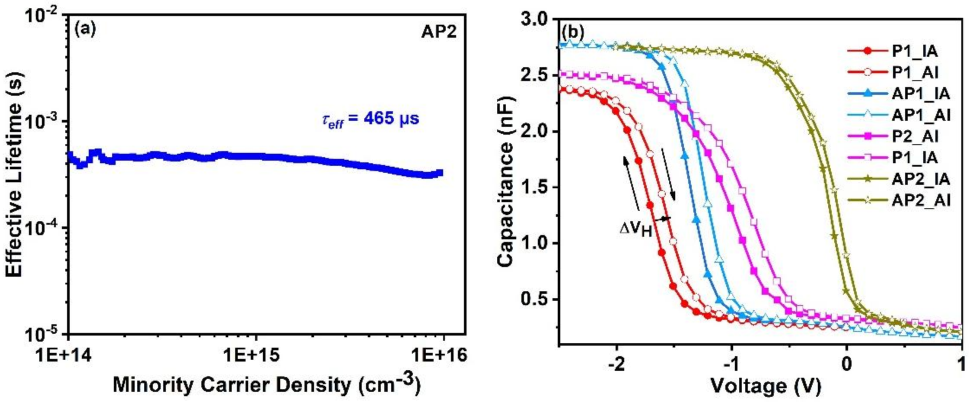

Figure-1 (a) Injection level dependence of minority carrier lifetime of annealed sample deposited at 50 cycles (b) High-frequency (1 MHz) CV curves for as deposited and annealed samples from inversion to accumulation (IA) with reverse sweep accumulation to inversion (AI).

Eco-Friendly Synthesis and characterization of ZnO Nanoparticles Using Neem Extract for Improved Structural and Optical Performance

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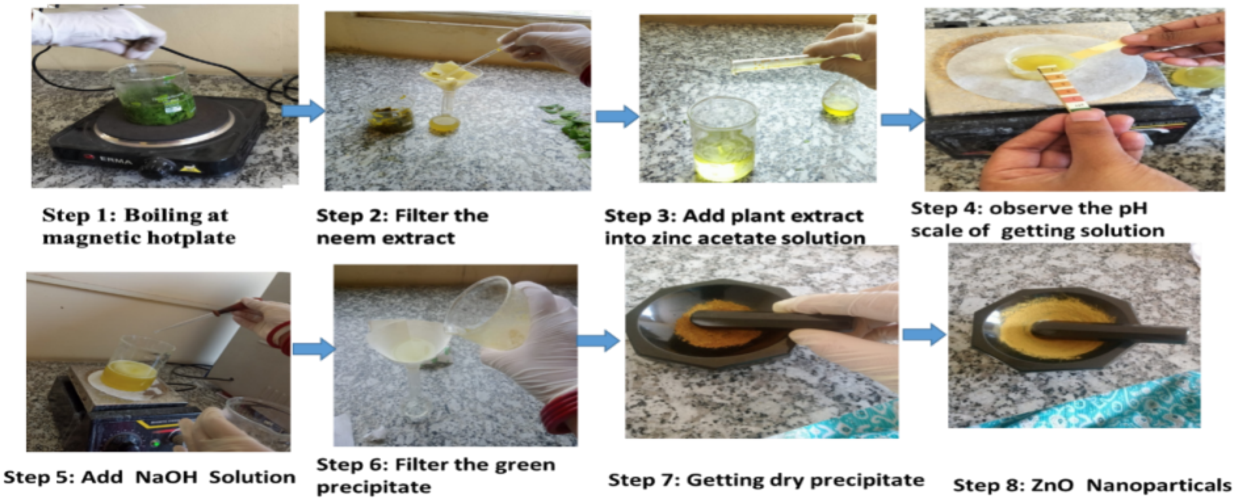
ABSTRACT

In this study, zinc oxide (ZnO) nanoparticles were synthesized through an eco-friendly green synthesized route using neem leaf extract as a natural reducing and stabilizing agent. The phytochemicals present in neem extract effectively facilitated the formation of ZnO nanoparticles without the use of toxic chemicals, making the process sustainable and environmentally benign. The synthesized nanoparticles were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) and UV-Visible spectroscopy to analyze their structural, morphological and optical properties. XRD analysis confirmed the formation of crystallite wurtzite hexagonal phase with an average crystallite size of 42 nm. SEM images revealed nearly spherical to hexagonal shaped nanoparticles with a grain size of 35.5 nm and uniform distribution, indicating effective capping by bioactive compounds from the neem extract. Optical analysis showed strong absorption in the UV region and reduced band gap suggesting improved optical activity. The optical band gap was found to be in the range of 1.65 eV, confirming the conducting nature of the ZnO nanoparticles. The results demonstrate that neem-extract-mediated green synthesis is an efficient, cost effective and sustainable method for producing ZnO nanoparticles with superior structural, optical properties suitable for optoelectronics devices applications

Keywords: Nanoparticles, Green synthesis, Optical, Optoelectronics, Crystallite.



Step 1: Boiling at magnetic hotplate

Step 2: Filter the neem extract

Step 3: Add plant extract into zinc acetate solution

Step 4: observe the pH scale of getting solution

Step 5: Add NaOH Solution

Step 6: Filter the green precipitate

Step 7: Getting dry precipitate

Step 8: ZnO Nanoparticals

(Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts)

Oxygen vacancy modulated neuromorphic behaviour in pulsed laser deposited yttrium iron garnet thin films

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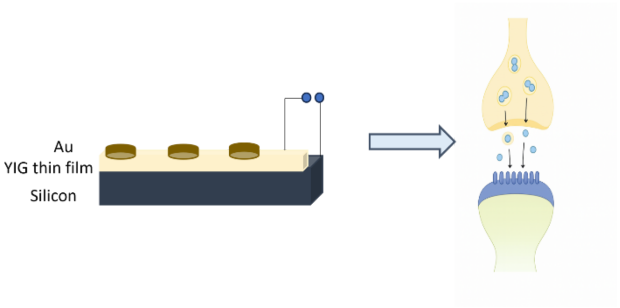
ABSTRACT

Yttrium Iron Garnet (YIG) thin films, traditionally valued for their low magnetic damping and superior spin wave properties, are increasingly being explored for their tunable electrical characteristics in neuromorphic computing applications. Introduction of oxygen vacancies during the growth phase can help modulate the behaviour of the material from insulating, to conducting. In this study, we investigate the role of oxygen vacancies in modulating the resistive and memristive behavior of YIG thin films grown via pulsed laser deposition (PLD) under controlled oxygen partial pressures. The optimised film is fabricated into a device to carry out electrical characterisation. Electrical transport measurements reveal a transition from highly insulating to semiconducting behavior with increasing oxygen deficiency, enabling non-volatile resistance states suitable for synaptic weight modulation. Furthermore, current–voltage (I–V) analysis shows clear evidence of hysteresis, indicative of potential for memristive synaptic devices. The vacancy-induced charge transport mechanisms are correlated with structural and chemical changes confirmed through X-ray photoelectron spectroscopy (XPS) and X-ray diffraction patterns (XRD). The results demonstrate that oxygen vacancy engineering in YIG not only expands its functional landscape beyond magnetics but also establishes a pathway toward multifunctional neuromorphic elements combining spintronic and electronic control.



Keywords: Thin films; Neuromorphic behaviour; Yttrium iron garnet; Pulsed laser deposition.

Domain : Microelectronics and Optoelectronic Devices

Dual-Mode Quantum Dot-Based Optoelectronic Physical Unclonable Function for Secure Authentication and Anti-Counterfeiting Applications

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Nanoparticle (NP)-based Physical Unclonable Functions (PUFs) represent a rapidly advancing frontier in hardware security, harnessing nanoscale randomness and the tunable optoelectronic characteristics of quantum materials to generate tamper-resistant, high-entropy identifiers. In this work, we demonstrate a dual-mode optoelectronic PUF utilizing Br-rich $CsPbC_xBr_{3-x}$ mixed-halide perovskite NPs that simultaneously exhibit stochastic optical emission and electrical conduction behavior. The proposed architecture exploits substrate-induced disorder as the fundamental source of entropy, where substrate topography (glass, mica, and Si/SiO_2) and spin-coating dynamics lead to a random nanoparticle assembly, governing both optical brightness distribution and inter-particle electrical connectivity. This inherent physical randomness defines the unclonable device signature that serves as the foundation for secure encoding. A two-pronged strategy combining MeOAc ligand stripping for enhanced nanoparticle interconnectivity and PMMA encapsulation for environmental protection ensures improved charge transport, photoluminescence retention, and long-term stability of the device. The resultant network demonstrates distinct, reproducible responses under optical excitation (365 nm UV illumination) and electrical probing (two-terminal current measurement under a fixed 10 V bias in dark conditions), both of which are digitally encoded to generate unique and complementary binary fingerprints. Statistical analysis of the extracted responses reveals excellent biasness (uniformity), high uniqueness with inter-device Hamming distances near the ideal 0.5, and superior reliability under repeated measurements, highlighting the robustness of the optoelectronic encoding. The fabrication process is entirely solution-based, relying on scalable spin-coating and mild post-treatment steps, while the readout requires only conventional optical microscopy and current–voltage measurements, underscoring the simplicity, low-cost nature, and practical deployability of this system. The synergy of optical and electronic randomness within a single nanoparticle ensemble offers a powerful route to multidimensional encoding, bridging the gap between quantum materials research and secure microelectronic device engineering. This dual-mode perovskite NP-PUF platform thus enables a new class of scalable, physically unclonable identifiers suited for diverse hardware security and anti-counterfeiting applications, ranging from secure device-to-device authentication in Internet-of-Things (IoT) networks to traceable, tamper-evident labeling of high-value products and digital assets. By coupling the rich disorder physics of perovskite nanomaterials with robust device-level readout and data encoding, this work establishes a practical foundation for next-generation microelectronic and optoelectronic devices where security, functionality, and scalability converge.

Keywords: optoelectronic PUF; substrate-induced disorder; hardware security; anti-counterfeiting; IoT

(Abstract Domain: 3)

Temperature-Induced Synaptic Fatigue in $BiFeO_3$-Based Electronic Synapses

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ABSTRACT

Neuromorphic devices are a type of devices that are designed to emulate the processing and memory functionality of biological neurones and synapses. Similar to the neurons in our brain, these devices are also sensitive to temperature, which can affect how charges move inside the device, which eventually decides how stable they are. In this study, we deposited $BiFeO_3$ (BFO) thin films using Pulsed Laser Deposition technique and examined the neuromorphic properties of Au/BFO/FTO devices at different temperatures (40°C, 60°C, 80°C, 100°C, and 120°C) to understand how temperature influences the behaviour of the synaptic device. At lower temperatures, the devices showed strong neuromorphic responses; however, from 100°C onwards, the devices could no longer maintain their neuromorphic behaviour. In addition, we trained and tested these devices at different temperatures for pattern recognition applications, which depict that at higher temperatures, the prediction efficiency of the devices significantly reduces. At lower temperatures, the charges mostly move due to an applied electric field (drift), but at higher temperatures, diffusion dominates, making the device less reliable. This is similar to how biological neurones lose efficiency when they are at high temperatures. These results suggest that temperature plays an important role in determining how well neuromorphic devices work in practical environments, and highlight that there is an upper temperature limit for these devices, beyond which their neuromorphic functional ability degrades.

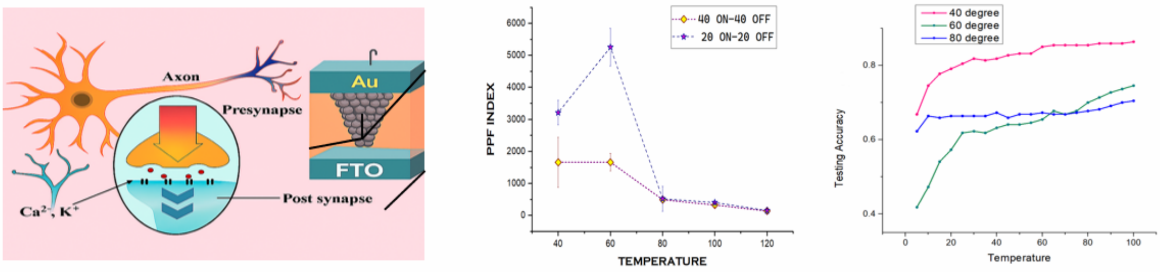

Fig : Schematic illustration of the biological-to-electronic synapse analogy, showing the temperature-driven variation in PPF index and the corresponding change in learning accuracy across different thermal conditions.

Keywords: Pulsed laser deposition (PLD); BiFeO thin films; Neuromorphic devices; Synaptic fatigue

(Computational Modeling & Simulations)

Designing and analysis of D–π–A–π–D and A–D–A structured π-conjugated organic compounds for utilization as field effect transistors

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ABSTRACT

In this work, a series of novel organic semiconducting molecules were computationally designed and analyzed for utilization as potential candidates for high-performance organic field effect transistors (OFETs). The studied molecular systems are based on two different electronic architectures viz. D–π–A–π–D and A–D–A. Here, D, π and A represent electron donor, π bridge and electron acceptor moieties respectively. Indacenodithiophene (IDT) and benzodithiophene (BDT) were used as electron donor units, and perylenediimide (PDI) and naphthalenediimide (NDI) were used as electron accepting units. Geometry optimization and electronic structure analyses were carried out using *Gaussian* and GaussView softwares. All calculations were performed using density Functional theory (DFT). Key charge transport parameters, namely adiabatic and vertical ionization potentials (IP_a and IP_v), adiabatic and vertical electron affinities (EA_a and EA_v), and reorganization energies for holes (λ) and electrons (λ_e), were evaluated to determine their suitability as efficient OFET materials. The results reveal that the D–π–A–π–D systems exhibit lower λ values and higher IP values, suggesting strong hole transport characteristics suitable for *p*-type semiconducting behaviour, whereas A–D–A systems demonstrate lower λ_e and higher EA values, indicative of *n*-type transport properties. The balanced λ /λ_e ratios and tunable frontier molecular orbital energies in both architectures underscore their potential for ambipolar OFET performance. Overall, this study establishes the reliability of *Gaussian*-based DFT analysis in predicting charge transport efficiency and provides a rational molecular design pathway for developing next-generation organic semiconductors with tailored electronic properties.

Keywords: OFET; IDT; BDT; NDI.

Atomic Layer Deposition of Hf:ZnO with Tailored Work Function and Dual Conducting–Dielectric Behavior

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In this study, a detailed investigation on the transparent conducting oxide (TCO) and dielectric properties of undoped ZnO and Hf-doped ZnO (HZO) thin films has ben presented. ZnO-based TCOs are highly valued in optoelectronic and photovoltaic applications due to their unique combination of high optical transparency and electrical conductivity. Hafnium doping introduces an additional degree of tunability, enabling ZnO films to demonstrate both conducting and dielectric characteristics depending on stoichiometry as well as the doping concentration. This dual behaviour enhances the versatility of HZO for a wide range of technological applications, including solar cells, sensors and capacitive devices.

Atomic layer deposition (ALD) method was used to deposit ZnO and HZO films, because ALD offers precise control over film thickness, doping concentration and uniformity at the atomic scale. ALD's self-limiting reaction mechanism ensures conformal growth on complex surfaces, enabling the production of high-quality, reproducible TCO and dielectric films. The deposition was performed on cleaned glass and p-Si substrates, maintaining a consistent film thickness of approximately 50 nm, which was confirmed through spectroscopic ellipsometry. Prior to the deposition, the substrates were cleaned using standard cleaning procedures. ZnO and HZO films with varying Hf doping concentrations were deposited at 250 ° C using diethylzinc (DEZ), deionized water, and tetrakis(ethylmethylamino)hafnium (TEMAHf) as the zinc, oxidant and hafnium precursors, respectively. The structural properties of the films were analysed using grazing incidence X-ray diffraction (GIXRD), confirming that ZnO and HZO films with low Hf doping (10:1 ratio) exhibit a polycrystalline hexagonal wurtzite structure. However, higher Hf doping concentrations (1:1 ratio) led to a reduced crystallinity and conductivity of the films, which are due to the limited solubility of Hf in the ZnO matrix, as confirmed by elemental analysis. Surface morphology and topography were analyzed using field-emission scanning electron microscopy (FESEM) and atomic force microscopy (AFM), revealing smooth and uniform film surfaces. Optical measurements performed using UV– Vis-NIR spectroscopy demonstrated an optical transmittance > 80% across the visible spectrum for all films, highlighting their suitability for optoelectronic applications. Electrical measurement results showed that undoped ZnO and Hf-doped ZnO films at higher doping concentrations exhibited high resistivity, whereas low Hf-doped ZnO films displayed enhanced conductivity with a minimum resistivity of 1.4 mΩ-cm. For electrical characterization, Al contacts were thermally evaporated onto both sides of ZnO/p-Si and HZO/p-Si heterojunctions. Current-voltage (I-V) measurements revealed a transition from rectifying to Ohmic behaviour with decreasing Hf concentration, which was attributed to variations in the work function of HZO film. Kelvin probe measurements further validated these findings by confirming changes in the work function of HZO films with the doping concentration. The interface properties of these heterostructures were studied using capacitance-voltage (C-V) measurements at different frequencies and impedance spectroscopy.

Overall, this study demonstrates that ALD-grown Hf-doped ZnO films at lower doping concentrations are promising TCO materials for photovoltaic and optoelectronic devices due to their superior conductivity and optical transparency. Conversely, highly Hf-doped ZnO films exhibit enhanced dielectric properties, making them suitable for advanced electronic applications such as capacitors and memristors. These findings provide valuable insights into the tunability of ZnO-based materials for multifunctional applications. Detailed results and analyses will be presented at the conference.

Keywords: TCO, dielectric, ALD, Hf-doped ZnO, work function

Reference

1. Geng, Y., Xie, Z. Y., Yang, W., Xu, S. S., Sun, Q. Q., Ding, S. J., ...&Zhang, D. W., Structural, optical and electrical properties of Hf-doped ZnO films deposited by atomic layer deposition. Surface and Coatings Technology 2013, 232, 41-45.

Influence of Film Thickness on the Performance of CuS-Based Resistive Switching Devices

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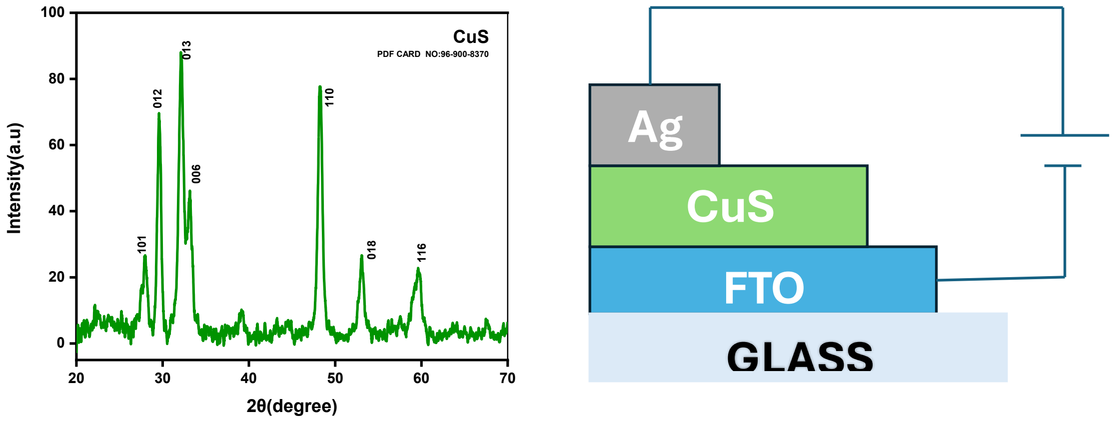
ABSTRACT

We investigate the influence of film thickness on the structural, optical, and electrical properties of Copper Sulfide (CuS) thin films and their application in memristive devices. CuS thin films with varying thicknesses were deposited on Fluorine-doped Tin Oxide (FTO) glass substrates at a temperature of 523 K using a co-evaporation method. Structural and compositional analysis confirmed the successful synthesis of the material. X-ray Diffraction (XRD) measurements verified the formation of the covellite phase of CuS, which is in good agreement with PDF card number 96-900-8370. Furthermore, Energy-Dispersive Spectroscopy (EDS) confirmed the presence of the constituent elements, copper (Cu) and sulfur (S), in the deposited films. Optical and electrical characterization revealed thickness-dependent properties. Optical studies showed that the direct optical band gap decreases from 2.18 eV to 1.6 eV with the decrease in film thickness. Electrical measurements confirmed the p-type conductivity of the CuS films, and analysis of parameters such as charge carrier mobility and electrical conductivity demonstrated a clear dependence on film thickness. Two-terminal memristor devices with structure of <FTO/CuS/Ag> are fabricated and evaluated their resistive switching characteristics. The highest on/off ratio of 96 was observed for devices fabricated with lowest CuS film thickness.

Keywords: copper sulfide; co-evaporation; memristor



(a) (b)

Fig. (a) XRD pattern of CuS thin film (b) schematic diagram of <FTO/CuS/Ag> device

(Abstract Domain: Thin Films/Nano-materials Growth, Novel techniques and concepts)

Long-term photovoltaic study of AZO, ITO, and FTO electrode-based Dye-Sensitised Solar Cells

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This study presents a detailed one-month investigation of long-term photovoltaic performance and corrosion resistance of Dye-Sensitised Solar Cells (DSSCs) fabricated using three different transparent conducting oxide (TCO) electrodes—Aluminium-doped Zinc Oxide (AZO), Indium Tin Oxide (ITO), and Fluorine-doped Tin Oxide (FTO). The photovoltaic parameters were initially evaluated to assess short-term efficiency and charge transport characteristics. During the early phase, DSSCs based on ITO and FTO exhibited higher power conversion efficiencies due to their superior conductivity and well-aligned energy levels. However, after a month of continuous testing under identical conditions, a significant decline in the performance of ITO and FTO devices was observed, primarily due to interfacial degradation and corrosion effects at the electrode–electrolyte interface. To further understand these changes, the cells were disassembled and subjected to detailed Electrochemical Impedance Spectroscopy (EIS) and corrosion analysis. The results revealed that AZO retained its electrochemical integrity with lower charge-transfer resistance and stronger corrosion resistance compared to ITO and FTO. This enhanced durability led to better long-term photovoltaic stability in AZO-based DSSCs, despite its initially lower efficiency. Overall, the findings highlights the importance of balancing initial performance with long-term stability when selecting TCO electrodes. The improved corrosion resistance and sustained performance of AZO make it a promising candidate for reliable and cost-effective DSSC applications.

Keywords: DSSCs, Corrosion, TCOs and EIS

Design of novel dopant free thiophene based hole transport material for perovskite solar cells: A DFT and SCAPS-1D simulation

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Abstract

Hole transport Layers (HTLs) play a vital role in perovskite solar cells (PSCs) towards increasing their overall efficiency. The corresponding compounds used to prepare HTLs are termed as hole transport materials (HTMs). They help in hole extraction and transport from active layer of PSCs, thereby improving PSC efficiency. In present work, molecular structures of $(TP)_n$-BZ ME(n=1,2….5) have been theoretically simulated to determine whether they can function as HTMs. Here, TP, BZ and ME represent thiophene, benzene and 2-(2-methoxyethoxy)ethoxy groups respectively. These compounds are based on polythiophenes structures reported by Andersson et al. Subject molecules were optimized under the framework of density functional theory (DFT) using B3LYP hybrid functional and 6-31G (d,p) basis set in *Gaussian 16W* software. The DFT methodology is utilized for investigating various important electrical, optical, and efficiency-related features of molecules. The doping free molecule was demonstrated by the proposed HTMs ($(TP)_n$-BZ-ME(n=1,2….5)), which made them suitable for faster hole mobility. The results confirm that the holes mobility is higher for the designed molecule in comparison to the electron's mobility whose values are (mobility for holes is 1.7 cm^2/V-s, mobility for electrons is 2.2 cm^2/V-s. Moreover, the performance of perovskite with novel HTMs was investigated using the Solar Cell Capacitance Simulator (SCAPS-1D) software. Moreover, the existence of imperfections in the electron transporting layer (ETL)/perovskite and HTL/perovskite interfaces was taken into account, and their influence on performance was also analyzed. The designed PSC after optimization has a practically achievable efficiency of 22.48%. Comparative analysis of title compounds shows most suitable molecule $(TP)_3$-BZ-ME which has good ability to behave as HTM.

Keywords: Perovskite, Hole transport material, DFT, SCAPS-1D

Study on the Structural and Electrical Properties of Polypyrrole Conducting Films Synthesized via Green Ultrasonication-Assisted and Conventional Chemical Methods

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ABSTRACT

The development of green and sustainable conducting polymers has gained immense interest for next-generation electronic and energy applications. In this study, polypyrrole (Ppy)—a versatile conjugated polymer—was synthesized via two environmentally benign routes: conventional chemical oxidative polymerization and green ultrasonication-assisted chemical oxidative polymerization, using ammonium persulfate as the oxidant at different oxidant-to-monomer (O/M) ratios. The work focuses on evaluating how synthesis pathways influence the structural, optical, and electrical characteristics of Ppy while emphasizing sustainability, cost-effectiveness, and energy efficiency.

The X-ray diffraction patterns confirmed the amorphous nature of the synthesized Ppy with an average chain separation of approximately 4.5 Å, indicating close molecular packing favourable for charge transport. FTIR spectra exhibited characteristic Ppy vibrational bands such as C=C, C–N, and N–H stretching modes, validating successful polymerization. Notably, ultrasonicated samples displayed sharper peaks and minor wavenumber shifts, signifying improved molecular ordering and dopant interaction due to the ultrasonic environment. UV–Vis spectra revealed distinct π–π* and polaron/bipolarons transitions. The ultrasonication method yielded a higher absorbance intensity and extended tail absorption beyond 600 nm, indicating improved conjugation, delocalization, and charge mobility.

The optical band gap (Eg) increased with the O/M ratio up to 0.5 and then decreased, highlighting an optimal oxidation level before over-oxidation. SEM analysis revealed that morphology was strongly influenced by the O/M ratio; ultrasonicated samples exhibited uniform, granular, and interconnected surfaces with enhanced particle connectivity, whereas chemically synthesized Ppy appeared less compact. Electrical conductivity measurements indicated that ultrasonication improved homogeneity and charge transport compared to the conventional route.

The findings confirm that ultrasonication-assisted polymerization is not only a green and sustainable synthesis method but also an energy-efficient and economically viable approach for producing high-quality Ppy films with superior structural and electrical properties. This method minimizes reagent consumption, reduces processing time, and enhances material performance, making it an excellent candidate for scalable, eco-friendly production of Ppy for applications in sensors, energy storage devices, and flexible electronics.

Keywords: Polypyrrole, Ultrasonication, Conductivity, bandgap

Biomass derived activated carbon from Apricot leaves as a potential electrode for supercapacitor

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The continuous depletion of natural resources promotes us to move towards renewable sources of energy and supercapacitor is emerging as great energy storage devices [1,2]. In the present work, we have prepared activated carbon from Prunus armeniaca (apricot leaves) by physical and chemical activation using $ZnCl_2$ as an activating agent. The area, pore structure characteristics and surface functionality of the activated carbons were evaluated using various characterization techniques namely BET, XRD, FESEM, Raman and XPS to investigate the influence on electrochemical performance. The BET surface area was found to be 891.63 $m^2 g^{-1}$. The performance of the activated carbon-based electrodes in electric double layer capacitor (EDLC) was studied via Electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV) and galvanostatic charge–discharge (GCD) measurements using a gel polymer electrolyte-cum-separator, comprising of PVdF-HFP/$NaClO_4$/EC-PC. The optimised potential window of the device was 2.7 V and the specific capacitance (C_{sp}) was found to be 166 F g^{-1}. The energy density and power density were also calculated from GCD measurements and found to be 42 Wh kg^{-1} and 0.66 kW kg^{-1}, respectively. It also shows good cyclic stability up to 10,000 cycles with coulombic efficiency of ~100%. Hence, the activated carbon.

References:

1. Yadav, N., Singh, M.K., Yadav, N. and Hashmi, S.A., 2018.
2.Jain, A., Ghosh, M., Krajewski, M., Kurungot, S. and Michalska, M., 2021.

(Abstract Domain: Materials and coatings for batteries, super-capacitors, and fuel cells)

Strategies for Enhancing Zinc-Iron Hybrid Redox Flow Battery

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ABSTRACT

Redox flow Batteries (RFBs) have attracted much attention due to their modular scalability, intrinsic safety, decoupling of energy and power, good cycle life, and large-scale energy storage range (> MWh). In recent times, Zn-based RFBs, specifically Zn-Fe, have been widely investigated for their high capacity and cell voltage, as well as for the earth-abundant Zn & Fe and low cost. However, the zinc dendrite formation, dead Zn-ion formation, hydrolysis of the Fe^{3+} reaction, hydrogen evolution, and unbalanced reaction kinetics, etc., are constraining further development of these Zn-Fe RFBs. To improve cell performance, the electrode and electrolytes have been modified, along with a suitable flow design. As a result, the Zn-Fe flow cell performance has been enhanced. However, it still needs further investigation to meet the commercial domain. Therefore, in this work, we aim to modify the electrode and optimize the electrolyte performance to improve the flow cell performance. The schematic representation of the Zn-Fe system (Figure 1) is shown below. The metal oxide attached to the graphite electrode shows significantly improved electrode kinetics, thereby improving the rate current and cycle life of the RFB cell.

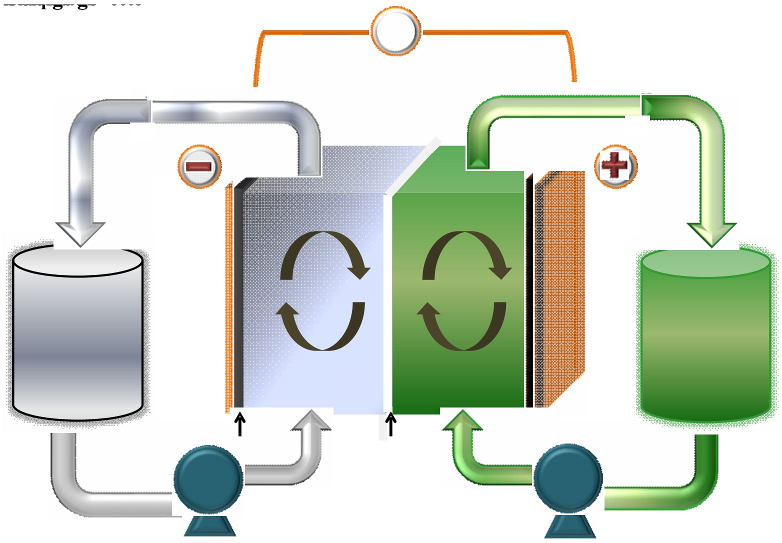

Figure 1: Schematic representation of the Zn-Fe redox flow cell

Keywords: Redox Flow cell; High energy; Electrolyte; Electrode Modification.

Optimal Selection of Surface Functionalized SnO_2 Dispersed Lubricants using Bootstrap based Statistical Methods for Tribology in Energy Applications

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ABSTRACT

Friction (~ 20%) and wear (~ 3%) are the major contributors to global energy consumption (~ 23%). Optimization of friction, wear and lubrication occupies a pivotal role in minimizing energy deficits, and economic detriments contributing to enhanced machinery durability. SnO_2 based novel lubricant additives are potential candidates for sustainable lubrication. These materials have shown substantial improvement in the tribological behavior of conventional lubricants due to its environmental friendliness, non-toxicity and thermo-chemical stability. In the current work, two materials, SnO_2 rods and Fe-doped SnO_2 rods are synthesized, and these additives are dispersed in transformer oil at different weight percentages using oleic acid and oleyl amine as surfactants. Anti-friction and anti-wear behavior are notably improved at a low additive weight percentage of 0.025. Coefficient of friction (~ 40%), wear scar diameter (~ 43 %), surface roughness (~77 %), and wear depth (~ 89%) substantially decreased attributing to a boost in lubrication performance. This is supported by tribo-sintered patchy film with high hardness and high dispersion stability of the developed lubricants. Fe-doped SnO_2 rods showed better performance in comparison to SnO_2. Recently, developed bootstrap methods based on ANOVA models have been applied on the friction and wear data set generated from our experiments. These novel test procedures have been used to detect trends in effect values. Optimal materials and concentrations were selected based on the outcomes of the ordering obtained from the advanced statistical simulations. Quite robust statistical computations show highly consistent results with the experimental values. This study opens doors for design and development of optimized sustainable lubricants for reducing energy losses in various domains related to efficient energy applications.

Ambient-Tolerant Mechanochemical Powder Strategy Combined with Alkali-Metal-Integrated HTLs for Stable, Solvent-Minimal Perovskite Devices

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ABSTRACT

Perovskite photovoltaics continue to face reproducibility and stability bottlenecks as long as liquid-phase dopants and trace additives remain indispensable for both the perovskite and hole-transport layers. We replace this paradigm with a fully solid-state route that embeds MACl into mechanochemically synthesized perovskite powder, steering crystallization and suppressing compositional drift from the outset. The resulting powder retains structural integrity even after prolonged exposure to 85% RH and 100 °C, dissolves cleanly into precursor inks, and reliably evolves into α-phase films without reliance on solution-side precision. In parallel, alkali-metal-integrated carbazole-based Hole Transport Layers (HTLs) provide dipole alignment and moisture-tolerant hole extraction without Li-TFSI or t-BP, eliminating the most instability-prone steps in conventional HTL doping. Under solvent-minimal fabrication with ultra-low anti-solvent loading (<10 μL), devices consistently exceed 20% PCE, and the fully powder-based configuration reaches 24.33% while retaining 96.8% of its initial efficiency after 800 h of continuous operation (AM1.5G, 25 °C, dry air). By transposing both the absorber formation and interfacial energetics into intrinsically defined powders, this approach renders perovskite fabrication markedly less sensitive to ambient humidity, operator handling, and dopant chemistry pushing the technology closer to reproducible, industrial-scale deployment.

Keywords: Perovskite powder; Mechanochemical synthesis; Alkali-metal HTL; Dopant-free

Pulsed laser deposition of bulk-like (111)- and (001)- NiO thin films

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Abstract

Nickel oxide (NiO) is recognized as a wide-bandgap transparent insulator, exhibiting a bandgap of 3.6 eV to 4.0 eV. It is an antiferromagnetic material with a Néel temperature of 523 K, substantially above room temperature. NiO crystallizes in a NaCl-type face-centered cubic (FCC) structure with a lattice parameter of 0.417 nm. The antiferromagnetic order in NiO is due to the antiferromagnetic alignment of ferromagnetic (111)-planes along the [111] crystallographic direction. Below the Néel temperature, magnetic ordering induces a rhombohedral distortion.

This study presents the growth of (111)- and (001)-oriented NiO thin films on (0001)-sapphire and (001)-MgO substrates, respectively, using pulsed laser deposition (PLD). DC magnetic susceptibility measurements of the films (~120 nm thick) confirm that they maintain antiferromagnetic ordering at room temperature. Additionally, this finding is supported by the observation of two-magnon Raman scattering, which persists in films with thicknesses down to at least 30 nm at room temperature. The relative intensity of this two-magnon mode compared to a neighboring phonon mode further highlights the bulk-like antiferromagnetic state in the thin films.

The optical properties of the NiO films were investigated using UV-vis spectroscopy, spectroscopic ellipsometry, and photoluminescence (PL) spectroscopy. The bandgap of the films was determined to be 3.6 eV, consistent with reported values for bulk NiO. Photoluminescence measurements on NiO(111)/Al_2O_3(0001) films, excited at 345 nm, revealed two emission bands centred at 385 nm and 405 nm, respectively. The linewidth of the 405 nm emission band displayed temperature-dependent broadening, indicative of exciton-magnon coupling. Furthermore, the UV-vis spectra, along with the films' refractive indices and extinction coefficients, suggest that their optical properties are bulk-like, making them suitable for optoelectronic applications.

Overall, this work demonstrates the successful deposition of (111)- and (001)-oriented NiO thin films via PLD, exhibiting magnetic and optical properties resembling those of bulk NiO. These findings underscore the potential of NiO thin films for exploring fundamental magnetic interactions and developing optoelectronic applications.

High-Performance VOC Detection via Ru and Rh-Tailored $Ti_3C_2O_2$ MXene: A DFT and NEGF-Based Insight into Breast Cancer Sensing

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Abstract

Early detection of breast cancer, the most prevalent malignancy in women, is constrained by invasive and insensitive conventional diagnostics, prominence the crucial need for non-invasive methods. Exhaled breath analysis, leveraging volatile organic compounds (VOCs) as molecular fingerprints, has developed as a promising approach. Here, density functional theory (DFT) joined with non-equilibrium green function (NEGF) method is employed to explore Ru and Rh adatom tailored $Ti_3C_2O_2$ MXene as innovative nano-biosensors. Both tailored surfaces demonstrate strong thermodynamic stability, with formation energies of –8.519 eV and –8.505 eV. AIMD simulations at 300 K confirm the structural stability of Ru and Rh- tailored $Ti_3C_2O_2$, with adsorption configurations conserved under thermal fluctuations. Ru and Rh-Tailored $Ti_3C_2O_2$ exhibits significantly stronger adsorption of BC associated VOCs 3,3-dimethylpentane,2-methylpentane and heptanal induces pronounced charge transfer, orbital hybridization and magnetic modulation. Remarkably, 2-methyloctane on Ru tailored $Ti_3C_2O_2$ and heptanal on Rh tailored $Ti_3C_2O_2$ exhibits the highest magnetic moment induced of 1.74 and 1.73 μ_B, with consistent sensing response of 89% and 78%, respectively. Transport calculation further discloses distinct modulation of transmission spectra and low-bias I-V curve characteristics with optimal sensitivity attained at bias voltages of 0.4 V and 0.1 V, respectively. By analysing adsorption strength, charge transfer, electron difference density (EDD), electron localization function (ELF), recovery time and transmission spectra, these insights establish Ru and Rh tailored $Ti_3C_2O_2$ as a robust platform for breath based and early-stage breast cancer detection in women.

Keywords: Breast Cancer, volatile organic compounds, density functional theory, Rhodium, Ruthenium, ab into molecular dynamics, non-equilibrium green function,

Abstract Domain: Thin films/ Nano-materials growth, Novel techniques and concepts

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 $CsPbBr_3$ 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 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 presents 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.

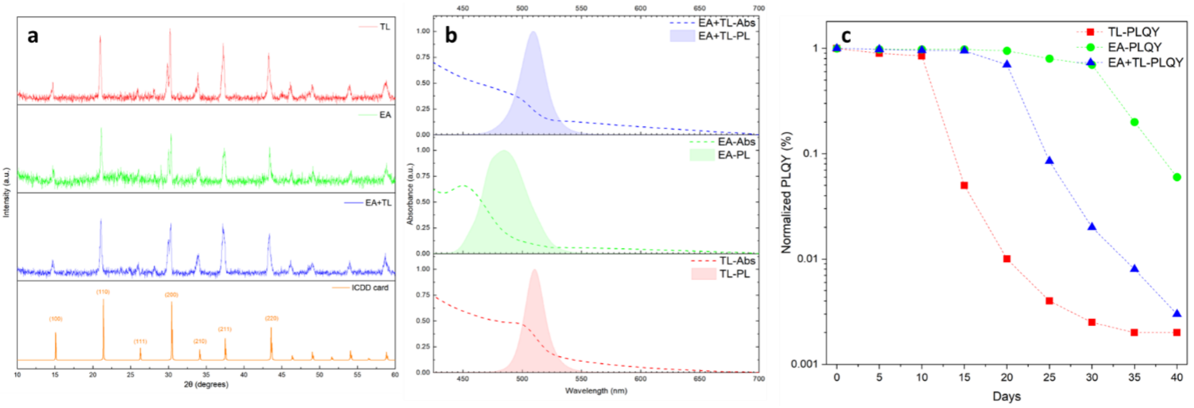

Figure 1: (a) X-Ray diffraction pattern of the synthesized PNCs under different polar environments show a consistent cubic structure. (b) UV-visible absorption spectra and respective PL curves excited at 400 nm at 300 K. (c) Stability studies portraying rate of decrease in the PL quantum yield of the PNC under different environments.

Bio-waste derived activated carbon for energy storage applications

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The depletion of natural resources demands exploration of alternative energy sources that are sustainable, eco-friendly, and also non-toxic. To meet the ever-growing energy needs, scientists have developed various energy storage devices such as batteries and supercapacitors [1]. Particularly, activated carbon electrodes-based supercapacitors have been studied vigorously and have been proved to be viable devices as commercial power sources. The bio-waste derived activated carbons are efficient electrode materials for supercapacitor application [2]. In the present work, the activated carbon has been prepared from Platanus Orientalis leaves and used as electrode materials. The chemical and physical activation have been performed by $ZnCl_2$ followed by CO_2 flow through carbon material which resulted in the substantial enhancement in the specific surface area. The surface area of activated carbon, pore size distribution, structural identification was analysed using various characterization techniques, including BET analysis, XRD, and Raman spectroscopy. The surface area of the activated carbon has been achieved up to ~1876 $m^2 g^{-1}$. The performance of activated carbon-based supercapacitor fabricated with a gel polymer electrolyte (PVdF-HFP/$NaClO_4$/EC-PC) has been tested via electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV) and galvanostatic charge discharge (GCD) measurements. The potential window of the device has been optimized at ~2.5 V. The specific capacitance has been found to be ~199 Fg^{-1} which corresponds to an energy density of ~43 Wh kg^{-1}. The device has been tested for long term cycling via galvanostatic charge discharge measurements and was found to be an excellent device for energy storage.

Key words: supercapacitor, electrochemical impedance spectroscopy, energy storage.

References:

1. Hor, A.A. and Hashmi, S.A., 2020. Optimization of hierarchical porous carbon derived from a biomass pollen-cone as high-performance electrodes for supercapacitors. Electrochimica acta, 356, p.136826.

2. Taslim, R., Apriwandi, A. and Taer, E., 2022. Novel moringa oleifera leaves 3D porous carbon-based electrode material as a high-performance EDLC supercapacitor. ACS omega, 7(41), pp.36489-36502.

Effect of Applied Electric Field During Spray Deposition on the Properties of ZnO Thin Films

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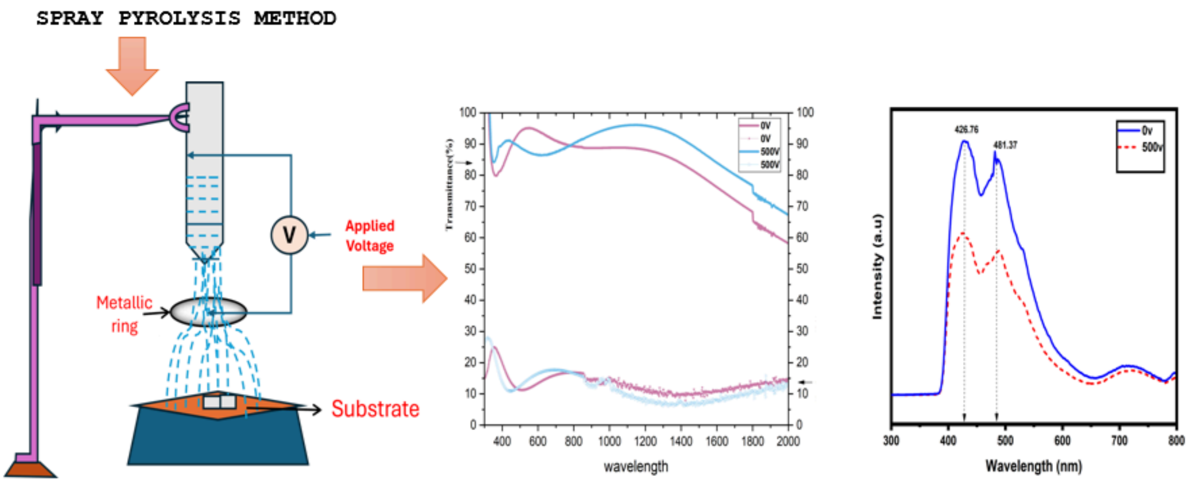
The present study investigated the influence of an externally applied electric field on the structural and optical properties of zinc oxide (ZnO) thin films deposited by the spray pyrolysis method. An external electric field ranging from 0 V to 500 V was applied between the spray nozzle and a metallic ring placed near the nozzle tip. UV-vis spectroscopy of the ZnO thin films demonstrate high transmittance around 80% to 90% in the visible to near-infrared region, for the sample deposited at lower voltage. The reflectance spectra show low reflectance values below 20% for the samples across the visible region.PL spectroscopy revealed that both samples show emission peaks in the ultraviolet region, most notably between 400–500 nm, which is characteristic of the near-band-edge (NBE) emission from ZnO. The film deposited at 0V shows the highest PL intensity. With the help of Spectroscopy Ellipsometry, we get the information about the refractive index, extinction coefficient, roughness and film thickness. The results showed that applying an electric field increase the thickness of the film. At 0V films roughness and thickness was measured around 7.31nm and 79.38nm respectively whereas for 500V roughness and thickness was measured as 21.25nm and 143.19nm respectively. The results showed that applying an electric field increase the thickness and roughness of the film. The observed variation suggest that the application promotes improved nucleation dynamics and film quality. These findings highlight the crucial role of electric field assisted spray pyrolysis in tailoring the structural and optical properties of ZnO thin film for advanced optoelectronic applications.

Keywords: Zinc oxide (ZnO), Spray pyrolysis, Electric field, thin films, optoelectronic.



Machine Learning-Based Colorimetric Detection of Mercury via Nanozyme Activity of MOF Nanocomposite

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Mercury is one of the most hazardous environmental pollutants due to its extreme toxicity, persistence, and bioaccumulative nature, posing serious risks to human health, particularly in the neurological, renal, and developmental systems. Its presence in industrial wastewater, even at trace levels, necessitates rapid, selective, and cost-effective monitoring technologies. In this study, a hybrid nanocomposite of two-dimensional MXene and ZIF-L, functionalized with chitosan, was engineered to exhibit enhanced peroxidase-like nanozyme activity for rapid and selective colorimetric detection of mercury ions (Hg^{2+}). The synergistic interaction between MXene's high electrical conductivity, ZIF-L's high surface area, and chitosan's surface functional groups facilitated efficient charge transfer and catalytic sites, leading to an intensified oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB). The developed sensing platform exhibited a distinct blue-to-colourless transition proportional to mercury concentration, enabling both visual and spectrophotometric quantification within minutes. For reliable and rapid on-site detection, machine learning algorithms were employed to correlate absorbance features with Hg^{2+} concentrations, achieving high prediction accuracy. The k-NN model demonstrated superior predictive accuracy, recording Mean Absolute Error (MAE) of 0.1200, Root Mean Square Error (RMSE) of 0.1350, and the Coefficient of Determination (R^2) score of 0.9693. Hence, the developed ML-enhanced colorimetric platform integrated with MOF nanozyme activity offers a cost-effective, portable solution for mercury detection, addressing urgent global needs for real-time environmental monitoring and public health protection.

References:

- Zehra, F., Mittal, H., & Khanuja, M. (2025). Exploration of the photocatalytic activity of various zeolitic imidazolate frameworks (ZIF-8, ZIF-9, ZIF-67, and Co-ZIF-L) on organic dye crystal violet. Journal of Materials Science: Materials in Electronics, 36(27), 1778.
- Zehra, F., Fatima, T., & Khanuja, M. (2025). Colorimetric Sensing of Mercury with Machine Learning Based on Nanozyme Activity of Chitosan Functionalized MXene/ZIF‐L Nanocomposite. Advanced Materials Technologies, e00519.

(Abstract Domain: 5. Perovskite, Silicon and CdTe thin films solar cells)

Fluorinated Two-Dimensional Interfacial Layers for Grain-Boundary Passivation and Enhanced Stability in Perovskite Photovoltaic Devices

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Perovskite solar cells (PSCs) hold immense promise for next-generation photovoltaics, thanks to their high-power conversion efficiencies, tunable optoelectronic properties, and compatibility with perovskite/silicon tandem architectures. However, their commercial potential remains constrained by long-term instability under ambient and operational conditions. Two-dimensional (2D) perovskite capping/passivation layers have emerged as a compelling solution, offering environmental resilience and interfacial passivation. This work investigates the implementation of 4-fluoro-phenylethylammonium (FPEA)-based 2D capping layers atop three-dimensional (3D) perovskite absorbers. Two fabrication strategies were explored: direct deposition and solvent-washed formation at multiple spacer cation concentrations. The latter approach enabled superior film uniformity and orientation control, as confirmed by grazing-incidence wide-angle X-ray scattering (GIWAXS). Solvent-washed layers exhibited a horizontal alignment, which was optimal for moisture resistance and minimised perovskite ion transport barriers across interfaces. The fluorine substitution-induced dipole field at the interface reduces recombination and aids charge separation, confirmed via recombination dynamics using time-resolved photoluminescence and diode quality factor extraction using Suns-VOC measurement. Conductive atomic force microscopy (c-AFM) highlighted enhanced conductivity pathways at grain boundaries, where FPEA cations passivate the trap sites and recombination centres, and suppress the non-radiative losses. These effects contributed to significant gains in the perovskite solar cell's open-circuit voltage and fill factor. Critical optoelectronic parameters, carrier mobility, trap density, and energy levels were experimentally extracted and integrated into charge carrier drift-diffusion simulations in a solar cell for tandem solar cell optimisations. These simulations accurately simulated internal fields, recombination dynamics, and charge transport. In 2-terminal PIN perovskite/silicon tandem configurations, coupling optical modelling with electrical simulations mitigated parasitic absorption losses and theoretical efficiencies exceeding 39% and open-circuit voltages above 2 V were projected.

Keywords: PSCs; Passivation and interfacial engineering; Conductive atomic force microscopy.

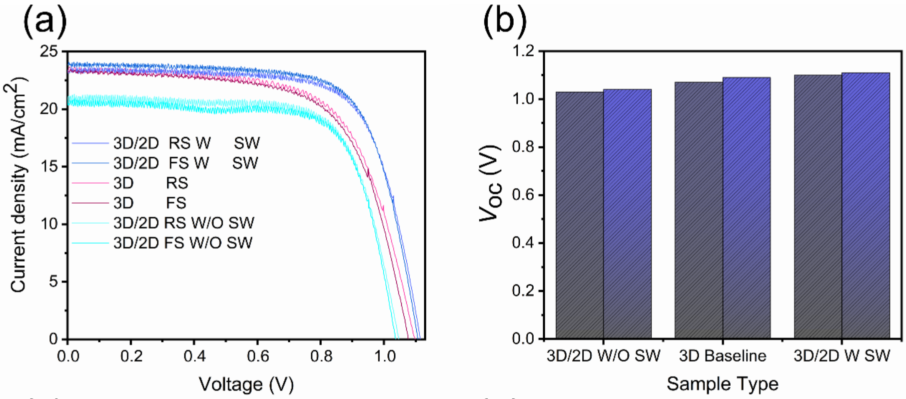

Fig. (a) *JV* response of PSCs showing SW 3D/2D perovskite exhibits the best performance compared to the pristine 3D perovskite and the W/O SW 3D/2D perovskite, (b) Improvement in V_{OC} for the solvent-washed 3D/2D perovskite compared to the other samples.

Tailoring Structural, Morphological, Magnetic, and Optical Properties of Mn and Fe-Doped TiO_2 Nanoparticles for Next-Generation Functional Materials

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Abstract

We report Pristine TiO_2 (Titanium dioxide) and synthesis of its doped variants with Mn and Fe i.e. $Ti_{0.98}Mn_{0.02}$ (manganese doped Titanium dioxide) and $Ti_{0.98}Fe_{0.02}$ (iron doped Titanium dioxide) by solid-state reaction method in this study. The experiments were sintered at various temperatures ranging from 500 °C to 1000 °C in air and argon ambient, respectively. Without the production of any impurity phases, X-ray diffraction investigations show the formation of the anatase phase of TiO_2 fitting to the 141/AMD space set in both samples. The crystal structure does not change when 5 at. % Mn content is added, revealing the precise replacement of Mn & Fe atoms at their locations. The variation in ionic radii is responsible for some of the observed changes in lattice characteristics and crystallite dimension in Mn & Fe-doped structures. The size of the crystallites as determined by X-ray diffraction analysis is comparable with the grain size as determined by scanning electron micrographs. The integration of Mn and Fe content in the TiO_2 structure has been verified by energy-dispersive X-ray analysis. Ferromagnetic behavior found in Mn and Fe-doped TiO_2 composition is consistent with the significant contribution of the Mn d-shell. The field of electric polarization (P–E) Glass-ceramic composites have a very low energy loss, according to hysteresis loops. The findings demonstrate that the sintering temperature and atmosphere had a significant impact on the magnetic properties.

Keywords: X-ray diffraction, TM-doped TiO_2, Diluted magnetic semiconductors, Magnetic properties.

Materials and coatings for batteries, super-capacitors, and fuel cells

Synthesis and characterization of ZnO/V_2O_5 nanocomposite through the ball milling process

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ABSTRACT

This study describes the simple procedure for synthesizing ZnO/V_2O_5 nanocomposite through planetary ball milling, which is a cost-effective method. X-ray diffraction (XRD) was used to examine the structural characteristics of the synthesized ZnO/V_2O_5 nanocomposite. Debye-Scherrer's formula was used to calculate the average crystallite size (D) of the synthesized ZnO/V_2O_5 nanocomposite, and the average crystallite size is 25.6 nm. The bandgap energy was calculated from Tauc's plots. The band gap energy was investigated using the ultraviolet visible spectra, scanning electron microscopy (SEM) was performed to examine the morphology of the nanocomposite material, and the existence of different functional groups and metal oxide (MO) linkages in the composite was investigated by FT-IR spectrum. The synthesized nanocomposite has expected promising supercapacitor performance and stability due to combination of V_2O_5 and ZnO. Vanadium pentoxide (V_2O_5) is considered one of the promising electroactive materials for supercapacitors due to its various oxidation states, low cost, low toxicity, broad voltage range, as well as its high capacitance and energy density. The electrochemical properties of V_2O_5-based electrodes are hindered by their poor conductivity and low cyclic stability, which also limits their applicability in supercapacitors. As a result, several modifications to structural, morphological, and electronic properties, along with the introduction of doping and the formation of nanocomposites, can improve the conductivity and stability of V_2O_5-based electrodes. Combining ZnO with V_2O_5 can improve tunable electronic band gaps, high surface area, and provide the capability to create stable structures for energy storage applications.

Keywords: ZnO, V_2O_5, nanocomposite, ball milling.

(Photocatalysis)

Hydrothermally assisted MXene based 2D nanocomposite for adsorption and photocatalytic immobilisation of Chromium (VI)

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ABSTRACT

This study utilises facile multistep approach for synthesis of Transition metal carbide/Transition metal oxide/conducting polymer-based nanocomposite, MVP comprising of MXene, V_2O_5 and Polypyrrole for the enhanced removal of heavy metal ion contaminant-Chromium (VI).The synthesised composite was well characterised using X-Ray Diffraction and Field Emission Scanning Electron Microscopy and High- Resolution Transmission Electron Spectroscopy which confirm the successful synthesis and increase in interlayer spacing of 2D MXene sheets in nanocomposite MVP. Polypyrrole spheres and Ball-milled V2O5 nanoflakes boosts the catalytic performance of MXene by acting as electron generating agents. Detailed photocatalytic degradation studies were done on removal of Chromium (VI) using MVP by varying the concentration of pollutant, dosage of photocatalyst, variation in pH etc. Compared to MXene, the higher performance of nanocomposite, MVP is ascribed to the optimised surface charge, reduced charge transfer resistance (R_{ct}), increased carrier concentration, and enhanced specific surface area. Electron paramagnetic resonance (EPR) confirmed the findings of scavenger study and it was concluded that superoxide radicals ($O_2^{-\cdot}$) are the primary species in the removal of chromium. The experimental determination of values of lande g-factor was also done using EPR plots and found to be equal to 2.03 ($O_2^{-\cdot}$) and ($OH^{\cdot}$) radicals, respectively which accounts to formation of single electron species formed at the interface of photocatalyst MVP and aqueous environment. It confirmed the role of the free radical species involved in redox reactions during removal of Chromium (VI) using MVP. Further, reusability experiment was done on the synthesised nanocomposite which validated the stability of the synthesised sample and offers significant potential for industrial applications in wastewater treatment, promoting sustainable development.

Keywords: MXene, V_2O_5, Chromium (VI), Photocatalysis.

(Sensors)

Colorimetric Detection of Mercury Ions Using $MoSe_2$/ZIF-L Nanocomposite with Peroxidase-Like Nanozyme Activity

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ABSTRACT

One of the latest developments in the detection of hazardous heavy metal ions is the nanozyme-based approach. However, the use of noble-metal-free nanozymes to develop an economical and environmentally friendly technique remains largely unexplored. In this study, a novel colorimetric sensing platform for rapid and selective detection of mercury ions (Hg^{2+}) is developed using a molybdenum disulfide/zeolitic imidazolate framework-L ($MoSe_2$/ZIF-L) nanocomposite and 3,3′,5,5′-tetramethylbenzidine (TMB).The sensing mechanism relies on the superior peroxidase-like activity of the $MoSe_2$/ZIF-L nanocomposite, which catalyzes the oxidation of TMB to generate a distinct blue-colored product. The presence of Hg^{2+} ions inhibits this catalytic reaction, leading to suppression of the color intensity in a concentration-dependent manner.The synthesis of the $MoSe_2$/ZIF-L nanocomposite is achieved via a solution mixing method, ensuring uniform ZIF-L distribution within $MoSe_2$ nanosheets to maximize active surface area and catalytic sites. The influence of Hg^{2+} concentration on TMB oxidation is investigated, revealing that Hg^{2+} disrupts electron transfer kinetics and inhibits the catalytic activity of the nanozyme. The extent of catalytic suppression is directly proportional to the Hg^{2+} concentration, enabling quantitative analysis. Parameters such as TMB molarity, nanocomposite concentration, and pH are systematically optimized to achieve high sensitivity and a broad linear detection range. The pH of the medium, which affects surface charge and catalytic stability, is identified as a critical factor determining optimal sensing performance. UV-Vis spectrophotometry is used to evaluate the colorimetric response of the material and its interaction with Hg^{2+}. Overall, this study presents an efficient noble-metal-free nanozyme platform for reliable detection of mercury contamination and contributes to the advancement of sustainable nanomaterial-based sensing systems.

Overall, the optimized noble metal-free nanozyme platform offers a simple, cost-effective, and rapid approach for reliable on-site detection of toxic mercury ions in aqueous samples, with significant potential for applications in environmental and public health monitoring, thereby contributing to the advancement of sustainable nanomaterial-based sensing systems.

Keywords: $MoSe_2$/ZIF-L nanocomposite; Colorimetric sensing; Nanozyme; Mercury detection.

Reference:

1-Mittal H, Ivaturi A, Khanuja M. MoSe2-modified ZIF-8 novel nanocomposite for photocatalytic remediation of textile dye and antibiotic-contaminated wastewater. Environ Sci Pollut Res Int. 2023 Jan;30(2):4151-4165. doi: 10.1007/s11356-022-22487-x. Epub 2022 Aug 13. PMID: 35963971; PMCID: PMC9376053.

(Perovskite, Silicon and CdTe thin films solar cells)

Identification and detection of reversible alterations in perovskite solar Cells by Electrochemical Impedance Spectroscopy

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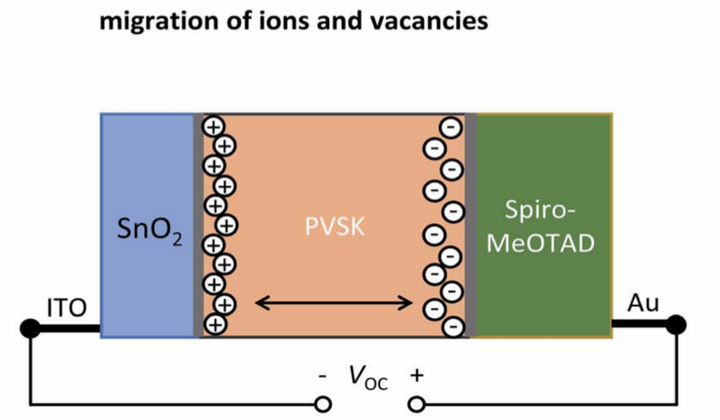
Abstract

The current understanding and application of electrochemical impedance spectroscopy (EIS) in analysing Perovskite solar cells (PSCs) remain limited, as most existing models lack the precision required to guide the design of more stable and efficient devices effectively. The intricate and slow dynamic processes within PSCs make accurate spectral interpretation challenging, and proper validation of the obtained impedance spectra is rarely performed. In this work, a comprehensive and reproducible EIS investigation was conducted at the open-circuit voltage (Voc) condition over an extended period exceeding 20 hours, producing a validated time series of 140 impedance spectra. The study reveals that the temporal variations in the impedance response are attributed to a transient reduction in the electronically active area of the device, as indicated by the inverse correlation between resistance and capacitance values. Notably, these changes are nearly completely reversible when the devices are kept in the dark for approximately one day. At the same time, the time constant associated with the high-frequency process remains stable throughout the entire measurement period. The tested full perovskite solar cells maintained operational stability for over 500 hours, confirming the structural robustness of the architecture. Moreover, the non-steady-state impedance behaviour reported here provides critical insight into the interpretation of previously published EIS data, highlighting the need for dynamic validation in spectral analysis. The findings demonstrate that the high-frequency semicircle observed in Nyquist plots can serve as a reliable diagnostic signature for tracking ionic migration and its consequences on device performance. These results offer a framework for quantifying ion migration at the device level and establishing new stability criteria and mitigation strategies for the long-term durability of Perovskite solar cells.

Keywords: Perovskite solar cells, Electrochemical impedance spectroscopy, Ionic migration, Device stability


migration of ions and vacancies
SnO2
PVSK
Spiro-MeOTAD
ITO
Au
-
V_OC
+

(Abstract Domain : Thin Films/Nano-materials growth, Novel techniques and concepts)

Tunable Insulator-to-Metal transition in epitaxial VO_2-based nanocomposite thin films *via* strain and defect engineering

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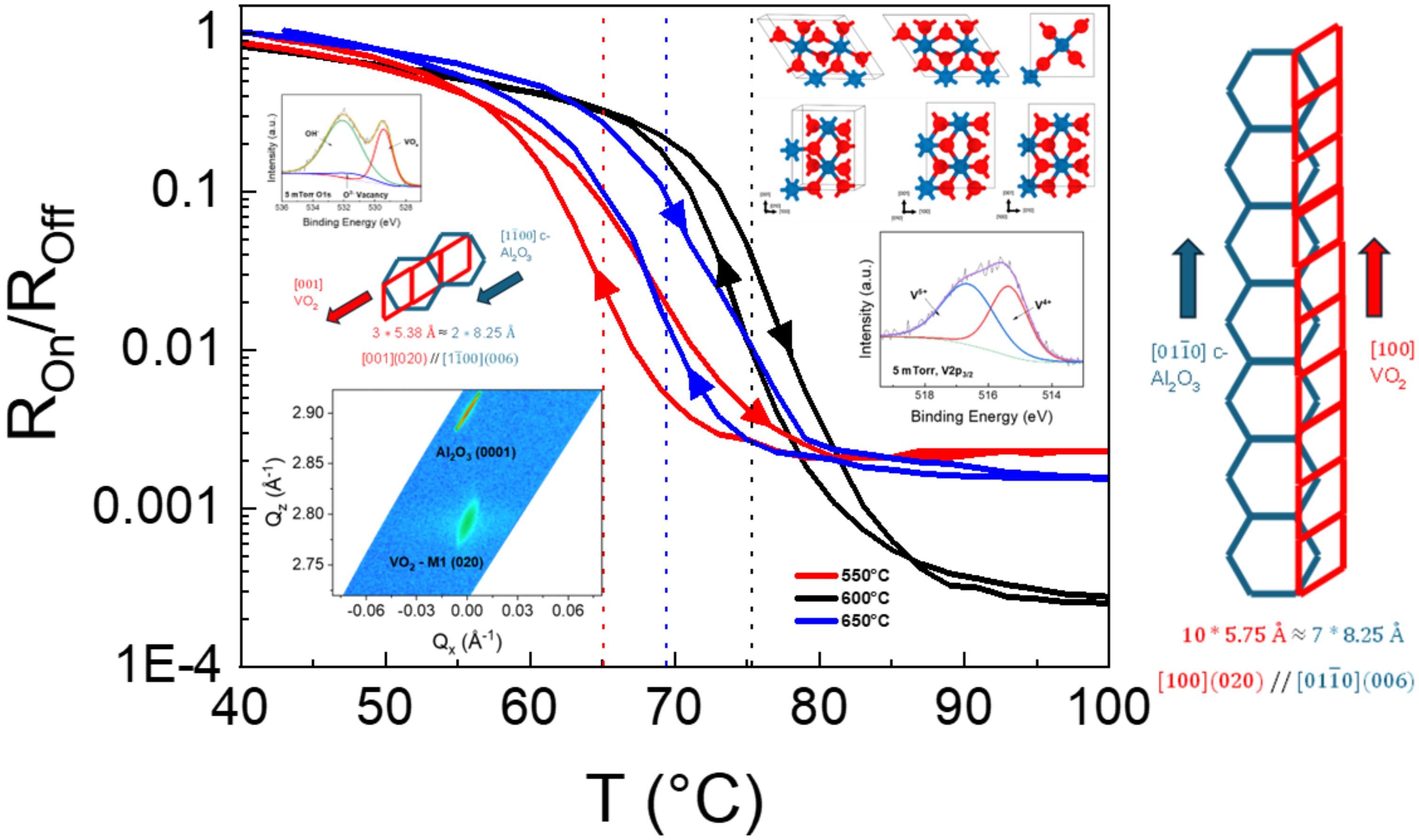
ABSTRACT

Vanadium Dioxide (VO_2), an Insulator-to-Metal (IMT) material has garnered significant research interest due to its potential applications in radiative coolers, optical memories, and optical switches. VO_2 exhibits MIT near 68°C, thereby requiring tuneable transition temperatures (T_c) in VO_2 thin films for practical device applications. In this work, we explore the role of strain and defect engineering in controlling the T_c in epitaxial VO_2 thin films deposited on c-cut sapphire using Pulsed Laser Deposition (PLD). The study involves varying growth parameters, mainly temperature and oxygen partial pressure. Strain engineering along the b-axis helped tune the transition temperature from 65°C to 82°C with the out-of-plane b-strain varying from -0.71% to -0.44%. Comprehensive structural and property analyses, including X-ray diffraction (XRD), Reciprocal Space Mapping (RSM), X-ray Dispersive Spectroscopy (XPS), Raman spectroscopy, and Resistivity-Temperature (R-T) measurements, were performed to correlate structural properties with T_c. Additionally, ab-initio DFT calculations were performed on Quantum Espresso using generalized gradient approximation of the revised Perdew-Burke-Ernzerhof (PBEsol) to provide theoretical validity to the experimentally obtained results. In addition, we also present a novel way to embed metallic nano-inclusions (W, Au and Ni) into the VO_2 film matrix to leverage greater tunability with regards to the transition temperature. All the VO_2 nanocomposite thin films showed reduced switching, enlarged hysteresis width and reduced T_c compared to pristine VO_2 epilayers grown on (0006) sapphire at similar deposition parameters. W-VO_2 thin films exhibited least switching ratio among all the combinations (0.028), along with least T_c (49.58°C). Our study provides critical insights on the interplay between strain and oxygen vacancies, as well as influence of metallic nano-inclusions, and their effects on the physical properties in VO_2 thin films with DFT calculations supporting the experimental findings.

Keywords: VO_2; PLD; Epitaxy; Nanocomposite


R_{On}/R_{Off}
1
0.1
0.01
0.001
1E-4
T (°C)
40
50
60
70
80
90
100
Intensity (a.u.)
OH⁻
VO_x
5 mTorr O1s
O^{2-} Vacancy
536
534
532
530
528
Binding Energy (eV)
[1$\bar{1}$00] c-Al_2O_3
[001] VO_2
3 * 5.38 Å ≈ 2 * 8.25 Å
[001](020) // [1$\bar{1}$00](006)
Q_z ($Å^{-1}$)
2.90
2.85
2.80
2.75
Al_2O_3 (0001)
VO_2 - M1 (020)
-0.06
-0.03
0.00
0.03
0.06
Q_x ($Å^{-1}$)
[001]
[010]
[100]
Intensity (a.u.)
V^{5+}
V^{4+}
5 m Torr, $V2p_{3/2}$
518
516
514
Binding Energy (eV)
550°C
600°C
650°C
[01$\bar{1}$0] c-Al_2O_3
[100] VO_2
10 * 5.75 Å ≈ 7 * 8.25 Å
[100](020) // [01$\bar{1}$0](006)

The significant role of CNT-ZnO core-shell nanostructures in the development of FDM-based 3D-printed triboelectric nanogenerators

Agneyarka Mohapatra

Cipet, BBSR

Abstract

A recent innovation in energy resource consumption has propelled the implementation of a green energy source in the form of triboelectric nanogenerators (TENGs). The combination of 3D printing with TENG has generated larger ripples in the field of energy storage and distributed power supply technology. The current research focuses on developing fused deposition modeling (FDM)-based TENG devices using feedstock materials such as polylactic acid (PLA) and acrylonitrile butadiene styrene as tribopositive and tribonegative layers, respectively. This study emphasizes the role of carbon nanotube-zinc oxide (ZnO) core-shell nanostructures reinforced into PLA by examining their impact on the final TENG output voltage. The presence of carbon nanotube -zinc oxide core shell (CNS) has enhanced the TENG output voltage (V_{oc}) from 1 V to 8 V. Furthermore, FDM 3D printing parameters such as filling rate (%), layer thickness, and printing patterns have engaging influence on $V_{oc.}$ Our research identifies PLA/CNS layers comprising 20% filling rate as having a layer thickness of 0.1 mm, and a donut pattern obtaining the highest V_{oc} (8.9 V). The reinforcement of CNS into PLA has also augmented its comprehensive properties including tensile strength and electrical conductivity. This research paves a path towards innovative fabrication strategies for TENG devices towards next generation portable electronic devices using FDM 3D printers.

(Abstract Domain: 3)

Design and Analysis of a Tri-Metal Double-Gate MOS Structure with Improved Electrical Control and Thermal Reliability

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ABSTRACT

In this work, two advanced three-dimensional MOS transistor structures were studied, one conventional single-material double-gate (SM-DG) structure and the other a proposed tri-metal double-gate (TM-DG) structure to compare their electrical and thermal behaviours. The SM-DG MOS structure was first analysed at 300 K to obtain its basic electrical parameters. Thereafter, a TM-DG MOS structure was designed using three different gate materials with optimised work functions to enhance gate controllability, suppress leakage, and improve device stability. The TM-DG MOS structure performs significantly better than the SM-DG MOS structure and achieve a lower leakage current (1.0×10^{-9} A) and subthreshold slope (99 mV/decade) against SM-DG structure. These 3D MOS structures were further analysed at different operating temperatures to evaluate its electrical and thermal performances at elevated temperature. The TM-DG structure maintains a stable operation with superior thermal reliability. As compared to SM-DG, the operating temperature in TM-DG structure is about 30 K less at $V_{DS} = 0.5$ V, VGS = 1.0 V. In addition to lower temperature the TM-DG transistor has also low output conductance of 2 µS, which enhances its intrinsic voltage gain, ensuring better power efficiency. Overall, the TM-DG MOS structure exhibits excellent electrical behaviour, effective thermal management, and strong stability, making it a highly promising candidate for future nanoscale, low-power, and high-performance integrated circuit applications.

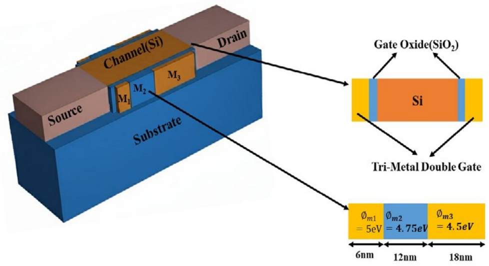

Fig. Sectional diagram of a Triple-material double-gate (TM-DG-MOSFET)

Keywords: Tri-Metal Double-Gate MOS transistor, Subthreshold Slope, Thermal Performance, MOSFET

High Output Piezo and Triboelectric generator based on MwCNT/Nd-doped ZnO/PVDF nanocomposite film for Energy Harvesting Application

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Abstract: -

The rising demand for renewable energy has driven intensive research on energy harvesting technologies. Among these, energy harvesting using Piezoelectric nanogenerators (PENGs) and Triboelectric nanogenerators (TENGs) stands out as a promising solution for powering electronic devices due to their high power and voltage generation capabilities. Neodymium-doped Zinc Oxide (NdZ) nanoparticles were synthesized via the co-precipitation method to enhance the energy output of the PENG and TENG devices. The structural characteristics of the synthesized NdZ powder were confirmed through X-ray diffraction (XRD), while their microstructural features were examined using Scanning Electron Microscopy (SEM). Flexible nanocomposite films were fabricated by incorporating varying weight percentages (0, 5, 10, 15, and 20 wt.%) of NdZ and MwCNTs into a PVDF matrix. These nanocomposite films were characterized using XRD, SEM, and Fourier-transform infrared spectroscopy (FTIR) to assess their crystallinity, morphological attributes, and β-phase content, respectively. After making the PENG devices from these composite films, we measured the voltage output, and the PENG of 10 wt.% produces the maximum output of 108 V from these 10 wt.% composite films we synthesized the triboelectric generator as one layer and the other layer of ITO-coated PET substrate film, and then measured the voltage output, which is about 340 V from this TENG. The practical utility of the PENG and TENG generator was demonstrated by powering light-emitting diodes (LEDs) and small-scale electronic devices. Overall, this work highlights the efficacy of MwCNT and NdZ nanoparticles as functional nanofillers in PVDF-based nanocomposites for the fabrication of high-performance PENG and TENG devices, thereby offering a promising route toward sustainable and portable energy solutions.

Keywords: Nd-doped ZnO; Piezoelectric; Triboelectric; Nanocomposite;

Solar-Energy-Driven Photocatalytic Performance of Perovskite Nanomaterial Composites for Wastewater Treatment: Advancements in Photocatalyst Design

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ABSTRACT

This study details the successful synthesis and characterisation of binary $BaTiO_3/SnS_2$ and ternary $BaTiO_3/SnS_2/TiO_2$ composite nanomaterials using a wet chemical method, emphasising their improved photocatalytic efficacy for the decomposition of methyl orange (MO) under visible light exposure. The wet chemical synthesis method has been used to synthesize nanocomposites. The prepared composites were characterized by X-ray diffraction (XRD), ultraviolet-visible (UV-vis) spectroscopy, Fourier transformed infrared (FTIR) spectroscopy, PL spectroscopy and FESEM. Methyl orange decomposition under ultraviolet light was used to assess the photocatalytic effectiveness of binary $BaTiO_3/SnS_2$ and ternary $BaTiO_3/SnS_2/TiO_2$ composites, which demonstrated enhanced activity than single-component materials. The photocatalytic degradation of binary and ternary composites is 61.5 % and 70%, respectively and following pseudo-first-order kinetics (Langmuir-Hinshelwood model) and linear $\ln(C/C\ )$ against time analysis was used to calculate their rate constant. Wet chemical synthesis makes it possible to customize the synthesis of efficient photocatalysts for solar-powered energy and environmental uses.

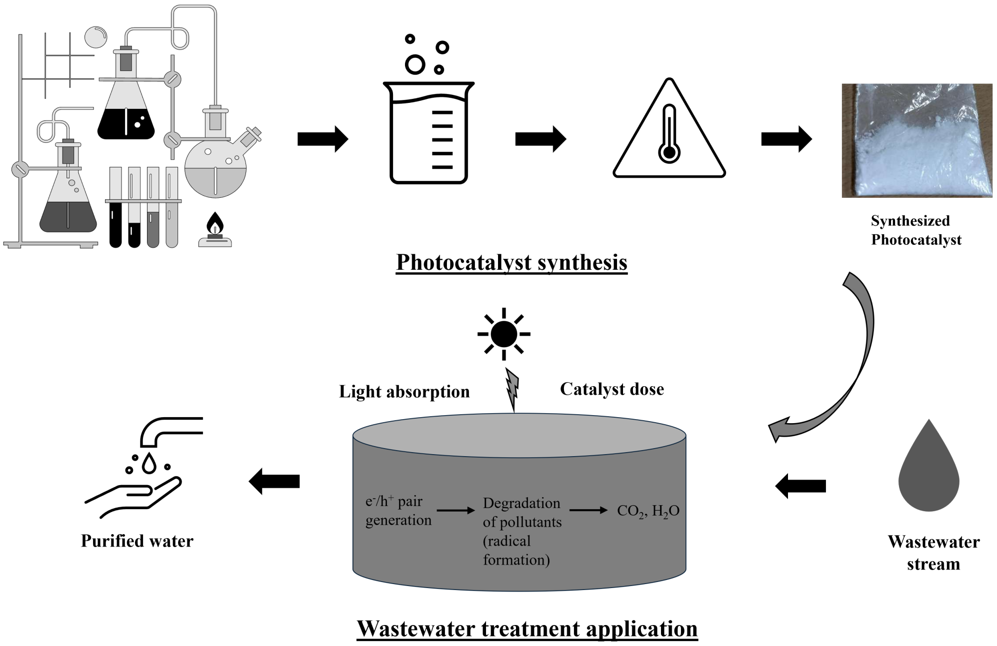

Fig. 1 Schematic of photocatalyst design and its application in wastewater treatment

Keywords: Methyl orange, Photocatalysts, Visible light, Degradation kinetics.

Abstract Domain: Computational Modelling And Simulations

A Comprehensive TCAD Investigation of Single-Fin and Dual-Fin 3D Bulk FinFETs Across Multiple High-K Dielectric materials

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ABSTRACT

This study presents a comprehensive simulation-based investigation of Single-Fin (Conventional) and Dual-Fin FinFET architectures using the Silvaco TCAD platform to evaluate their electrical characteristics with various high-k gate dielectric materials. The analysis emphasizes the influence of different dielectrics-such as SiO_2, Si_3N_4, Al_2O_3, HfO_2, ZrO_2, La_2O_3, and TiO_2 on key device parameters including drain current (I_D), threshold voltage (Vth), subthreshold swing (SS), Ion/Ioff ratio, and Drain-Induced Barrier Lowering (DIBL). The results demonstrate that dielectric materials with higher permittivity effectively enhance gate control, minimize leakage current, and improve switching efficiency. Comparative analysis between Single-Fin and Dual-Fin structures reveals that the Dual-Fin FinFET provides superior electrostatic integrity, lower SCEs, and higher drive current, making it highly suitable for nanoscale low-power applications. The study also explores structural optimization through Fin geometry and dielectric selection to achieve improved performance, ensuring compatibility with next-generation VLSI and ultra-scaled CMOS technologies. Overall, the work establishes that the integration of high-k dielectrics in multi-fin FinFETs enables enhanced electrical efficiency, thereby paving the path for future generations of energy-efficient semiconductor devices.

Keywords: FinFET; Dual-Fin FinFET; High-k Dielectric; Short-Channel Effects (SCEs); Subthreshold Swing (SS); Threshold Voltage (Vth); Ion/Ioff Ratio; DIBL; Silvaco TCAD Simulation;

Perovskite , Silicon and CdTe thin films solar cells

Performance Optimization of different ETLs and HTLs with perovskite $Cs_{0.17}FA_{0.83}PbI_3$

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ABSTRACT

In recent years, perovskite solar cells (PSCs) have emerged as a promising photovoltaic technology because of their rapid efficiency advancements, low manufacturing expenses, and suitability for large-scale production. Despite these advantages, achieving stable and reliable device performance remains a key challenge limiting their commercialization. I have done simulation of various ETLs and HTLs in Setfos software with the mixed-cation perovskite absorber $Cs_{0.17}FA_{0.83}PbI_3$. Various combinations of electron transport layers (ETLs: TiO_2, PCBM, and ZnO) and hole transport layers (HTLs: Spiro-OMeTAD, P3HT, and NiO) were evaluated to identify the most efficient configuration. Among these, the ZnO/NiO structure exhibited the highest performance with a PCE of 18.25%, reflecting superior charge extraction and lower recombination losses. To improve the overall device performance, the thickness of the perovskite absorber layer and its bulk defect density were systematically adjusted under the optimized ZnO/NiO structure.

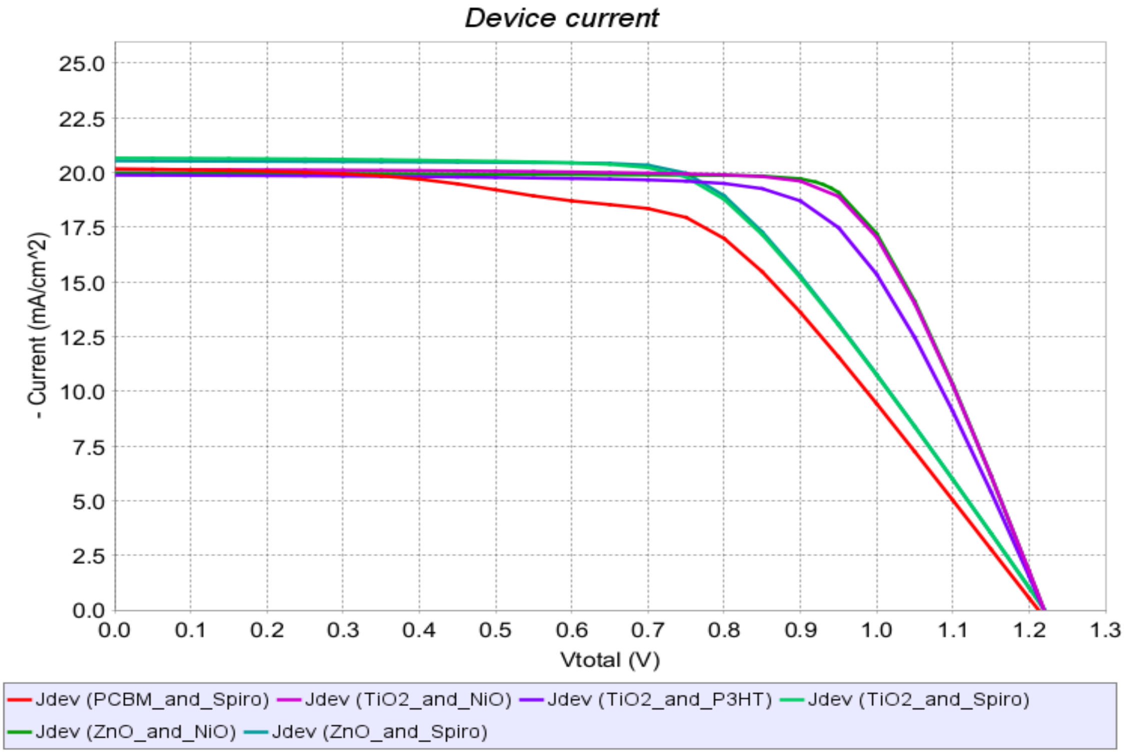

Figure: J-V of different combinations of ETLs and HTLs.

Synergistic $Ti_3C_2T_x$ MXene Quantum Dots/Nanosheets Hybrid: Elevating Supercapacitor Performance

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Abstract

Supercapacitors are promising energy storage devices, offering a unique combination of high energy and power densities. This study systematically investigates the synergistic effect of $Ti_3C_2T_x$ -MXene quantum dots (MQDs)/nanosheets hybrid on supercapacitor performance. $Ti_3C_2T_x$ MQDs are synthesized through a two-step process: first, $Ti_3C_2T_x$ MXene 2D sheets are prepared via acidic etching of precursor materials. Then, a combined hydrothermal (water-based) and solvothermal (ethanol-based) treatment at 150 °C reduces the sheet size, producing MQDs. The electrochemical performance of the MQDs/nanosheets hybrid is evaluated using a three-electrode configuration with 1M H_2SO_4 as the electrolyte. Galvanostatic charge-discharge (GCD) tests at current densities from 1-5 Ag^{-1} reveals significant improvement in specific capacitance under all tested conditions. Similarly, CV at scan rates of 10-200 mVs^{-1} demonstrates enhanced charge storage capability and superior rate performance, attributed to the synergistic effects of MQDs. EIS confirms reduced charge-transfer resistance and excellent capacitive behavior across a wide frequency range. The enhancement in the results are due to the high surface area, remarkable electrical conductivity, and abundant electrochemically active sites of MQDs. This study highlights the potential of $Ti_3C_2T_x$ MQDs/nanosheets hybrids as high-performance materials for next-generation supercapacitors, paving the way for their integration into advanced energy storage systems.

Keywords: MXene; $Ti_3C_2T_x$ QDs; Supercapacitors; Electrochemical properties; Energy Storage.

(Abstract Domain : Perovskite, Silicon and CdTe thin films solar cells)

Simulation of 2T & 4T Textured Silicon–Perovskite Tandem Solar Cell using SETFOS

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ABSTRACT

In this study, comprehensive optoelectronic simulations of two-terminal (2T) and four-terminal (4T) silicon–perovskite tandem solar cells are carried out using the commercial simulation tool SETFOS. The device structure employs $Cs_xFA_{1-x}PbI_3$ as the top perovskite absorber and a silicon heterojunction (SHJ) as the bottom sub-cell. The aim of the work is to understand the influence of optical texturization and perovskite thickness optimization on the current matching, light absorption, and overall power conversion efficiency (PCE) of tandem configurations.

The optical absorption spectra of both the perovskite and silicon layers were first analyzed individually and then incorporated into a tandem architecture to study photon distribution and parasitic losses. Two types of tandem cells—planar (bare) and textured—were designed and simulated. The texturization was modeled on both the front and rear interfaces of the silicon sub-cell to enhance light trapping and reduce reflection losses. The perovskite thickness was systematically varied in the range of 300–800 nm to achieve current matching between the sub-cells and to determine the optimum configuration for maximum efficiency.

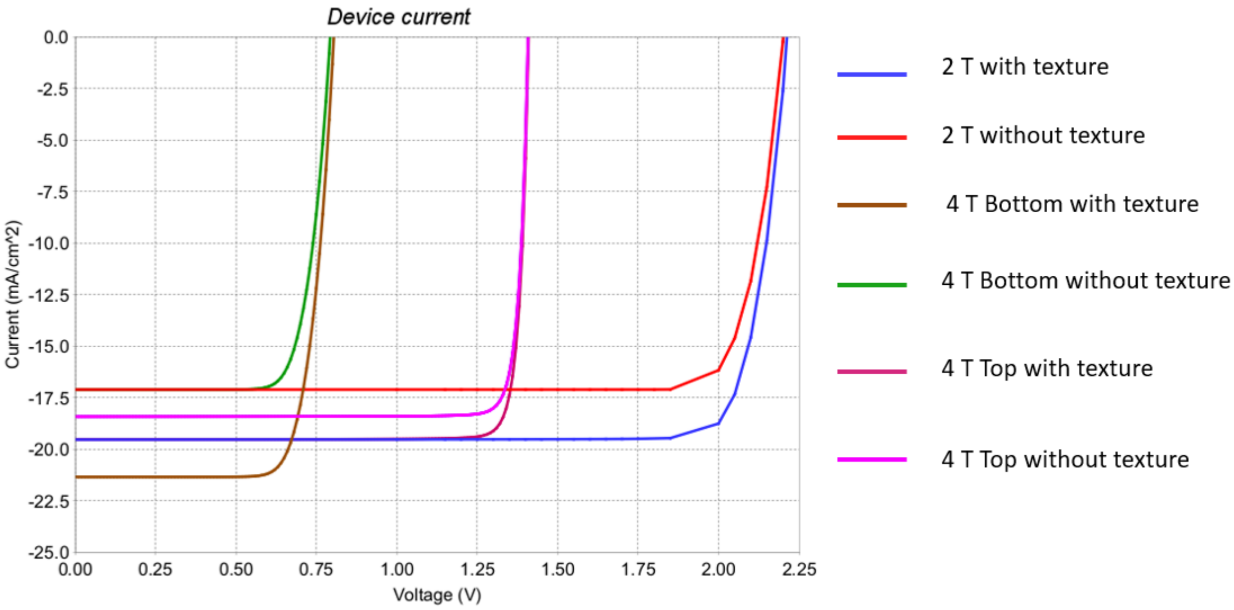
For the 2T tandem cell, a planar configuration achieved a power conversion efficiency (PCE) of 32.6%, while introducing texturing on both sides of the silicon layer enhanced the efficiency to 37.6% due to improved optical coupling and reduced transmission losses. Similarly, for the 4T tandem structure, the planar configuration exhibited an efficiency of 34.0%, and the dual-textured device achieved 36.6%. These results highlight the crucial role of interface texturization and optical optimization in achieving high-efficiency silicon–perovskite tandem devices.

Furthermore, the study investigates the effect of mobile ionic species within the perovskite absorber and their influence on transient device behavior, particularly under preconditioning and bias stress. The inclusion of mobile ions in the simulation framework revealed significant hysteresis effects and performance degradation trends, aligning well with experimental observations reported in literature. This demonstrates the potential of SETFOS as a reliable modeling tool for capturing both optical and electrical dynamics in hybrid perovskite systems.

The optimized 2T and 4T tandem solar cells simulated in this work show strong potential for future high-efficiency photovoltaic applications. The insights gained from this study will guide the design of next-generation tandem devices that combine cost-effectiveness, high stability, and scalability for commercial solar energy deployment.

Keywords: Perovskite–Silicon Tandem; Optoelectronic Simulation; Texturization; SETFOS

Figure 1. I-V Characteristics of 2T and 4T Devices with and without Texturisation



Understanding the Role of Densification on the Solid-State Electrolytes for Solid-State Batteries

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ABSTRACT

Solid-state sodium-ion batteries (SSSBs) have attracted growing attention as a potential alternative to lithium-ion batteries owing to the natural abundance, low cost, and environmental sustainability of sodium resources. The ionic conductivity of the solid electrolyte (SE) is a key parameter that determines the electrochemical performance of SSSBs, and it is highly influenced by the degree of densification achieved during pellet fabrication. This study aims to understand the role of densification on the ionic conductivity of a solid electrolyte by systematically varying the applied uniaxial pressure while keeping the sintering temperature constant. Electrolyte pellets were prepared under different pressures ranging from 50 MPa to 250 MPa, maintaining identical thermal conditions to isolate the effect of pressure on densification. The ionic conductivity of the samples was measured at room temperature using electrochemical impedance spectroscopy (EIS). From the Nyquist plots, bulk resistance values were extracted and used to calculate ionic conductivity ($\sigma = L / R_bA$), where L is the pellet thickness, A is the electrode area, and R_b represents the bulk resistance. The results showed a clear dependence of ionic conductivity on applied pressure. As the pressing pressure increased, the ionic conductivity initially increased, reaching a maximum at 150 MPa, and subsequently decreased beyond this point. The initial enhancement is attributed to improved particle contact, reduced porosity, and the formation of continuous ion transport pathways within the solid matrix. However, excessive pressure beyond the optimum level likely induced structural distortions, grain boundary constriction, or microcracking, which increased ion transport resistance and reduced conductivity. This study establishes that densification has a dual effect beneficial up to an optimal limit but detrimental when over-applied. The identified optimal pressure of 150 MPa provides a useful processing guideline for fabricating dense and highly conductive solid electrolytes. These findings underline the critical role of mechanical processing conditions in optimizing the performance of solid-state sodium-ion batteries and contribute to a deeper understanding of the relationship between microstructure and ionic transport. Such insights can be extended to other classes of oxide and sulfide-based solid electrolytes to guide the design of high-performance solid-state energy storage systems.

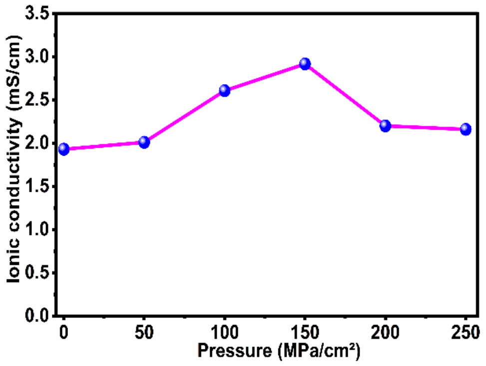

Fig: Ionic Conductivity vs pressure

Abstract Domain: Thin films/Nano-materials growth Novel techniques and concept

FTM-Controlled Aligned Organic Semiconducting Thin Films: Advances, Challenges, and Device Applications

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ABSTRACT

In this presents an o work discuss both the conventional and newly developed Floating Film Transfer Method (FTM) for fabricating oriented thin films at liquid interfaces. Traditional thin-film deposition methods often face limitations in achieving large-area uniformity, molecular orientation, and low-cost scalability—factors crucial for next-generation organic and flexible electronics. The single direction FTM overcomes these challenges through a solution-based process that enables thin-film formation at the liquid–air or liquid–liquid interface, followed by design slider. By optimizing casting parameters such as solvent volatility, surface tension, and film transfer rate, FTM allows precise control over thin-film morphology, crystallinity, and orientation.

The method is compatible with solution-processable organic and hybrid semiconductors, supporting large-scale and layer-by-layer film fabrication. Its simplicity and versatility make it particularly suitable for flexible, transparent, and printable devices, eliminating the need for vacuum systems or high-temperature processing. FTM-grown films exhibit high structural order and uniformity, directly translating into superior charge transport and device performance.

Applications of FTM-fabricated films include organic field-effect transistors (OFETs), phototransistors, and gas sensors, where enhanced carrier mobility and device stability have been demonstrated. Moreover, FTM-based photodetectors and nonvolatile memory switches highlight the technique's multifunctionality and adaptability. Beyond performance improvements, FTM supports environmentally friendly and low-cost production, aligning with the demands of sustainable electronics.

In summary, this technique offers a scalable and reproducible route to high-quality, oriented thin films with tunable properties. Its compatibility with diverse materials, facile transfer process, and suitability for flexible device architectures establish FTM as a promising platform for next-generation organic and hybrid electronic systems at large-area device fabrication.

Keywords: Floating Film Transfer Method (FTM); Thin-film deposition; Oriented thin films; Organic field-effect transistors (OFETs); Solution-processable techniques; Photodetectors; Gas sensors; Organic semiconductors;

SnO2/MXene/PVDF based Flexible Composite Triboelectric Nanogenerators (FCTENG) for sustainable wearable electronic device

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ABSTRACT

Triboelectric nanogenerators (TENGs) are extensively investigated as prominent energy harvesting platforms for wearable electronics, owing to their structural simplicity, high energy conversion efficiency, self-powered sensing functionality, and broad material selectivity, which collectively facilitate sustainable manufacturing. This study presents a dual-filler strategy that synergistically integrates surface-functionalized MXene and tin oxide (SnO2) nanoparticle into PVDF matrix engineered as a tribo-positive layer for high-performance, flexible TENGs. Fabricated via solution casting, these devices exhibit exceptional electrical output, generating a open circuit peak-to-peak voltage exceeding 150 V and open circuit peak-to-peak current (Ip-p) of ~18 μA under an applied force of ~20 N. A maximum power density of 6.0 μW/cm² was achieved at a load resistance of 3.0 MΩ, confirming efficient energy conversion. The TENGs successfully enabled continuous motion sensing of various body joints (knee, elbow, and fingers) upon direct epidermal application. Furthermore, the devices demonstrated operational stability over 2000 s, indicating robustness for prolonged use in practical applications.

Keywords: Triboelectric nanogenrators1; MXene2; Fabrication3; Keyword4.

(Abstract Domain : Material & coatings for batteries, super-capacitors and fuel-cells)

Investigating The Extended Interlayer MoS_2 Cathode Performance In Magnesium-Lithium Hybrid Electrolyte Cells

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ABSTRACT

This study reports the synthesis and in-depth electrochemical evaluation of 1T-phase molybdenum disulfide (MoS_2) as a cathode for rechargeable magnesium batteries employing a hybrid electrolyte. The hybrid electrolyte facilitates enhanced ionic conductivity and cooperative Mg^{2+} transport, promoting efficient intercalation within the layered dichalcogenide matrix. Structural analyses by XRD and Raman spectroscopy confirm formation of phase-pure 1T- MoS_2 with expanded interlayer spacing and superior electronic conductivity. Electrochemical testing reveals that 1T- MoS_2 exhibits significantly higher reversible capacity and coulombic efficiency compared to the 2H phase, demonstrating values of 249 and 136 $mAhg^{-1}$ at 100 mA g^{-1} after 100 cycles, respectively. The outstanding cycling stability and performance of the 1T phase are mainly ascribed to its improved conductivity and robust accommodation of Mg ions with limited structural degradation. Overall, this work demonstrates that engineering the MoS_2 phase and employing a dual-ion electrolyte strategy can effectively overcome the challenges of sluggish Mg^{2+} kinetics and interfacial incompatibility, positioning 1T- MoS_2 as a promising cathode for the development of high-performance, durable, and safe magnesium-based energy storage technologies.

Keywords: Rechargeable magnesium batteries; hybrid electrolyte; phase engineering.

(Abstract domain: Thin film/Nano-materials growth, Novel techniques and concepts)

In-situ phase transitions and strain evolution in freestanding $BaTiO_3$ epitaxial membranes *via* sacrificial $La_{2/3}Sr_{1/3}MnO_3$ assisted lift-off

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Abstract

Flexible and robust epitaxial architectures are vital for the development of next-generation electronic devices. In this work, we demonstrate the successful lift-off of a BaTiO (BTO) epitaxial layer through the selective etching of a sacrificial La / Sr / MnO (LSMO) layer from a SrTiO (001) single-crystal substrate. The as-grown BTO film exhibits a c/a ratio of 1.005, indicating out-of-plane compressive strain accompanied by in-plane tensile strain, relative to its bulk counterpart. Upon release, the freestanding membrane shows a slight relaxation of out-of-plane strain compared to the epitaxial stack. Surface morphology and chemical states were characterized using X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and optical profilometry. The temperature-dependent structural phase transitions of the freestanding BTO layer were systematically investigated using confocal Raman spectroscopy over a wide temperature range (-170°C to 200°C). A transition from the tetragonal to cubic phase is observed at elevated temperatures above 125°C, while at cryogenic temperatures, sequential transitions from tetragonal to orthorhombic (below 0°C) and to rhombohedral (around -80°C) are clearly identified.

Keywords: Epitaxy, freestanding membranes, phase transition, metal oxides

Double Modification (Mg, Ca, B & P) of Nano-ZSM-5: Effect on Acid Sites, Pore Narrowing, and Shape-Selective Toluene Methylation to p-Xylene

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Abstract.

Magnesium (Mg), Calcium (Ca), boron (B) & phosphorus (P) modified ZSM-5 zeolites were synthesized by Wet impregnation method. Commercial ZSM-5 was treated with ion exchange method (NH_4OH) to prepare hierarchical ZSM-5(H-ZSM-5). %wt of MgO, CaO, B_2O_3, & P_2O_5 in ZSM-5 was kept 3-5% in double modification. Pore narrowing and shape selectivity of Mg, Ca, B and P modified ZSM-5 was evaluated for toluene methylation to xylenes reaction. The parent, ion-exchanged and modified nano-sized zeolite catalysts were characterized using different analytical techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FE-SEM), Thermogravimetric analysis (TGA), Brunauer-Emmett-Teller method (BET) and; NH_3-TPD to analyze the crystallographic structure, surface area, porosity, morphology and particle size. Post synthesis modification of ZSM-5 with Mg, Ca, B and P generated new acid sites and narrowed the pore of ZSM-5. Besides this, there was change in acid site strength and total acid sites. These acid sites efficiently catalyzed toluene methylation with methanol and narrowed the pore opening resulting in para-selectivity. Decrease in total acid sites and pore volume by Mg and Ca modification has a direct correlation with increase in shape selectivity. Combination of 5%P+3%B/ZSM-5 gives the best result up to 19% toluene conversion and 80-90% para-xylene selectivity. It is anticipated that this process has good industrial prospective for high para-xylene production.

Keywords: Toluene methylation, p-Xylene, Pore size engineering, Single modification, Acid-sites reduction

References:

(1) Young, L. B.; Butter, S. A.; Kaeding, W. W. Shape Selective Reactions with Zeolite Catalysts. III. Selectivity in Xylene Isomerization, Toluene-Methanol Alkylation, and Toluene Disproportionation over ZSM-5 Zeolite Catalysts. J. Catal. 1982, 76 (2), 418–432. https://doi.org/10.1016/0021-9517(82)90271-8.
(2) Cavallaro, S.; Pino, L.; Tsiakaras, P.; Giordano, N.; Rao, B. S. Alkylation of Toluene with Methanol III: Para-Selectivity on Modified ZSM-5 Zeolites. Zeolites 1987, 7 (5), 408–411. https://doi.org/10.1016/0144-2449(87)90005-4.
(3) Giordano, N.; Pino, L.; Cavallaro, S.; Vitarelli, P.; Rao, B. S. Alkylation of Toluene with Methanol on Zeolites. The Role of Electronegativity on the Chain or Ring Alkylation. Zeolites 1987, 7 (2), 131–134. https://doi.org/10.1016/0144 2449(87)90074-1
(4) Breen, J.; Burch, R.; Kulkarni, M.; Collier, P.; Golunski, S. Enhanced Para-Xylene Selectivity in the Toluene Alkylation Reaction at Ultralow Contact Time. J. Am. Chem. Soc. 2005, 127 (14), 5020–5021. https://doi.org/10.1021/ja046421o.
(5) Breen, J. P.; Burch, R.; Kulkarni, M.; McLaughlin, D.; Collier, P. J.; Golunski, S. E. Improved Selectivity in the Toluene Alkylation Reaction through Understanding and Optimising the Process Variables. Appl. Catal. A Gen. 2007, 316 (1), 53–60. https://doi.org/10.1016/j.apcata.2006.09.017.
(6) Zhou, J.; Wang, Y.; Zou, W.; Wang, C.; Li, L.; Liu, Z.; Zheng, A.; Kong, D.; Yang, W.; Xie, Z. Mass Transfer Advantage of Hierarchical Zeolites Promotes Methanol Converting into Para-Methyl Group in Toluene Methylation. Ind. Eng. Chem. Res. 2017, 56 (33), 9310–9321. https://doi.org/10.1021/acs.iecr.7b02187
(7) Wang, Y.; Liu, M.; Zhang, A.; Zuo, Y.; Ding, F.; Chang, Y.; Song, C.; Guo, X. Methanol Usage in Toluene Methylation over Pt Modified ZSM-5 Catalyst: Effects of Total Pressure and Carrier Gas. Ind. Eng. Chem. Res. 2017, 56 (16), 4709–4717. https://doi.org/10.1021/acs.iecr.7b00318.

(Computational modelling and simulations)

Optimizing Hydrogen Adsorption on Graphene Oxide

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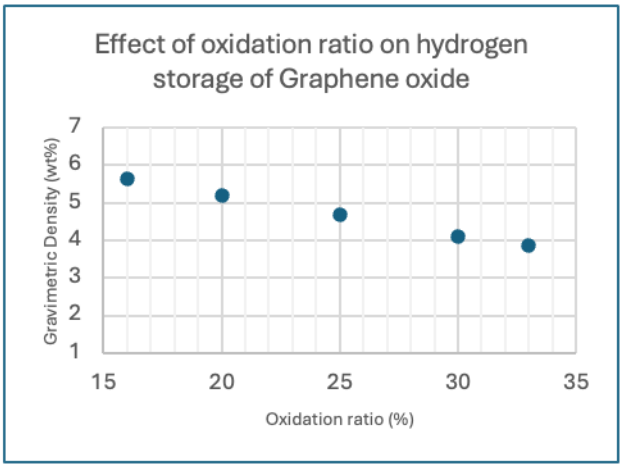
ABSTRACT

The efficient storage of hydrogen is a fundamental technological challenge critical for realizing its potential as a future energy source. GO is an attractive candidate because it is easy to synthesize, available in large quantities, and less expensive than pure graphene. GO is a chemically heterogeneous two-dimensional material composed of graphene sheets modified with various oxygen functional groups. While the presence of polar oxygen groups can enhance the H_2 binding energy beyond weak van der Waals forces, studies show that high oxygen content may reduce gravimetric capacity by adding weight and creating steric hindrance that obstructs the gas adsorption region. Computational modeling is indispensable to fully understand these complex structural-chemical relationships at the molecular level.

We report a ReaxFF molecular dynamics study on hydrogen physisorption in graphene oxide (GO). We systematically investigated the effects of sheet size (5-10 nm) and oxidation ratio (16-33%) on gravimetric density. Results indicate size-insensitivity above 8nm and an inverse relationship between oxidation and storage capacity.

We investigated the effect of GO sheet size on hydrogen storage, keeping the oxidation ratio (R) constant at approximately 16% and hydroxyl to epoxy ratio (OH/O) ~3%. Square sheets with side lengths of 5 nm, 8 nm, and 10 nm were simulated for production run of 1.2 ns. The resulting average gravimetric densities were 5.900 wt%, 5.656 wt%, and 5.642 wt%, respectively. The data show a slightly higher capacity for the smallest 5 nm sheet, likely due to a higher proportion of edge sites, but converge rapidly. The minimal difference between the 8 nm and 10 nm sheets suggests that edge effects become negligible and the storage capacity becomes size-insensitive for sheets of this size and larger.

Next, we studied the influence of the O/C ratio (R) on a fixed 10 nm GO sheet. Current results based on available production run lengths show a clear and consistent trend. Increasing oxidation leads to lower hydrogen storage. The gravimetric densities were 5.6 wt% for R=16%, 5.2 wt% for R=20%, 4.7 wt% for R=25%, 4.102 wt% for R=30%, and 3.863 wt% for R=33%. This inverse relationship suggests that while oxygen functional groups may enhance the binding energy of individual H_2 molecules, their steric hindrance at higher concentrations blocks access to the graphene basal plane, reducing the total number of available adsorption sites and thus lowering the overall storage capacity.



Keywords: Graphene oxide; Hydrogen storage; Atomic scale simulation; Gravimetric Density.

A Sustainable Binder for High-Voltage Graphite Cathodes in Sodium Dual-Ion Batteries

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Abstract

The role of binders in the performance of sodium dual ion batteries (SDIBs) has received limited attention, with polyvinylidene fluoride (PVDF) still predominantly utilised as a default choice for the electrodes. There are several water-based binders that have been explored for the anode; however, to date, there is no sustainable alternative capable of replacing the electrochemically stable PVDF binder for the graphite cathode for SDIBs. Herein, we propose a sustainable water-based binder composed of carboxymethyl cellulose (CMC) and sodium lignosulfonate (LgSA) as a promising substitute, which is compatible with graphite cathode operating above 4.5 V, for the development of SDIBs. As a result, the combination of these two binders for the graphite enables stable operation with comparable performance to that of the PVDF binder, with similar anion storage capacity. Beyond offering comparable performance, this binder combination paves the way for scalable SDIB technologies at low cost and enhanced safety.

Keywords: Sodium Dual Ion Batteries, Water-based Binders, Graphite cathode, anion-intercalation

Abstract Domain: Computational Modelling And Simulations

A Comprehensive TCAD Investigation of Single-Fin and Dual-Fin 3D Bulk FinFETs Across Multiple High-K Dielectric materials

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ABSTRACT

This study presents a comprehensive simulation-based investigation of Single-Fin (Conventional) and Dual-Fin FinFET architectures using the Silvaco TCAD platform to evaluate their electrical characteristics with various high-k gate dielectric materials. The analysis emphasizes the influence of different dielectrics-such as SiO_2, Si_3N_4, Al_2O_3, HfO_2, ZrO_2, La_2O_3, and TiO_2 on key device parameters including drain current (I_D), threshold voltage (Vth), subthreshold swing (SS), Ion/Ioff ratio, and Drain-Induced Barrier Lowering (DIBL). The results demonstrate that dielectric materials with higher permittivity effectively enhance gate control, minimize leakage current, and improve switching efficiency. Comparative analysis between Single-Fin and Dual-Fin structures reveals that the Dual-Fin FinFET provides superior electrostatic integrity, lower SCEs, and higher drive current, making it highly suitable for nanoscale low-power applications. The study also explores structural optimization through Fin geometry and dielectric selection to achieve improved performance, ensuring compatibility with next-generation VLSI and ultra-scaled CMOS technologies. Overall, the work establishes that the integration of high-k dielectrics in multi-fin FinFETs enables enhanced electrical efficiency, thereby paving the path for future generations of energy-efficient semiconductor devices.

Keywords: FinFET; Dual-Fin FinFET; High-k Dielectric; Short-Channel Effects (SCEs); Subthreshold Swing (SS); Threshold Voltage (Vth); Ion/Ioff Ratio; DIBL; Silvaco TCAD Simulation;

(Abstract Domain 1: Thin films/Nano-materials Growth, Novel techniques and concepts)

Type II Based Tise$_2$/Tio$_2$ Heterostructures for Hydrogen Evolution Reactions (HER)

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ABSTRACT

The hydrogen evolution reaction (HER) confers a sustainable method for producing hydrogen. The main goal of this work is to create a type-II heterostructure based on titanium diselenide/titanium dioxide ($TiSe_2/TiO_2$). For $TiSe_2$, selenium and titanium oxide powder were used via Chemical vapour deposition (CVD) on silicon and for TiO_2, hydrothermal synthesis in order to increase HER control. TiO_2 nanorods are combined with transition metal dichalcogenides, such as $TiSe_2$, which are renowned for their exceptional qualities, to create a potent photocatalytic system. Field-emission scanning electron microscopy (FE-SEM), Raman spectroscopy, and X-ray diffraction (XRD) were among the characterization methods used. Both ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS) provide a broad understanding of charge transport kinetics and electronic interactions. The UPS experiments demonstrate that an improvement in catalytic active sites is defined by a shift in peak positions in XPS spectra. It was confirmed that the heterostructure's enhanced energy environment to start the charge transfer strengthened the creation of hydrogen. According to the UPS research, the heterostructure minimum work function ($TiSe_2$) calls for improvement in charge transfer. $TiSe_2/TiO_2$ heterostructure is therefore deemed a likely material for sustainable hydrogen generation.

Keywords: $TiSe_2/TiO_2$ heterostructure; Chemical vapour deposition; Hydrothermal synthesis.

References:

[1] Dawood F, Anda M, Shafiullah GM. Hydrogen production for energy: an overview. Int J Hydrogen Energy Feb. 07, 2020;45(7):3847–69. https://doi.org/10.1016/j. ijhydene.2019.12.059. Elsevier Ltd.

[2] Lasia A. Mechanism and kinetics of the hydrogen evolution reaction. Int J Hydrogen Energy Jul. 26, 2019;44(36):19484–518.https://doi.org/10.1016/j. ijhydene.2019.05.183. Elsevier Ltd.

[3] Dincer I, Acar C. Review and evaluation of hydrogen production methods for better sustainability. Int J Hydrogen Energy Aug. 2014;40(34):11094–111.https://doi. org/10.1016/j.ijhydene.2014.12.035.

(Abstract Domain : Materials & coating for batteries, super-capacitors and fuel cells)

Architecture-driven Performance Enhancement in Lithium-ion Batteries

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ABSTRACT

The interplay between electrode architecture and electrochemical performance is increasingly recognized as a decisive factor in advanced lithium-ion (Li-ion) energy storage systems. Conventional monolithic electrodes, composed of a blend of multiple active materials, often suffer from redox overlap, sluggish ion diffusion, and localized potential mismatch, ultimately limiting rate capability and solid-phase lithium-ion diffusivity. To address these inherent constraints, we introduce a modular electrode design that spatially segregates distinct active material domains on a single current collector, thereby allowing independent lithiation–delithiation and minimizing intermixing of redox processes.

In this study, mesocarbon microbeads (MCMB) and reduced graphene oxide (rGO) were used as representative anode materials owing to their contrasting lithium intercalation and storage mechanisms. Monolithic electrodes (each of 15 mm diameter) and modular electrodes (each consisting of 4 smaller electrodes of 5 mm diameter) were fabricated as a function of ω_{MCMB} (where $\omega_{MCMB} = 0$ for pure rGO composition and $\omega_{MCMB} = 1$ for pure MCMB composition) and assembled into CR2016 half-cells versus Li/Li^+. Modular electrode fabrication was achieved by utilizing a polymer film coating. Comprehensive electrochemical characterization, including galvanostatic charge–discharge, Electrochemical Impedance Spectroscopy (EIS), Galvanostatic Intermittent Titration Technique (GITT), Incremental Capacity (dQ/dE) analysis, and X-ray Photoelectron Spectroscopy (XPS), was employed to delineate kinetic and thermodynamic characteristics arising from architectural configuration.

The rate capability results distinctly highlight the kinetic superiority of modular electrodes. At 2C, modular electrodes retained >30% of their initial capacity, compared to only ~17% for monolithic electrodes. EIS analysis revealed that pristine modular electrodes possessed a largely suppressed charge transfer resistance (R_{CT}) compared to their monolithic counterparts as a result of spatial decoupling. Incremental Capacity Analysis (ICA) further underscored architectural control over redox thermodynamics. Modular electrodes displayed a dynamic and adaptive lithiation behaviour, preserving individual redox identities and depicting more stable phase transformation kinetics as compared to monolithic electrodes. This preservation of distinct redox plateaus suggests minimized electronic cross-talk and better-defined thermodynamic states. Additionally, GITT-derived Li^+-ion diffusivity (D_{Li}) revealed that while D_{Li} diminished at higher MCMB compositions in monolithic electrodes, it exhibited a monotonic increase with increasing MCMB compositions in modular electrodes. Additionally, D_{Li} in pure MCMB-phase modular electrode was observed to be ~10^{-15} m^2 s^{-1}, nearly an order of magnitude higher than its monolithic counterpart, confirming the presence of shorter diffusion paths and enhanced ion transport kinetics. Post-cycling XPS analysis of monolithic electrodes revealed significant SEI thickening and increased Li_2CO_3 signals, whereas the modular electrodes maintained thinner, compositionally stable SEI layers. These observations, reinforced by SEM analysis, indicate that architectural segregation of active domains mitigates electrolyte decomposition during prolonged cycling.

Overall, this study establishes that electrode architecture functions as a systems-level design parameter governing both kinetic (transport, charge transfer, diffusivity) and thermodynamic (phase stability, redox potential distribution) properties in Li-ion batteries. The demonstrated modular electrode configuration offers a scalable route toward high-rate, durable anodes with sustained redox clarity and transport efficiency. These findings open new avenues for architecture-centric battery engineering, bridging material science and electrochemical systems design.

Keywords: Electrode design; Electrode architecture; Modular electrode; Incremental capacity

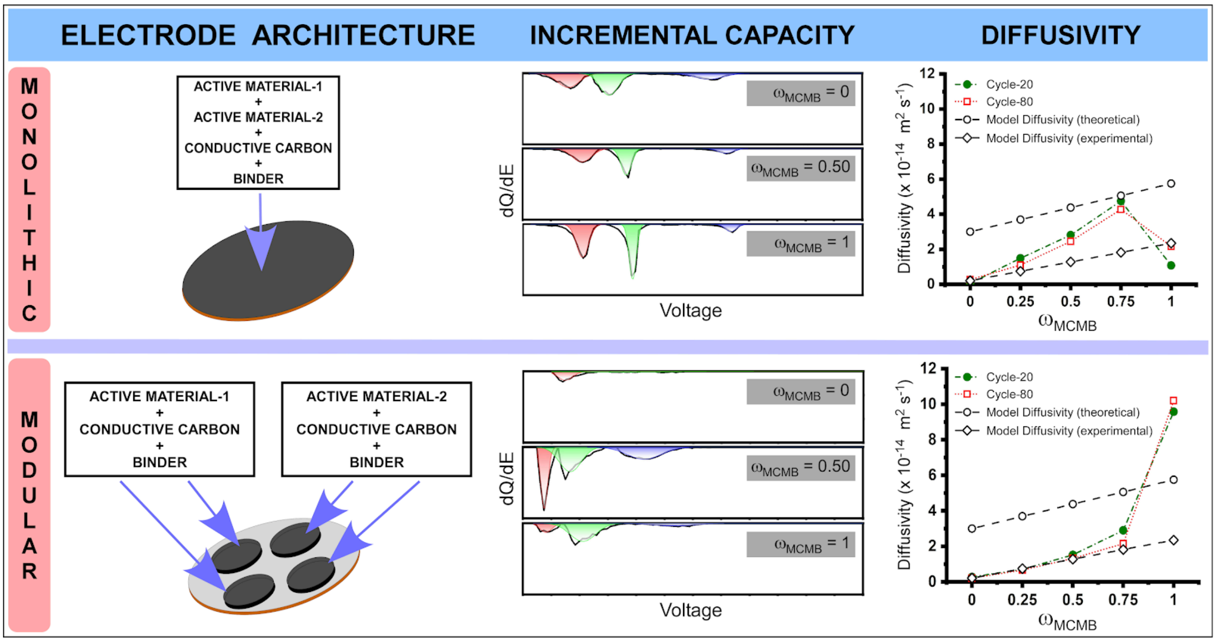

Figure 1: Architecture-driven differences in incremental capacity (dQ/dE) and Li-ion diffusivity (D_{Li}) between monolithic and modular electrodes, emphasizing adaptive lithiation behaviour and superior kinetics in the modular design

Interfacial Engineering of 1T-WS_2/rGO Nano-hybrid Heterostructure for Supercapacitor Application

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Keywords: 1T-WS_2, Electrochemical, (1T-WS_2) (rGO) nano-hybrid, supercapacitor, charge-discharge

Abstract: The rapid depletion of fossil resources, coupled with the escalating demand for sustainable and high-efficiency energy storage systems, underscores the necessity of engineering advanced electrode materials. In this context, the present work explores the design of 1T-WS_2/reduced graphene oxide (rGO) hybrid heterostructures to overcome the intrinsic limitations of pristine 1T-WS_2 in supercapacitor applications. The introduction of rGO as a conductive interlayer not only reinforces the mechanical and structural stability of 1T-WS_2 but also augments its electrochemical kinetics by providing a highly conductive nanoscale electron-transport network. 1T-WS_2 was derived from solvothermal process, subsequently integrated with rGO in ethanol at controlled ratios to fabricate 1T-WS_2/rGO composites. The rGO incorporation effectively mitigated volumetric strain during repetitive charge-discharge cycling while enhancing electronic conductivity through its role as a quasi–current collector. Comprehensive physicochemical analyses (SEM, TEM, XRD, Raman, and BET) validated the successful assembly of the heterostructure with improved microstructural robustness and hierarchical porosity. Electrochemical assessments, including cyclic voltammetry, galvanostatic charge-discharge, and impedance spectroscopy, revealed a pronounced enhancement in capacitive behaviour. Specifically, the (1T-WS_2) (rGO) nano-hybrid exhibited a high specific capacitance of 230 Fg ^{1} at 1 Ag ^{1}, surpassing the 161 Fg ^{1} of pristine 1T-WS_2 in electrolyte 1 M H_2SO_4. This study demonstrates the critical role of rGO as a conductive bridge in mitigating structural collapse and accelerating charge transport, thereby advancing TMDs-based supercapacitors toward next-generation, high-performance, and durable energy storage application.

Abstract Domain: Thin films/Nano-materials growth Novel techniques and concept

FTM-Controlled Aligned Organic Semiconducting Thin Films: Advances, Challenges, and Device Applications

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ABSTRACT

In this work discuss both the conventional and newly developed Floating Film Transfer Method (FTM) for fabricating oriented thin films at liquid interfaces. Traditional thin-film deposition methods often face limitations in achieving large-area uniformity, molecular orientation, and low-cost scalability—factors crucial for next-generation organic and flexible electronics. The single direction FTM overcomes these challenges through a solution-based process that enables thin-film formation at the liquid–air or liquid–liquid interface, followed by design slider. By optimizing casting parameters such as solvent volatility, surface tension, and film transfer rate, FTM allows precise control over thin-film morphology, crystallinity, and orientation.

The method is compatible with solution-processable organic and hybrid semiconductors, supporting large-scale and layer-by-layer film fabrication. Its simplicity and versatility make it particularly suitable for flexible, transparent, and printable devices, eliminating the need for vacuum systems or high-temperature processing. FTM-grown films exhibit high structural order and uniformity, directly translating into superior charge transport and device performance.

Applications of FTM-fabricated films include organic field-effect transistors (OFETs), phototransistors, and gas sensors, where enhanced carrier mobility and device stability have been demonstrated. Moreover, FTM-based photodetectors and nonvolatile memory switches highlight the technique’s multifunctionality and adaptability. Beyond performance improvements, FTM supports environmentally friendly and low-cost production, aligning with the demands of sustainable electronics.

In summary, this technique offers a scalable and reproducible route to high-quality, oriented thin films with tunable properties. Its compatibility with diverse materials, facile transfer process, and suitability for flexible device architectures establish FTM as a promising platform for next-generation organic and hybrid electronic systems at large-area device fabrication.

Keywords: Floating Film Transfer Method (FTM); Thin-film deposition; Oriented thin films; Organic field-effect transistors (OFETs); Solution-processable techniques; Photodetectors; Gas sensors; Organic semiconductors;

Thin films/Nano-materials Growth, Novel techniques and concepts

Synthesis of β-Ga_2O_3 Nanowires through Au-assisted VLS Growth

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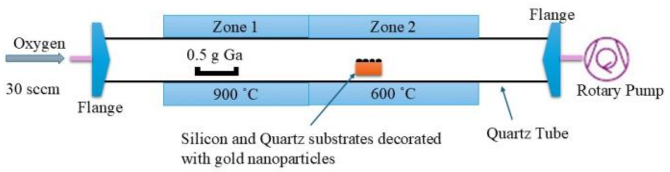
β-Ga_2O_3 is a promising ultra-wide-bandgap semiconductor (bandgap ~4.7–4.9 eV) with advantages over GaN (3.4 eV) and SiC (3.2 eV). Its wide bandgap makes it suitable for high-power electronics, solar-blind ultraviolet photodetectors, and gas sensors. One-dimensional nanowire (NWs) structures can offer large surface area and improved electrical transport, potentially enhancing device performance.

In this study, we focus on the vapor–liquid–solid (VLS) growth of β-Ga_2O_3 nanowires using gold (Au) catalyst nanoparticles. We aim to synthesize β-Ga_2O_3 nanowires and to characterize their structure and optical properties.

We deposited a thin gold film on silicon and quartz substrates and annealed it to form Au nanoparticles. Scanning electron microscopy (SEM) confirmed that after annealing, the Au film had dewetted, forming uniformly distributed Au nanoparticles (130–150 nm in diameter) on the substrates. These Au nanoparticles serve as effective catalytic sites for NWs growth. Next, β-Ga_2O_3 nanowires were grown using high-purity Ga metal as the source in a two-zone tube furnace. About 0.5 g of Ga metal was placed in a quartz boat in zone-1 (the upstream source zone), while the Au-coated silicon and quartz substrates were placed in a separate quartz boat in zone-2 (the downstream substrate zone) (see Fig. 1). The quartz tube was evacuated to vacuum and heated; zone-1 was raised to 900 °C to vaporize the Ga, while zone-2 was maintained at 600 °C to provide the growth temperature for the NWs on the substrates. After stabilizing these temperatures, oxygen was introduced into the system. Growth continued for 2 hours under these conditions, after which the furnace was allowed to cool naturally to room temperature.

After growth, field-emission scanning electron microscopy (FE-SEM) was used to examine the nanowire morphology. X-ray diffraction (XRD) was used to confirm the crystal phase, Raman spectroscopy to assess lattice vibrations, and UV–Vis absorption spectroscopy to measure the optical bandgap.

SEM images reveal a dense forest of long, straight nanowires covering the substrate. The nanowires have diameters on the order of a few hundred nanometers, and lengths of several tens of micrometers. X-ray diffraction (XRD) and Raman spectroscopy indicate that the nanowires are high-quality, single-crystal β-Ga_2O_3 (monoclinic) with no detectable secondary phases. UV–Vis absorption shows a sharp edge near 265 nm, corresponding to a direct bandgap of about 4.6–4.7 eV, in agreement with known values for β-Ga_2O_3.



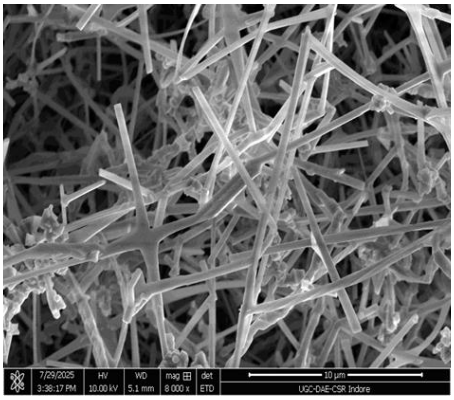


Fig. 1. Sketch of the synthesis setup, made of a two-zone furnace with Ga source is placed in the hottest point of the furnace while substrates decorated with gold nanoparticles are at lower temperature downstream. Fig. 2: Top-view FE-SEM micrograph of the as-grown β-Ga_2O_3 NWs, showing a dense and uniform distribution.

Keywords: β-Ga_2O_3 nanowires, CVD, ultra-wide-bandgap semiconductor.

Lithium source dependent structural evolution and electrochemical performance in NMC811 cathode material for lithium-ion batteries

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Abstract

Lithium-ion batteries are the backbone for the today's digital era and electric vehicles. NMC cathodes are commercially used for electric vehicles due to their high capacity and higher working potential. This study investigates the influence of different lithium precursors like carbonates, hydroxides, acetates, nitrates etc., with NMC-hydroxide ($Ni_{0.8}Mn_{0.1}Co_{0.1}(OH)_2$) to synthesise NMC811 ($LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$) cathode material for lithium-ion batteries. The NMC-hydroxide was synthesised via co-precipitation route and it was subsequently mixed with varied lithium sources, including carbonate, hydroxide, acetates and nitrates etc. Thermogravimetric analysis was employed to assess precursor decomposition and reaction behaviour of the precursor mixtures and then calcinated to form NMC811. The synthesised NMC811 cathode material was evaluated for phase formation and morphology using X-Ray diffraction and scanning electron microscopy. Electrochemical performance was systematically studied through electrochemical impedance spectroscopy, cyclic voltammetry, galvanostatic charge-discharge and galvanostatic intermittent titration technique to evaluate the redox potential, capacity, and lithium diffusion coefficient of the NMC811 cathode material synthesised using different lithium sources.

Keyword – NMC811, Cathode Material, Lithium precursor, Lithium-ion diffusion, Co-precipitation.

Electrical Characteristics of Al/n-MoS_2/p-Si heterojunction for ohmic Photo detector

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Abstract: Transition metal dichalcogenides (TMDs) have garnered significant attention for their unique optoelectronic properties, making them promising candidates for next-generation electronic and photo detecting devices. Among them, molybdenum disulfide (MoS_2) is one of the most extensively studied materials owing to its tuneable bandgap, strong light–matter interaction, and high carrier mobility. In this study, multilayer MoS_2 thin films were synthesized via chemical vapor deposition (CVD) through the sulfurization of thermally evaporated molybdenum trioxide (MoO_3) using sulphur (S) powder as a precursor in a single-zone tubular furnace on p-type Si (100) substrates. The deposition parameters were optimized to obtain high-quality crystalline films. Structural analyses by Raman spectroscopy showed characteristic E_{2g}^{1} and A_{1g} modes at 384 cm^{-1} and 411 cm^{-1}, confirming the formation of multilayer MoS_2. Morphological examination through field-emission scanning electron microscopy (FE-SEM) displayed uniform layered structures. The electrical behaviour of the Al/n-MoS_2/p-Si heterojunction was investigated through current–voltage (I–V), capacitance–voltage (C–V), and conductance–voltage (G–V) measurements under visible and ultraviolet (UV) illumination. The I–V characteristics exhibited nearly linear behaviour, indicating an ohmic contact between Al and MoS_2. Furthermore, C–V and G–V analyses revealed frequency-dependent responses and modulation of interface states under illumination. These findings confirm the successful synthesis of high-quality MoS_2 films with excellent electrical and optoelectronic properties, making them highly suitable for low-power photodetector and sensor applications.

[1] Y. H. Lee, X. Q. Zhang, W. Zhang, M. T. Chang, C. T. Lin, K. D. Chang, *et al.*, "Synthesis of large-area MoS_2 atomic layers with chemical vapor deposition," *arXiv preprint*, arXiv:1202.5458, 2012.

[2] J. V. Pondick, J. M. Woods, J. Xing, Y. Zhou, and J. J. Cha, "Stepwise sulfurization from MoO_3 to MoS_2 via chemical vapor deposition," *ACS Applied Nano Materials*, vol. 1, no. 10, pp. 5655–5661, 2018.

[3] C. Yim *et al.*, "Electrical devices from top-down structured platinum diselenide films," *npj 2D Materials and Applications*, vol. 2, no. 1, p. 7, Feb. 2018, doi: 10.1038/s41699-018-0051-9.

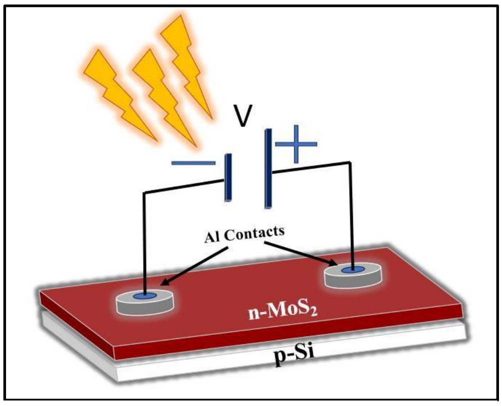

Fig.1 Schematic Diagram for Al/n-MoS_2/p-Si

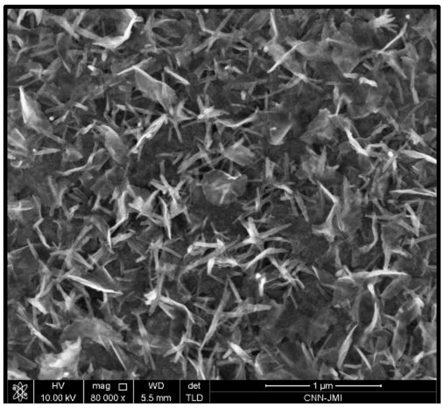

Fig.2 FE-SEM image of Al/n-MoS_2/p-Si

Direct Growth of Na-ion Conducting $Na_3O_{15}Si_6Y$ Solid Glass Electrolyte with Reduced Interfacial Resistance for Room-temperature Sodium-Sulfur Pouch Cells

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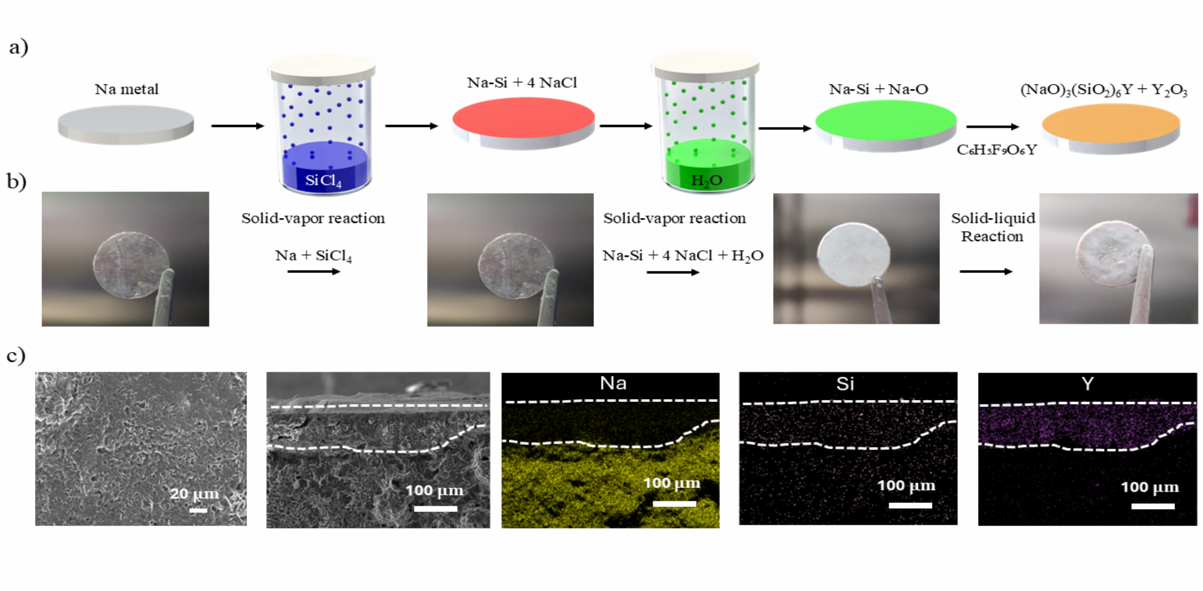
ABSTRACT:

The stability of the solid electrolyte/electrode interface is critical for the solid-state batteries. Traditionally developed solid electrolytes are prone to high interface resistance due to how electrolyte is placed on the electrodes; no effective method has been devised to solve this problem. Here, we report a solid-vapor growth method for directly growing a Na^+-ion conducting solid electrolyte on the sodium metal anode, thereby minimizing interfacial resistance. As a result, the solid electrolyte (i.e. $Na_3O_{15}Si_6Y$) exhibits a significantly reduced interfacial resistance of $\sim 6.2\ \Omega\ cm^2$, accompanied by an improved room-temperature Na-ion conductivity of ~1.6 mS/cm. Due to reduced interfacial resistance, sodium symmetric cells exhibit an extremely low stripping/plating overpotential of about 180 mV. *Ab initio* molecular dynamics (AIMD) simulations suggest that the Na^+-ions are the primary charge carriers in the $Na_3O_{15}Si_6Y$ system and attain a low activation energy barrier (~0.25 eV) for Na-ion diffusion. A full-cell comprising Na metal anode with as-grown solid electrolyte and metal sulfide cathode functions reversibly for over 400 cycles with an average coulombic efficiency about 99%. Moreover, a pouch cell ($3 \times 3\ cm^2$) can reversibly be cycled with a high discharge capacity, demonstrating the stability and scalability of the solid vapor-grown solid electrolyte.



Inspiration from Roof Leaks to understand cathode material degradation: Building Moisture-Resistant Cathodes

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Abstract

The wide commercialization of sodium-ion batteries (SIBs) is hindered by the poor air-stability of transition metal layered oxide cathode materials. These materials, particularly Na_xTmO_2 (where Tm = transition metal like Co, Ni, Mn, Fe), are very promising because they have low cost, high reversible specific capacity, and rich sodium contents. But they are degraded by exposure to water, which is a big issue in the practical applications of SIBs. Na-vacancies are

either present in pristine O3-phase $NaMn_xNi_{1-x}O_2$ (x=0.1 to 0.5) materials or produced during the charging process.[1–3] These Na-vacancies are prone to detrimental intercalation of water, carbon dioxide and other reactive molecules in these Na-vacancies. Historically, scientists have studied doping or elemental substitution in the transition metal slabs to limit this degradation. The first approaches utilized structure-based descriptors, i.e., dopant cations that cause a diminution of the Na-layer distance by increasing the Tm-layer and thus making water intercalation geometrically less desirable.[1] These structural characteristics, augmented by charge and size of transition metals, were retrieved from first-principles calculations, impressively often without the direct inclusion of the energetic aspect of water-material interactions within water-free systems.[3]

To make the otherwise computationally costly rigorous thermodynamic computations of sampling large numbers of water configurations feasible, the work concentrates on the initial stages of water insertion. The corresponding energy change, ΔE, calculated from the various water (in Na-vacancies) inserted configurations is demonstrated to be a more accurate material stability descriptor than structure-based descriptors for instance Na-layer separations in O3-

Na-ion layered based cathode materials. A comprehensive effort, the study involved nearly over 135 DFT calculations using PBE+U+D3 functional (Vienna ab initio simulation package (VASP)), amounting to 1,063 CPU hours, highlighting our rigorous analysis.[4] The most important finding is water insertion into bulk O3-NMNO (O3-$NaMn_{0.5}Ni_{0.5}O_2$) and O3-NTNO

(O3-$NaTi_{0.5}Ni_{0.5}O_2$) systems were energetically unfavorable (positive ΔE values of +0.75 eV and +0.78 eV respectively). [4] In particular, quite similar values of ΔE in bulk systems countered the previously known instability of O3-NMNO towards degradation, proving that bulk systems are unreliable for the study of water insertion and stability.[4]

In contrast to water insertion into bulk O3-NMNO and O3-NTNO systems, water insertion at the material surface was energetically favorable for NMNO and quite unfavorable for NTNO.

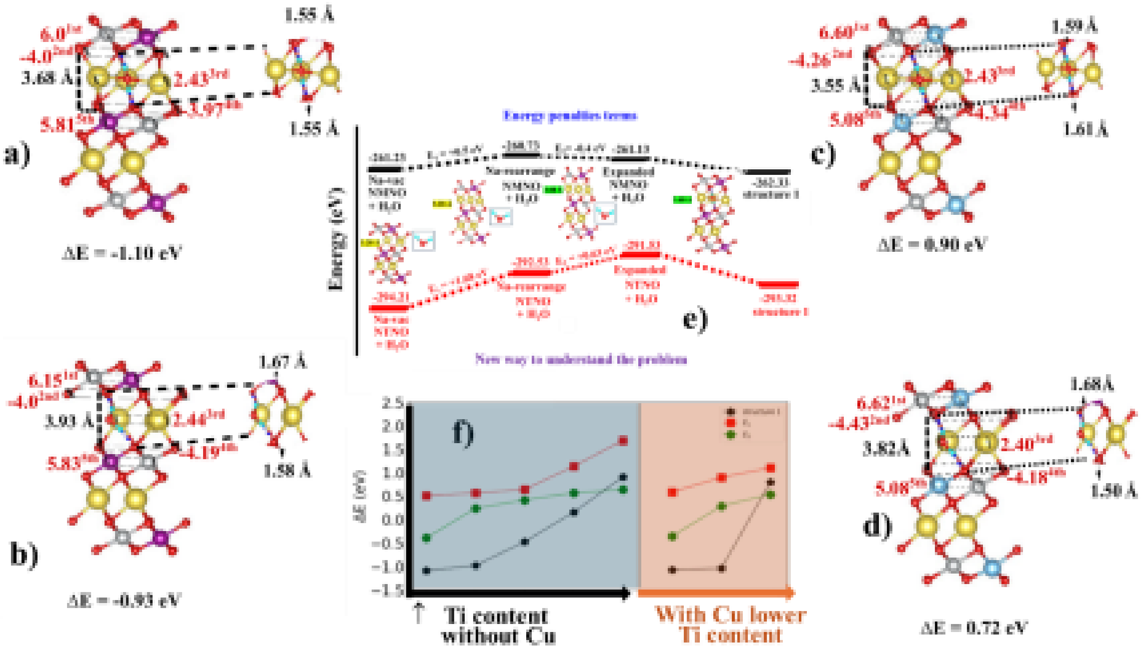

Figure 1. a) O3-NMNO slab showing Na-rearrangement in water inserted configuration ((H_2O)$Na_7Mn_6Ni_6O_{24}$), b) O3-NMNO slab showing water inserted configuration without Na rearrangement ((H_2O)$Na_7Mn_6Ni_6O_{24}$), c) O3-NTNO slab with water inserted configuration (H_2O)$Na_7Ti_6Ni_6O_{24}$), d) O3-NTNO slab showing water inserted configuration without Na rearrangement ((H_2O)$Na_7Ti_6Ni_6O_{24}$), e) Energy penalties term explanation, and f) ΔE, E_1 and E_2 (eV) for slab with Na-rearrangement in water inserted configurations.[4]

For surface interactions, symmetrical surface slab structures and appropriate vacuum regions were built. DFT For O3-NMNO slab, three stable orientations of water molecules were observed. The ΔE values of -1.1 eV, and -0.93 eV for structure 1 (see Figure 1a), and structure 2 (see Figure 1b) respectively, indicated that water insertion is energetically favorable in structure 1 and structure 2. One of the most important factors in stabilization is the orientation of the water molecule, so that proper H-bonding between the hydrogen atoms of the water molecule and the oxide layer oxygen atoms is achieved. This typically requires the water molecule to point at an angle relative to the Na layer normal, with acceptable H-O distances.[4]At water insertion, the structural reorganizations include the displacement of sodium ions from initial positions and opening of Na layer gaps. These interruptions are costly in terms of energy. To make room for favorable insertion of water into NMNO, the material prefers relaxing less ionic, minimizing charge separation among layers. But there is a counterbalancing factor that is more negative charge on the oxide layer is favorable for hydrogen bonds, less negative charge is favorable for expanding Na layer spacing to allow water inside the materials. A similar calculation for the O3-NTNO system (with Mn-ions replaced by Ti-ions) indicated that water insertion is generally energetically unfavorable (ΔE values 0.90 eV, and 0.72 eV for structure 1 (see Figure 1c) and structure 2 (see Figure 1d) respectively). Although structural reorganizations like Na rearrangement and Na expansion of the layer in NTNO are like NMNO, the values of ΔE vary exceedingly (-1.10 eV for NMNO structure 1 vs. 0.90 eV for NTNO structure 1). This contrast highlights that ΔE, and not structural or charge quantities, is more connected to material stability. Interestingly, water insertion renders the NTNO system more ionic, the opposite of NMNO.

The study concludes that five factors collectively determine the overall energetics of water insertion:

1. Penalty due to Na rearrangement.
2. Penalty due to increase of Na-layer spacing, even if the initial one is large.
3. Orientation of the water molecule to assist in the formation of hydrogen bond between the oxide layer and water.
4. Na, oxide, and Transition Metal (Tm) charges, influencing the ease with which the Na-layer opens (lower charge preferred).
5. Higher charge on the transition metal, which can lead to more compact spacing of the Na-layers (e.g., Ti as compared to Mn).

All of these are connected and normally interact with each other. For instance, shifting the Na ions to place water in the correct way has an energy cost. Computing these penalties, the study finds that in NMNO, the energy penalty of Na-layer rearrangement (E_1 = +0.5 eV) and expansion (E_2 = -0.4 eV) is countered largely by the creation of stable hydrogen bonds, thereby facilitating water insertion (see Figure 1e). For NTNO, though, the greater energy penalties (E_1 = +1.68 eV, E_2 = +0.63 eV) are not compensated by hydrogen bonding and thus insertion of water is not favorable (see Figure 1e). The Na ion displacement (E_1 term) is described as the most unfavorable factor. [4]

For doping, the progressive substitution of Mn with Ti ions indicated that higher content of Ti renders water insertion harder (ΔE ranges from -1.1 eV for O3-NMNO to 0.9 eV for O3-$Na_7Ti_6Ni_6O_{24}$). The optimal Mn:Ti ratio of water stability was 1:1, beyond which water insertion is energetically unfavorable (ΔE turns positive). Also, the study investigated the effect of Cu-doping, which was shown experimentally to reduce hygroscopicity in NMNO cathodes alongside Ti-ions. Even when charge-based explanation failed to fully explain the phenomenon, the DFT calculations revealed that replacement of a single Ni atom by Cu and stepwise replacement of Mn by Ti makes water insertion even less favorable. For example, O3- $Na_7Mn_3Ti_3Ni_5CuO_{24}$ is 0.79 eV in ΔE and far more stable than the Cu-free system (see Figure 1f). Notably, air stability of dopant Cu is achieved predominantly by inhibiting hydrogen bond formation, so water insertion is less favorable. Non-overlap of ΔE-vs.-Na layer thickness plots of Cu-free and Cu systems also confirmed the poor correlation between structural parameters and energy, which corroborates the energy-based descriptors role. The trend towards hydrogen bonding formation was found to be Mn > Mn,Ti > Mn,Ti,Cu > Ti, providing a simple approach to predict air stability (see Figure 1f).

In short, it is of utmost importance to solve the water stability of Na-ion-based layered transition metal oxides in order to place them in actual battery applications. The research focuses on the water stability of Na-ion-based layered transition metal oxides for battery applications. It provides an energy-based descriptor for measuring air-stability and informs dopant choice. Visualize a material's stability to moisture like a home being resistant to a leak. Structure-based descriptors like checking the house by making sure its doors and windows are closed tight - it gives some sense of potential entry points. But this study's energy-based descriptor is like actually pushing water into the home and seeing how difficult it is, considering not just the doors but also how the water would be influenced by the inside furniture (Na ions) and walls (oxide layers) once inside, and how the inside forces (hydrogen bonds) would reject or accept it. A house (material) is truly stable if the effort to let water in (ΔE) is large, because the internal processes (Na rearrangement, weak hydrogen bonding) actively resist the intruder, not just relying on gap size.

References

[1] Y. You, A. Dolocan, W. Li, A. Manthiram, *Nano Lett.* **2019**, *19*, 182–188.

[2] Y. Zhang, M. Wu, W. Teng, J. Ma, R. Zhang, Y. Huang, *ACS Appl. Mater. Interfaces* **2020**, *12*, 15220–15227.

[3] Y. Zhang, R. Zhang, Y. Huang, *Front. Chem.* **2019**, *7*, 1–15.

[4] R. Kumar, A. Chatterjee, *Inorg. Chem. Front.* **2025**.

Functional Oxide Thin Films for Next-Generation Electronics and Photonics: A Multi-Material Perspective

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ABSTRACT

Complex metal oxides are a class of functional oxides whose importance arises from a diverse range of tunable physical properties that can be engineered through techniques such as strain engineering, stoichiometry control, and doping. Functional oxides such as Vanadium Oxide (VO_2), Hafnium Zirconium Oxide ($Hf_{0.5}Zr_{0.5}O_2$), and $BaTiO_3$ (BTO) are particularly interesting as they exhibit important phenomena such as electrically and thermally controlled metal-insulator transition (VO_2), thickness-dependent ferroelectricity (HZO), and non-linear optical properties (BTO) which allow them to be used in a wide range of applications including non-volatile memory, piezoelectric devices, optical sensors, and neuromorphic computing components. Further, obtaining the freestanding epitaxial thin films offer huge potential for flexible electronics and heterogeneous integration with next-generation devices. In addition, Deep learning and Natural Language Processing (NLP) are transforming materials science by enabling efficient data analysis, property prediction, and design optimization. In this work, we present an overview of the phase evolution and stability, as well as various methods for tuning the physical properties of these functional oxides. We also explore deep learning and NLP-driven approaches for accelerating materials discovery, particularly in the field of complex oxides. The importance of point defects, materials processing and their influence in tuning the physical properties will be discussed.

Keywords: Functional oxides, thin films, freestanding, ferroelectrics, phase-change materials, Natural Language Processing (NLP), materials discovery

Impact of structural transitions on the local spin environment and lattice dynamics in K_2IrBr_6

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K_2IrBr_6 is a transition metal compound with 5d Ir ions in an ideal local octahedral environment with J_{eff} = ½ Mott insulating state. It undergoes structural phase transitions from cubic to tetragonal to monoclinic phases towards low temperatures. We have studied the impact of such transitions on the local spin environment and lattice dynamics using temperature-dependent electron paramagnetic resonance (EPR) and Raman scattering, respectively. At room temperature in the cubic phase, EPR revealed anisotropic g-factor that suggests the entangled spin and lattice due to strong spin-orbit interaction of Ir-ions. EPR further reveals that the local spin structure and dynamics are strongly interlinked to the structural transitions. Our Raman scattering experiments did not obtain any new phonon modes as the structural transitions happen. However, a soft phonon anomaly has been observed across the cubic-to-tetragonal phase transition. In summary, our study obtains how the structural transitions affect the local spin structure and lattice dynamics in K_2IrBr_6.

Design and development of organic hole transport materials for n-i-p structure perovskite solar cells

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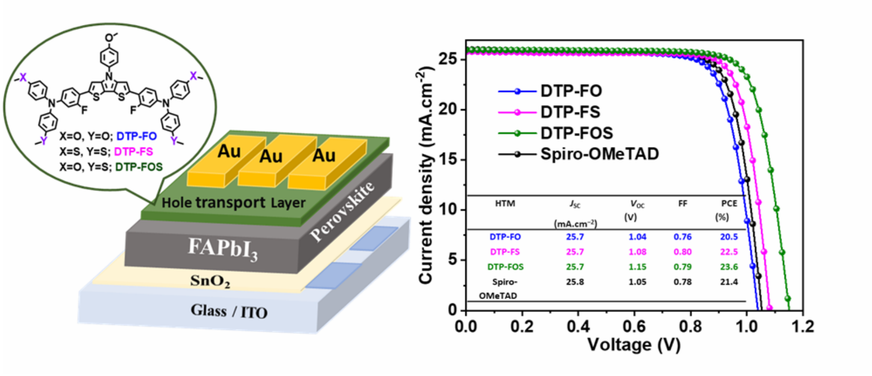
ABSTRACT:

Organic hole-transport materials (HTMs) play complementary and crucial roles in high-performance perovskite solar cells by controlling charge extraction, interfacial energetics, and device stability. Moreover, HTMs (small molecules and polymers) provide the contiguous transport network that selectively extracts and transports photogenerated holes to the anode while blocking electrons. Herein, we introduce novel HTMs featuring a D-π-D molecular structure. These HTMs have 3-fluoro-*N,N*-bis(4-(methylthio)phenyl)aniline (TPASF) peripheral terminal groups, which are linked with various π-core moieties. Our investigation reveals that altering the π-linkers affects the film morphology of the HTMs, significantly influencing device performance. HTMs. In the similar molecular architecture (D-π-D), incorporating a dithieno[3,2-*b*:2',3'-*d*]pyrrole (DTP) core functionalized with various *ortho*-fluorinated triarylamine donor units. Through systematic modification of the terminal groups, we designed three distinct HTMs: DTP-FO (methoxy terminal group), DTP-FS (methylthio), and DTP-FOS, a hybrid structure incorporating both methoxy and methylthio substituents [4,4'-(4-(4-methoxyphenyl)-4*H*-dithieno[3,2-*b*:2',3'-*d*]pyrrole-2,6-diyl)bis(3-fluoro-*N*-(4-methoxyphenyl)-*N*-(4-(methylthio)phenyl)aniline)]. These tailored structural modifications induce intramolecular noncovalent interactions that effectively regulate the optoelectronic properties, crystallinity, and charge transport characteristics of the HTMs. PSCs fabricated with DTP-FO, DTP-FS, and DTP-FOS achieved average power conversion efficiencies (PCEs) of 20.5%, 22.5%, and 23.6%, respectively. Remarkably, the DTP-FOS-based device retained 75% of its initial efficiency after 2500 hours of continuous illumination under maximum power point tracking at 25°C. Furthermore, both DTP-FS and DTP-FOS outperformed the benchmark 2,2',7,7'-tetrakis-(*N,N*-di-4-methoxyphenylamino)-9,9'-spirobifluorene (spiro-OMeTAD) (PCE of 21.4%) not only in terms of PCE, but also in thermal and photostability, indicating their considerable potential for realizing stable and scalable PSC technologies.



HTM	J_{SC} (mA.cm^{-2})	V_{OC} (V)	FF	PCE (%)
DTP-FO	25.7	1.04	0.76	20.5
DTP-FS	25.7	1.08	0.80	22.5
DTP-FOS	25.7	1.15	0.79	23.6
Spiro-OMeTAD	25.8	1.05	0.78	21.4

Fig. 1 Chemical structures of the newly developed HTMs.

Keywords: perovskite; hole transport material; stability; efficiency.

References:

1. T. B. Raju, C. A. M. Senevirathne, M. Watanabe, Y. Fujita, D. Senba and T. Matsushima, *J. Mater. Chem. C,* 2025,**13**, 15082-15090.
2. T. Wu, T. B. Raju, J. Shang, L. Wu, J. T. Song, C. A. M. Senevirathne, A. Staykov, S. Wang, S. Ida, N. Shibayama, T. Miyasaka, T. Matsushima and Z. Guo, *Adv. Mater.*, 2025, **37**, 2414576.

3. M. Zhai, N. Shibayama, T. B. Raju, T. Wu, C. Chen, Z. Guo, T. Matsushima, T. Miyasaka and M. Cheng, *Small,* 2025, 2505961.

Designing Layered Halide Perovskites for Optoelectronics: Insights from ab initio and data-driven modeling

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ABSTRACT

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

References:

1. Nayak et al. Nano Lett, **2025**, 25, 5520
2. Ghosh et al. J. Mater. Chem. C, **2022**, 10, 9563
3. Ghosh et al. J. Mater. Chem. A **2020**, 8, 22009
4. Ghosh et al. J. Phys. Chem. Lett, **2020**, 11, 2955
5. Bhatt et al. ACS Nano, **2024,** 18, 24484

Keywords: Layered halide perovskites; ML; excited-state dynamics; carrier lifetime

Computational modelling & simulations

Design and Parametric Optimization of 4H-SiC Schottky Diode for High-Power Applications

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ABSTRACT

High-power semiconductor devices have emerged as a key component of modern power electronics, where exceptional material properties are required to ensure stable operation under extreme thermal and electrical conditions. In this work, the structure of a high-power 4H-SiC Schottky diode has been studied and optimized to achieve improved device performance. The design employs a 4H-SiC substrate because of its excellent ability to sustain high temperature and voltage stresses. A detailed parametric investigation has been performed to analyze the effect of nickel Schottky contact, epitaxial layer thickness, and doping concentration on forward current and breakdown voltage. The simulations are carried out using Silvaco TCAD software to understand the physical behavior and internal mechanisms of the device. The optimized results show a trade-off between forward current and breakdown voltage, obtained at an epitaxial layer thickness of 50 µm, doping concentration of 1×10^{15} cm^{-3}, and Schottky contact diameter of 4.8 mm. The final optimized structure shows an ideality factor of 1.02, forward current of 23A at 5V, breakdown voltage of 2750 V, leakage current of 5 uA, turn-on voltage of 0.9 V, and barrier height of 0.25eV. These results demonstrate that the optimized 4H-SiC Schottky diode can serve as a reliable high-power device for applications in power converters, rectifiers, electric vehicles, and power switching circuits.

Keywords: 4H-SiC, Schottky power diode, high-power devices, TCAD simulation.

Development of PVP:PEG-Based Solid Polymer Electrolyte for Safer Sodium Metal Batteries

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Abstract

Sodium metal batteries (SMBs) have emerged as promising alternatives to lithium-based systems due to the abundance and low cost of sodium resources. However, the use of conventional liquid electrolytes poses significant safety challenges, including flammability, leakage, and dendrite formation, which hinder their practical deployment. To address these issues, solid polymer electrolytes (SPEs) offer a safer and more stable solution by eliminating liquid components while enabling flexible and compact cell configurations. In this work, a polymer blend matrix composed of polyvinylpyrrolidone (PVP) and polyethylene glycol (PEG) is developed and optimized as the host framework for sodium-ion conduction. The PVP:PEG system is selected for its complementary properties—PVP contributes high polarity and strong sodium ion solvation, while PEG enhances segmental motion and ionic conductivity through its ether oxygen sites. The resulting SPE films are prepared via a simple solution casting method and characterized for their structural, thermal, and electrochemical properties. Fourier-transform infrared (FTIR) analysis confirms the complexation between sodium salt and polymer functional groups, while impedance spectroscopy reveals enhanced ionic conductivity with optimized PVP:PEG ratios. The developed SPE demonstrates good mechanical integrity, wide electrochemical stability, and improved interfacial compatibility with sodium metal. Overall, the PVP:PEG-based solid polymer electrolyte presents a promising pathway toward safer, more reliable, and cost-effective sodium metal batteries, aligning with the growing demand for sustainable energy storage technologies.

(Computational Modeling & Simulations)

Computational investigations on oligomeric charge transport materials having $(D_1)_n$–π–D_2 (n = 1, 2, … 5) type of molecular architecture for perovskite solar cell applications

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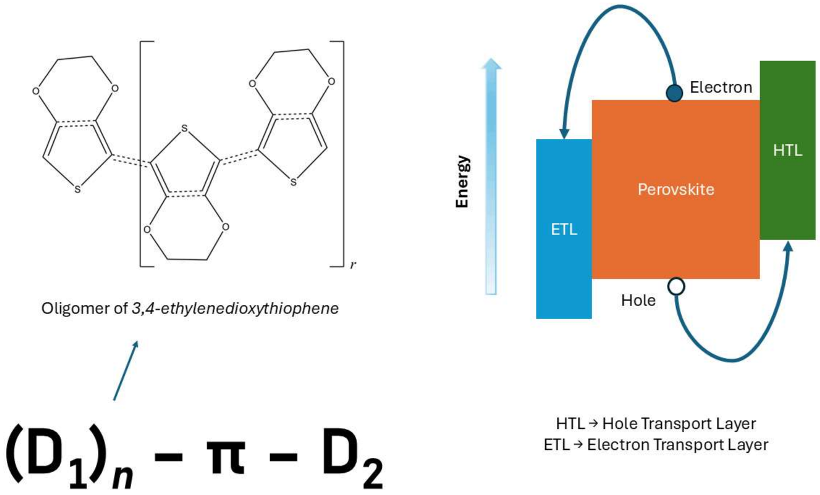
ABSTRACT



Charge transport layers facilitate extraction and movement of electrons and holes (generated by photovoltaic effect) from the active material to their respective electrodes. The corresponding materials used for transportation of electrons and holes are known as electron transport material (ETM) and hole transport material (HTM) respectively. Organic compounds based on the D–π–D structure have been widely investigated for development of HTM. In current investigation, charge transport materials based on a modified structure $(D_1)_n$–π–D_2 (n = 1, 2, … 5) have been simulated and analyzed. Here, D_1 and D_2 represent electron donor moieties which are connected together through π-conjugated bridge. The D_1 unit is composed of increasing monomers of *3,4-ethylenedioxythiophene* (EDOT) forming oligomers. *Gaussian 16W* quantum chemical software was used for simulating reorganization energies, frontier molecular orbitals and other relevant properties of title compounds. All calculations were performed using the density functional theory along with B3LYP functional and 6-31G(d,p) basis set. The properties were used to predict whether the subject molecules will behave as ETM or HTM. A theoretical perovskite based solar cell containing selected title compounds as charge transport layer was constructed. The results obtained from DFT calculations were used in the solar cell simulator SCAPS-1D to determine the output characteristics.

Keywords: Charge Transport Material; Oligomer; Electron Donor; Perovskite.

Study of Multifunctional Characterization of Titanium Dioxide Nanoparticles Synthesized via Sol–Gel Method

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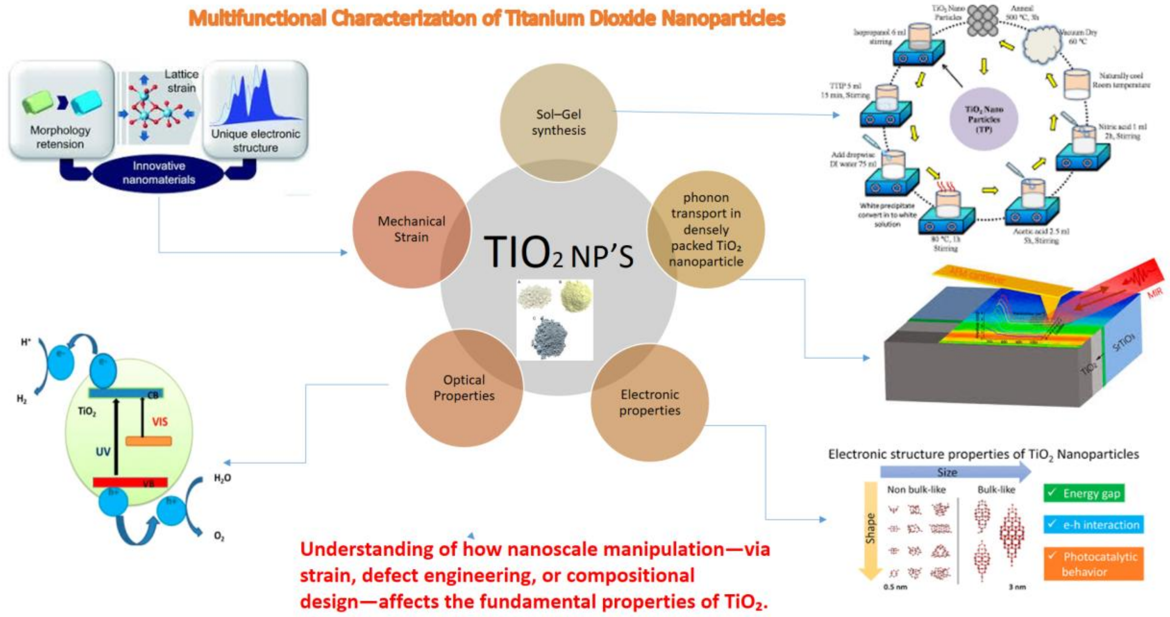
Abstract

Titanium dioxide (TiO_2) nanoparticles have emerged as multifunctional materials with exceptional physical, optical, and electronic properties, making them integral to advanced technologies in energy harvesting, catalysis, and optoelectronic systems. The present research investigates TiO_2 nanoparticles from a multifunctional perspective, exploring how structural, mechanical, and electronic factors influence their performance at the nanoscale. Study of X-ray diffraction (XRD) confirmed the formation of anatase phase TiO_2 with high crystallinity and average particle size in the nanometer range. The study encompasses several experimental approaches aimed at uncovering the interplay between structure and properties. In one direction, TiO_2 nanoparticles were embedded in a flexible polymer (PDMS) matrix to study the effect of mechanical strain on optical and electronic properties. Systematic strain application revealed measurable band gap shifts, confirmed through optical absorption and photoluminescence spectroscopy, demonstrating the feasibility of strain-engineering band structures in oxide nanomaterials. In a complementary study, core–shell TiO_2 nanoparticles with varying amorphous shell thicknesses were fabricated to explore carrier recombination dynamics using ultrafast time-resolved spectroscopy. Results indicated that the shell morphology significantly affects trap density and carrier lifetime, providing a route to control charge dynamics in photocatalytic and photovoltaic systems. Collectively, these investigations offer a comprehensive understanding of how nanoscale manipulation—via strain, defect engineering, or compositional design—affects the fundamental properties of TiO_2. The combination of sol–gel synthesis, strain modulation, ultrafast spectroscopy, and thermal-optical analysis presents a practical and scalable framework for designing multifunctional nanomaterials. This research highlights the potential of TiO_2-based systems for flexible electronics, energy-efficient devices, and next-generation quantum and optical technologies.

Keywords

Titanium dioxide, Nanoparticles, Sol–Gel synthesis, Optical, Electronic

Graphical Abstract:



A Shuttle-Free Sodium–Sulfur Battery via Effective Polysulfide Confinement Strategy

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ABSTRACT

Sodium–sulfur batteries (NaSBs) are gaining attention as next-generation rechargeable energy storage systems because of their high energy density, low cost, abundance, and environmental friendliness. However, their practical application is limited by the dissolution of sodium polysulfides in the electrolyte and the unstable sodium anode, which require excess electrolyte and sodium metal — lowering the overall energy density. Quasi-solid-state NaSBs help reduce these issues by confining sulfur in carbon matrices, but low sulfur loading (<40 wt%) and incomplete sulfur utilization (<70%) still restrict their performance. In this work, we have developed a high-loading sulfur cathode by uniformly dispersing sulfur within an oxygen-rich carbon framework through strong C–S and O–S chemical interactions. This molecular-level bonding effectively stabilizes sulfur and enhances its electrochemical activity. When combined with an all-fluorinated lean electrolyte, the system promotes a stable solid-state sodiation/desodiation process after forming a protective solid electrolyte interphase during the first cycle, completely preventing polysulfide shuttling. The optimized C/S composite delivers a high reversible capacity of 680 mAh·g ^{1} (based on total composite mass) and maintains excellent cycling stability over 400 cycles under lean electrolyte conditions. This study demonstrates that chemically bonded sulfur–carbon composites can achieve both high energy density and long cycle life, providing a promising strategy for the development of practical sodium–sulfur batteries.

Abstract Domain: Materials & coatings for batteries, super-capacitors, and fuel cells.

Study of Nickel-Doping in Mn-based Prussian Blue Analogues as High-Performance Cathodes for Sodium-Ion Batteries.

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The increasing global shift toward renewable energy necessitates efficient, cost-effective, and sustainable energy storage systems. Sodium-ion batteries (SIBs) have emerged as a promising alternative to lithium-ion technology owing to sodium's natural abundance, low cost, and similar intercalation chemistry. Among potential cathode materials, Prussian Blue Analogues (PBAs) stand out due to their open framework, facile ion diffusion, and ease of synthesis. However, their practical performance is often hindered by the Jahn–Teller distortion caused by Mn^{3+} ions, leading to lattice instability and capacity fading over prolonged cycling.

In this study, Nickel-doped Sodium Manganese Hexacyanoferrate (NaMnHCF) cathodes were synthesized via a co-precipitation route employing an ethanol-assisted solvent system, which uniquely minimizes interstitial and coordinated water content, thereby enhancing structural and electrochemical stability. Three Ni doping concentrations (0.1 M, 0.05 M, and 0.025 M) were explored to investigate the correlation between doping level, capacity, and stability. The 0.05 M Ni-doped cell exhibited a capacity retention of 78.6 % after 960 cycles, while the 0.025 M Ni-doped cell showed a capacity retention of 93.44 % after 680 cycles. While higher Ni content reduced the active Mn contribution and overall capacity, moderate Ni incorporation markedly improved structural robustness and capacity retention. The presence of Ni also promoted the formation of a stable voltage plateau, indicating suppressed degradation and improved electronic conductivity during long-term cycling. Furthermore, cyclic voltammetry (CV) analysis revealed distinct and reversible redox peaks corresponding to Fe^{2+}/Fe^{3+} and Mn^{2+}/Mn^{3+} couples, confirming multi-electron activity. X-ray diffraction confirmed the formation of a single-phase, highly crystalline cubic PBA structure, verifying the successful incorporation of Ni without the presence of secondary phases. Ongoing experiments are focused on refining the Ni concentration window to achieve an optimized balance between capacity and cyclic stability, thereby further strengthening the applicability of these materials for high-energy sodium-ion battery configurations.

Keywords: Sodium-ion batteries, Prussian Blue Analogues, Nickel doping, Ethanol-assisted synthesis, Jahn–Teller effect, Cyclic stability.

Room-Temperature Sodium-Sulfur (RT/Na-S) Batteries: Cathode Design Strategies

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Abstract

Sodium–sulfur (Na–S) batteries have attracted great attention as next-generation energy storage systems due to their high theoretical capacity, low cost, and environmental friendliness. However, their practical application is hindered by the poor electronic conductivity of sulfur and the severe polysulfide shuttle effect. To overcome these issues, iron pyrite (FeS) coated with conductive carbon (FeS @C) has been developed as an efficient cathode material. The FeS @C composite was synthesized through a simple hydrothermal process followed by carbonization, where the carbon coating not only enhances the intrinsic conductivity of FeS but also provides strong chemical interaction and physical confinement for soluble sodium polysulfides, effectively suppressing their shuttle effect during cycling. The synergistic coupling between FeS and the carbon layer facilitates fast ion/electron transport, accelerates redox kinetics, and ensures excellent structural stability. Consequently, the FeS @C cathode exhibits a high initial discharge capacity of 1003.68 mAh g^{1} and maintains a stable capacity of 590 mAh g^{1} after 25 cycles, demonstrating remarkable electrochemical reversibility and long-term cycling stability. This study highlights the potential of FeS @C composites as high-performance cathode materials for room-temperature sodium–sulfur batteries.

Keywords: sodium batteries, sodium-sulfur batteries, sulfur cathode, amorphous carbon, short chain sulfur.

(Abstract Domain: 5. Perovskite, Silicon, and CdTe thin films solar cells)

Curing temperature optimization for screen printed Silicon Heterojunction Solar Cell

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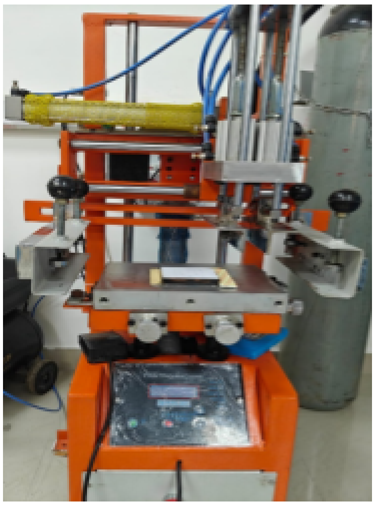
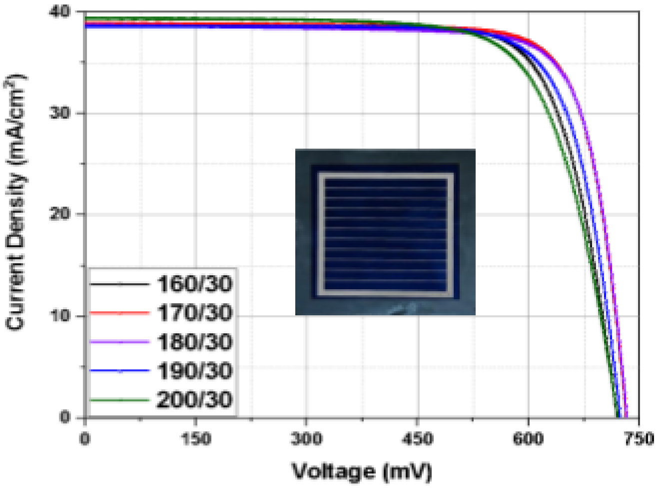
Silicon heterojunction (SHJ) solar cells have emerged as a leading photovoltaic research area, primarily due to their strong passivation, high-efficiency potential, superior temperature coefficient, higher bifaciality, and low-temperature fabrication. However, Metallization plays a vital role in solar cell parameters. Among the various metallization methods such as sputtering, thermal evaporation, e-beam evaporation, screen printing, and lithography, screen printing continues to widely use in industrial production due to its reliability, easy handling, high throughput, and low cost.

Study investigates the impact of curing temperature on solar cell parameters. Through the screen printer, width of finger, which is measured ~65 µm, giving metal coverage area ~3.57%.

At 170 ℃, optimized solar cell parameters has been achieved with the FF of 79%, and efficiency 22.49%.





Keywords: Silicon heterojunction solar cell, screen printing, curing temperature

Mitigating Interfacial Defects with Discotic Liquid Crystal Interlayer: A Dual Function Strategy for Efficient and Durable Perovskite Solar Cells

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Abstract:

Perovskite/Spiro-OMeTAD interfaces in perovskite solar cells (PSCs) are often plagued by defect states, poor wettability, and dopant induced degradation, which collectively hinder hole extraction and compromise long-term device stability. To overcome these interfacial limitations, a functional interlayer was strategically introduced to passivate defects, improve interfacial conformity, and suppress dopant diffusion. In this work, a discotic columnar liquid crystal, anti-bis(4,5-dialkoxybenzimidazole) (**PB20**), was employed as an interfacial modifier between the perovskite and Spiro-OMeTAD layers. The incorporation of **PB20** resulted in a well-organized interfacial structure that significantly enhanced film morphology and reduced interfacial trap densities, thereby serving as an effective passivation layer. The columnar stacking of **PB20** facilitated intimate interfacial contact and promoted efficient hole transfer across the perovskite/HTL interface. Consequently, **PB20** treated devices exhibited an enhanced power conversion efficiency (PCE) of 18.56 %, compared to 17.32 % for the pristine counterparts corresponding to a relative improvement of approximately 7.2 %. In terms of environmental stability, **PB20** based devices retained 82% of their initial efficiency after 60 days of storage, whereas pristine devices preserved only 58 %. This stability enhancement is attributed to the hydrophobic alkoxy side chains of **PB20,** which impart moisture resistance and effectively shield the perovskite layer from ambient degradation. Overall, the introduction of **PB20** offers a dual advantage of efficiency enhancement and durability, underscoring its potential as a robust interfacial engineering strategy for high performance perovskite solar cells.

Keywords: Perovskite solar cells, Interfacial passivation, Charge transport, Discotic Liquid Crystals, Defect Mitigation, Stability Enhancement.

“Regulating Zn^{2+} Solvation Environment using hybrid Electrolyte Engineering for Durable and Reversible Zinc Metal Batteries”

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ABSTRACT

Zinc-metal batteries (ZMBs) have emerged as viable alternatives for large-scale energy storage due to their inherent safety, economic efficiency, and significant theoretical capacity. Nonetheless, their practical application is frequently obstructed by parasitic side reactions, dendritic formation, and the constrained cycle stability of the Zn anode. In this study, we presented a dimethyl sulfoxide (DMSO)–tri-methyl phosphate (TMP)-water hybrid electrolyte that efficiently stabilises the Zn–electrolyte interface, facilitating dendrite-free and highly reversible zinc plating and stripping. The optimised hybrid electrolyte displays a minimal nucleation overpotential of merely 20 mV and showcases exceptional long-term cycle stability exceeding 3000 hours in symmetric Zn‖Zn cells, sustaining a low overpotential of 60–70 mV. The enhanced interfacial behaviour is ascribed to the controlled Zn^{2+} solvation environment and the inhibited hydrogen evolution reaction in the hybrid electrolyte system. When paired with a Ni-doped Prussian blue (Ni-PBA) cathode, the Zn‖PB full cell exhibits an initial discharge capacity of 72.5 mAh g^{-1} and maintains 78% of its capacity after 100 cycles at a C/2 rate. Furthermore, at an elevated rate of 1C, the cell shows an initial discharge capacity of 62 mAh g^{-1} and good cycling stability over 1000 cycles. The findings underscore the synergistic impact of DMSO–TMP-Water hybrid solvation in improving the reversibility of the Zn anode and the stability of the cathode, presenting a promising path for safe, high-performance, and durable zinc-based energy storage systems.

Keywords- Zinc-metal batteries, Dendrites, Overpotential, Hybrid Electrolyte

Abstract Domain: Materials & coating for batteries, super-capacitors, and fuel cells.

In The Quest For a high-capacity, air-stable layered oxide cathode for sodium ion batteries.

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The high penetration of renewable energy has led to the need for more energy storage, as sodium-ion batteries (SIBs) have emerged as a viable alternative and complementary technology to lithium-ion batteries (LIBs), sharing a similar operating mechanism and component structure. Transition metal layered oxides are identified as the most suitable electrode candidate for SBI due to their higher theoretical specific energy, abundance, and cost-effectiveness. The development of stable, high-performing layered oxide cathode materials presents a significant challenge, primarily due to the extensive diversity in their chemical compositions and intricate crystal structures. These materials are particularly susceptible to moisture exposure in open air, which can compromise their integrity and performance. In this study, titanium and manganese-based layered oxide cathodes with the general composition $Na_{.85}Ni_{.38}Zn_{.04}Mn_{.58-x}Ti_{x}o_{2}$ $(x = 0.1, 0.15\ \&\ 0.28)$ were synthesised using a conventional solid-state reaction method followed by calcination in open air. The open-air synthesis route not only simplifies fabrication but also enhances the air stability of the resulting materials by promoting uniform oxidation and structural integrity. The Ti/Mn ratio was meticulously optimized by progressively increasing the titanium content while concurrently decreasing the manganese concentration. This careful adjustment aimed to mitigate the Jahn–Teller distortion induced by Mn^{3+} ions and enhance the stability of the layered structure. X-ray diffraction (XRD) confirmed the formation of various phases in the synthesized materials, which are highly crystalline layered oxides with excellent resistance to air-induced degradation from moisture. Among the synthesised compositions, $Na_{.85}Ni_{.38}Zn_{.04}Mn_{.43}Ti_{.15}O_{2}$ was found to be the optimised sample, as compositions with relatively higher titanium content $Na_{.85}Ni_{.38}Zn_{.04}Mn_{.3}Ti_{.28}O_{2}$ and a proportionately lower titanium content $Na_{.85}Ni_{.38}Zn_{.04}Mn_{.45}Ti_{.1}O_{2}$ exhibited comparatively lower specific capacities w.r.t the optimised sample. The results demonstrate that open-air calcination, combined with optimized titanium substitution, is an effective and scalable strategy for developing air-stable and high-performance layered oxide cathodes for next-generation sodium-ion batteries.

Keywords: Energy storage, Sodium-ion, Sodium Layered oxides, open-air calcination, chemical composition.

The Role of Anions in Regulating Zn Deposition toward a Reversible and Stable Zn-Metal Anode

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Abstract

Thermodynamic instability and dendrite growth limit the commercial viability of aqueous Zn metal batteries (ZMBs). Although non-aqueous electrolytes can partially alleviate anode instability, they remain ineffective in suppressing dendrite formation. Electrolyte engineering to regulate Zn deposition offers a promising strategy for mitigating dendrites in non-aqueous systems, yet it has not been explored. In this work, the local chemistry of Zinc trifluoromethanesulfonate ($Zn(OTf)_2$) in trimethyl phosphate (TMP) electrolyte is modified with zinc chloride ($ZnCl_2$) to control Zn deposition. The presence of Cl^- alters the de-solvation dynamics of Zn^{2+}, leading to the formation of a chloride-rich interphase. Theoretical calculations suggest that Cl^- ions influence Zn^{2+} solvation, resulting in a more compact structure with higher binding energy. This promotes uniform Zn^{2+} deposition at the anode. Increasing Cl^- concentration further enhances the binding energy of the solvation shell; notably, 0.1 M Cl^- enables smooth Zn^{2+} deposition. Zn half-cells containing Cl^- exhibit stable cycling with high initial Coulombic efficiency. The effect of the co-salt anion is more pronounced in Zn||Zn symmetric cells, which demonstrate stable operation with low overpotential for over 2000 hours at 1 $mA\ cm^{-2}$. Overall, this electrolyte design approach

highlights the importance of tailored chemistries for multivalent batteries and advances the development of novel electrolytes for high-performance ZMBs.

Perovskite Solar cells

AI/ML driven studies of perovskite solar cells for Indoor Applications

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ABSTRACT

Solar energy is one of the finest renewable and abundant energy resource in 21st centuries and out of various types of solar cell technologies perovskite solar cells are favourite research field for solar cell researchers due to it's flexibility and higher efficiencies in both indoor and outdoor conditions. Metal-halide perovskites, with tunable bandgaps, low-temperature processing, and high absorption coefficients, are front-runners for this regime. However, indoor optimization is a multi-dimensional, non-convex problem spanning composition, film formation, interfaces, device architecture, and measurement protocols. AI/ML has emerged as the fastest route to navigate this design space, accelerate discovery, and enforce reproducibility. For indoor spectra, optimal single-junction bandgaps typically skew wider (1.7–2.0 eV) than outdoor PV to minimize thermalization and maximize voltage at low irradiance. ML pipelines—ranging from Gaussian-process (GP) surrogate models to neural networks (CNN/ANN)—are trained on curated datasets of A-site cations (FA/MA/Cs), mixed halides (I/Br/Cl), and B-site dopants (Pb/Sn/Ge traces) to predict phase stability, tolerance factors, and band edges. Regularization by physics-informed priors constrains the search away from segregation-prone or photo-unstable chemistries. Indoor PCE is dominated by non-radiative recombination and shunt pathways that are exacerbated at low photocurrent.. Here we are predicting band gaps by training these models for Indoor air applications. In further research we will predict the various parameters novel perovskite structures and optimization techniques

Keywords: Perovskite solar cells; Band gaps; Machine learning;

Perovskite Solar cells

AI/ML driven studies of perovskite solar cells for Indoor Applications

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Solar energy is one of the finest renewable and abundant energy resource in 21st centuries and out of various types of solar cell technologies perovskite solar cells are favourite research field for solar cell researchers due to it's flexibility and higher efficiencies in both indoor and outdoor conditions. Metal-halide perovskites, with tunable bandgaps, low-temperature processing, and high absorption coefficients, are front-runners for this regime. However, indoor optimization is a multi-dimensional, non-convex problem spanning composition, film formation, interfaces, device architecture, and measurement protocols. AI/ML has emerged as the fastest route to navigate this design space, accelerate discovery, and enforce reproducibility. For indoor spectra, optimal single-junction bandgaps typically skew wider (1.7–2.0 eV) than outdoor PV to minimize thermalization and maximize voltage at low irradiance. ML pipelines—ranging from Gaussian-process (GP) surrogate models to neural networks (CNN/ANN)—are trained on curated datasets of A-site cations (FA/MA/Cs), mixed halides (I/Br/Cl), and B-site dopants (Pb/Sn/Ge traces) to predict phase stability, tolerance factors, and band edges. Regularization by physics-informed priors constrains the search away from segregation-prone or photo-unstable chemistries. Indoor PCE is dominated by non-radiative recombination and shunt pathways that are exacerbated at low photocurrent.. Here we are predicting band gaps by training these models for Indoor air applications. In further research we will predict the various parameters novel perovskite structures and optimization techniques

Keywords: Perovskite solar cells; Band gaps; Machine learning;

Unveiling Structure–Performance Relationships in Synthetic and KS6 Graphite Cathodes for Sodium Dual-Ion Batteries

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Abstract

Rechargeable sodium dual-ion batteries are gaining interest for stationary storage applications due to their low cost, high-energy efficiency, and superlong cycle life. A comprehensive analysis is necessary to understand the intercalation and de-intercalation mechanisms of PF_6^-. This study presents a comparison between synthetic graphite (SG) and KS6 graphite as positive electrode materials in rechargeable sodium dual-ion batteries. By combining Raman spectroscopy and BET analysis, we found that the irreversibility of graphite materials is significantly influenced by factors such as porosity, surface area, and defects that can trap intercalated species within the graphite structures. Additionally, these systems are characterized using ex-situ wide-angle X-ray spectroscopy (WAXS) and atomic force microscopy (AFM) to elucidate the intercalation mechanisms of PF_6^- and stress experienced during cycling. We also investigate the electrochemical performance to understand the electrode behaviour, and X-ray photoelectron spectroscopy (XPS) is conducted to assess the impact of the cathode material on the cathode electrolyte interphase (CEI). This work provides new insights into graphitic intercalation compounds (GICs) for sodium dual-ion batteries.

Enhanced Infrared Detection Sensitivity in VO_2-Based Bolometers Through Phase Transition Engineering

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Sonika Singh[2], Ankur Goswami[1], Krishna B. Balasubramanian[1]

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Abstract

VO_2 based bolometers exhibit remarkable detection sensitivity, particularly when operated near their insulator–metal transition temperature. In this work, we demonstrate a tuneable sensitivity bolometer with an extended operational range, realized through a specially engineered gated meander device structure employing VO_2 thin films. Although the applied electric field does not directly shift the transition temperature of the meandering VO_2 microwire, it induces the formation of a two-dimensional confined electron layer at the interface. This field-induced modulation significantly enhances the photosensitivity by up to 50%, across a broad range of incident laser powers, even in the absence of external thermal bias. These findings reveal that electric-field control in VO_2 can enable low-power, high-performance bolometric operation, opening new possibilities for energy-efficient and durable infrared detection technologies.

Keywords:- Phase transition, VO_2 thin film, Micro-meander, 2-D electron gas.

References

[1] F.J. Morin, "Oxides Which Show a Metal-to-Insulator Transition at the Neel Temperature," Phys Rev Lett **3**(1), 34–36 (1959).

[2] S.A. Corr, D.P. Shoemaker, B.C. Melot, and R. Seshadri, "Real-space investigation of structural changes at the metal-insulator transition in VO 2," Phys Rev Lett **105**(5), 056404 (2010).

[3] J. Zhang, X. Tan, M. Liu, S.W. Teitelbaum, K.W. Post, F. Jin, K.A. Nelson, D.N. Basov, W. Wu, and R.D. Averitt, "Cooperative photoinduced metastable phase control in strained manganite films," Nat Mater **15**(9), 956–960 (2016).

[4] J. Cao, E. Ertekin, V. Srinivasan, W. Fan, S. Huang, H. Zheng, J.W.L. Yim, D.R. Khanal, D.F. Ogletree, J.C. Grossman, and J. Wu, "Strain engineering and one-dimensional organization of metal–insulator domains in single-crystal vanadium dioxide beams," Nat Nanotechnol **4**(11), 732–737 (2009).

(Abstract Domain: 5. Perovskite, Silicon, and CdTe thin films solar cells)

Impact of reduced wafer thickness on the performance of the Silicon Heterojunction Solar Cell.

Arnab Jyoti Mandal[1], Shahnawaz Alam[1], Silajit Manna[1], Kishan Bajpai[1], Asish Samanta[1], Niraj Yadav[1], Manisha[1], Manvendra Sigh Gangwar[1], Son Pal Singh[1], **Vamsi Krishna Komarala** [1,*]

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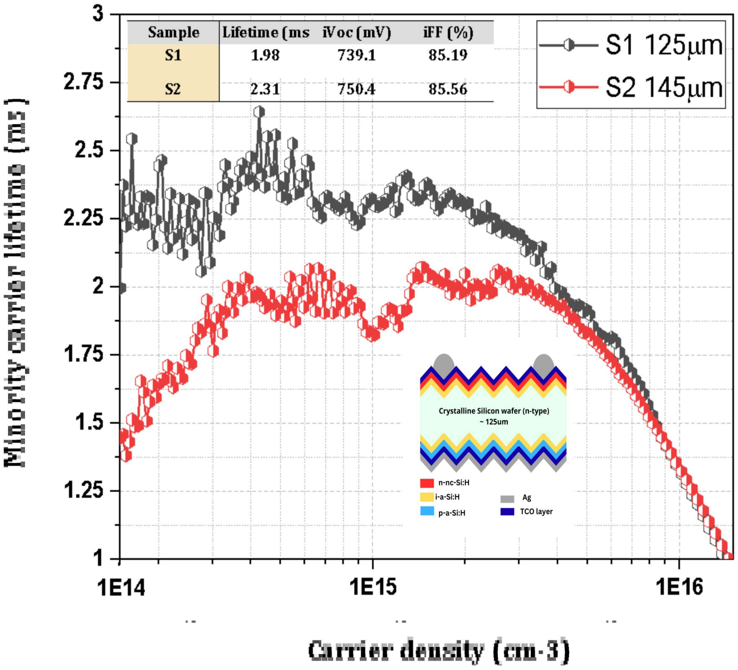
Abstract: Crystalline silicon (C-Si) wafers encounter a significant issue with saw damage during the fabrication of high-efficiency Silicon Heterojunction (SHJ) solar cells. Research has shown that it is possible to get an unwanted thin amorphous silicon phase on top of crystalline silicon (c-Si) wafers. Which, in turn, creates additional resistance for carriers. Fabrication of such c-Si wafers by slicing c-Si ingots with a diamond-edged blade or a wire saw often results in damage at the interface between the stacks. Whereas the fabrication of such ingots also contributes to the formation of similar damage. Such damages, found from surface/interface level to several micrometres deep into the wafer bulk, act as a shunting path for the generated charge carriers. This can further hinder the passivation of the silicon wafer and fail to reduce the dangling bonds. To minimise such saw damage, researchers have employed a saw damage removal (SDR) process that involves etching the silicon surface with an acid solution. This study proposes a unique ratio for the acidic SDR solution to optimise the SDR process, which mitigates the saw damage with a substantial reduction in the wafer thickness [2]. This study also highlights the additional improvements in the SHJ device performance with the processed c-Si wafers of reduced thickness. The study was conducted on the characteristics of c-Si wafers with varying wafer thicknesses by the mentioned SDR ratio, followed by the formation of a a i-a-Si:H/n-nc-Si:H/p-a-Si: H (i-p-n) stack. It was found that reducing the thickness reduces the bulk resistivity as it removes the amorphous silicon phase on the surface of the c-Si wafer. The result showed a gain in the open-circuit voltage (iVOC) of ~ 11 mV with the reduction in thickness after the i-p-n stack. Further experiments were carried out with 125 μm and 145 μm c-Si wafers, where a VOC of ~737 mV was obtained with a bulk resistivity of ~0. 65Ω.cm for the 125 μm wafer. This shows a reduction of ~ 0.2 Ω cm in the resistivity. The study was also compared using SEM images of both samples, yielding a more uniform pyramid distribution in the 125μm thin wafers. This outcome further suggests that a thin wafer can produce a higher Voc with no reduction in short-circuit current, as confirmed by the spectral response of both samples.- Such a reduction in thickness also enhances the economic viability of this technology for future industrial upscaling, resulting in reduced material usage.

Keywords: SDR; Pyramid distribution; iVoc; Resistivity.



Sample	Lifetime (ms	iVoc (mV)	iFF (%)
S1	1.98	739.1	85.19
S2	2.31	750.4	85.56

Figure 1 Minority carrier lifetime with different thickness wafer [S1-125µm & S2-145µm]

(Abstract Domain: Materials & coatings for Batteries, supercapacitor & Fuel cells)

Electrochemical properties modification by chemical pressure in Fe, Ni, and Co doped Lanthanum Silver Manganite-based electrode for Supercapacitor

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Abstract:

A-site and B-site modified manganite-based materials are promising electrodes to increase pseudocapacitance behaviour in a supercapacitor because of their rich electronic and ionic conductivity proerties due to the existence of multiple valencies of metal ions and oxygen vacancy. These properties in manganites can initiate a faradic reversible redox reaction between the electrode and electrolyte, which enhances the overall specific capacitance as well as energy density of the supercapacitor. Hence, B-doped lanthanum silver manganite (B = Nickel, Iron and Cobalt) nanoparticles are successfully synthesised to explore their redox-active pseudocapacitance behaviour in a supercapacitor. The morphological analysis of the material synthesised by the solid-state method was done by FESEM and BET analysis. Electrochemical properties have been explored using cyclic voltammetry (CV), galvanometric charge discharge (GCD) and electrochemical impedance spectroscopy (EIS). This can be explained by the changed Lanthanum-Silver Manganites' microstructure and chemical environments. The practical application of B-site and A-site modified manganites for energy storage applications in supercapacitors is demonstrated.

Keywords: Energy storage device; Perovskite oxide; Energy density; Mixed ionic and electronic conductivity.

Abstract Domain: Computational Modelling And Simulations

Design of Energy-Efficient and High-Speed 16T Hybrid Full Adder using 7nm FinFET Technology

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ABSTRACT

The primary goal of this work is to utilise simultaneous XOR–XNOR generation while eliminating the need for complementary input signals. This study introduces and analyses two compact 1-bit full adder (FA) circuit structures: a full-swing configuration and a hybrid logic-based configuration. The first hybrid adder (HFA-1) employs an XOR–XNOR module, followed by a network of pass transistors and inverters that computes the sum and carry responses. HFA-2 integrates an XOR–XNOR block followed by a pass-transistor and inverter circuitry to obtain the sum signal, with a 2–1 MUX responsible for determining the carry output. Both adders target reduced circuit complexity and significantly minimise transistor usage compared to conventional FA implementations. The circuits are realised using 7-nm FinFET devices with a 0.7-V operating voltage and verified through HSPICE simulations. The 7-nm FinFET node delivers superior electrostatic control, substantially reduced leakage, and enhanced switching efficiency compared to larger-node FinFETs and conventional CMOS technologies. As a result, circuits implemented in this technology exhibit significantly improved performance metrics, including reduced delay, lower average power consumption, and highly optimised power-delay product values. The simulation results reveal that HFA-1 achieves delay improvements ranging between 17.35% and 99.05%, PDP enhancement from approximately 57.76% to well above 100%, and average power reduction up to 34.62%. Similarly, HFA-2 demonstrates delay reduction in the same 17.35%–99.05% range, PDP improvement between 60.45% and beyond 100%, and average power savings ranging from 4.316% to 38.80%. These findings confirm that the proposed hybrid FA designs offer superior efficiency and reduced hardware complexity over existing full-adder circuits. The proposed architectures are highly suitable for next-generation nano-scale VLSI systems, particularly in applications demanding ultra-low power consumption and high-speed arithmetic computation.

Keywords: FinFET; CMOS; Hybrid Full Adder; XOR-XNOR;

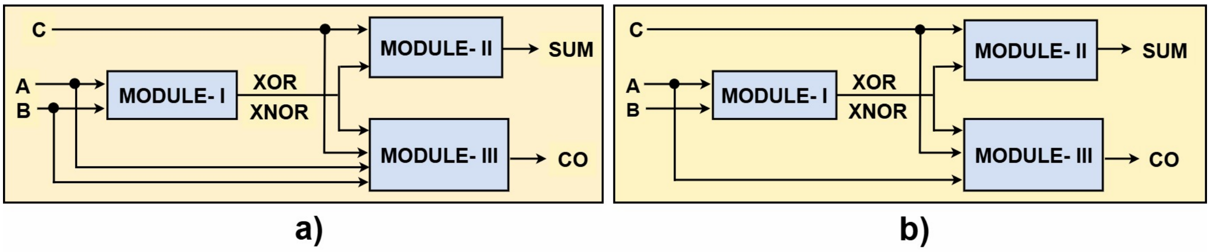

Figure. Proposed Hybrid Full Adders Schematics

Abstract Domain: Computational Modelling And Simulations

A Comprehensive TCAD Investigation of Single-Fin and Dual-Fin 3D Bulk FinFETs Across Multiple High-K Dielectric materials

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ABSTRACT

This study presents a comprehensive simulation-based investigation of Single-Fin (Conventional) and Dual-Fin FinFET architectures using the Silvaco TCAD platform to evaluate their electrical characteristics with various high-k gate dielectric materials. The analysis emphasizes the influence of different dielectrics-such as SiO_2, Si_3N_4, Al_2O_3, HfO_2, ZrO_2, La_2O_3, and TiO_2 on key device parameters including drain current (I_D), threshold voltage (Vth), subthreshold swing (SS), Ion/Ioff ratio, and Drain-Induced Barrier Lowering (DIBL). The results demonstrate that dielectric materials with higher permittivity effectively enhance gate control, minimize leakage current, and improve switching efficiency. Comparative analysis between Single-Fin and Dual-Fin structures reveals that the Dual-Fin FinFET provides superior electrostatic integrity, lower SCEs, and higher drive current, making it highly suitable for nanoscale low-power applications. The study also explores structural optimization through Fin geometry and dielectric selection to achieve improved performance, ensuring compatibility with next-generation VLSI and ultra-scaled CMOS technologies. Overall, the work establishes that the integration of high-k dielectrics in multi-fin FinFETs enables enhanced electrical efficiency, thereby paving the path for future generations of energy-efficient semiconductor devices.

Keywords: FinFET; Dual-Fin FinFET; High-k Dielectric; Short-Channel Effects (SCEs); Subthreshold Swing (SS); Threshold Voltage (Vth); Ion/Ioff Ratio; DIBL; Silvaco TCAD Simulation;

(Abstract Domain: Materials & coating for batteries, super-capacitors and fuel cells)

A Density Functional Theory Study of NbX_2 (X=Se, Te) monolayers for Electrodes of Energy Storage Devices

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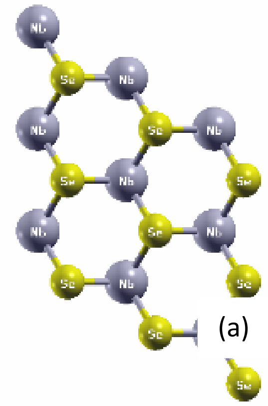
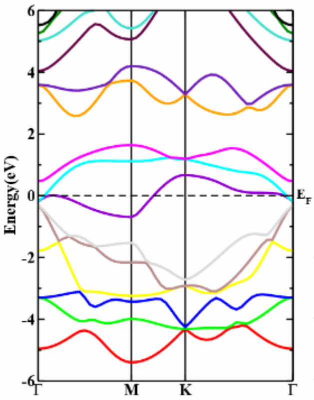
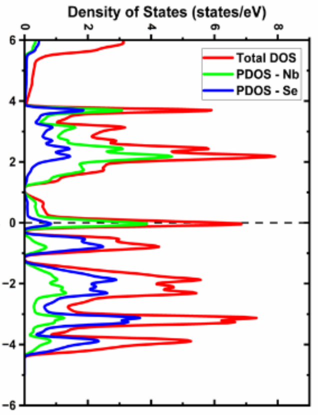
ABSTRACT

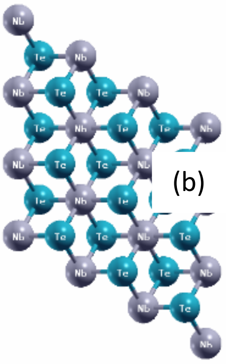
In this study, electronic, optical and thermoelectric properties of NbX_2 (2H-$NbSe_2$ and 1T-$NbTe_2$) monolayer were investigated using Density Functional Theory (DFT) calculations for electrode applications of battery and supercapacitors. The 2H-$NbSe_2$ shows a peak value of DOS (6 states/eV) near Fermi level while 1T-$NbTe_2$ has a uniform distribution of DOS. The obtained band structure and DOS indicates the metallic nature of the monolayer NbX_2 structures which indicates the suitability of these materials as electrodes of batteries and supercapacitors. The 1T-$NbTe_2$ shows very high electrical conductivity in the order of ~10^{20} $ohm^{-1}m^{-1}sec^{-1}$ when compared to 2H-$NbSe_2$ at higher chemical potentials. The high value of dielectric function (Real part) and very small energy loss function also promotes the suitability of the 1T-$NbTe_2$ material over 2H-$NbSe_2$ as a candidate for electrode applications. These observations show the applicability of the monolayer NbX_2 materials for the electrode application of energy storage devices.

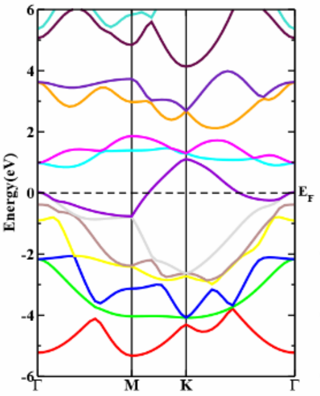
Keywords: Density Functional Theory, $NbSe_2$, $NbTe_2$, 2D-Materials;

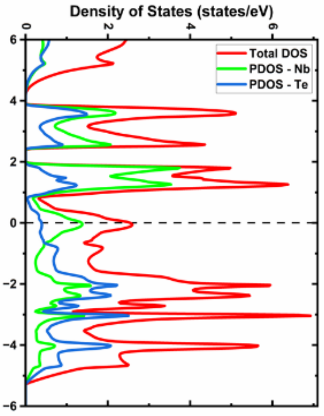












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(Abstract Domain: Perovskite, Silicon and CdTe thin films solar cells)

Numerical analysis of $CsGeI_3$-based perovskite solar cell for indoor light harvesting

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ABSTRACT

The advancement of efficient and stable photovoltaic materials for indoor applications is essential for self-sustaining portable and Internet-of-Things (IoT) gadgets. Lead-free halide perovskites have emerged as appealing substitutes for traditional absorbers due to their environmental friendliness and adjustable optoelectronic characteristics. CsGeI , an inorganic, lead-free perovskite, has a straight bandgap and robust absorption properties that align well with the emission spectra of prevalent indoor light sources such as LEDs, fluorescent lights etc. In this work, the performance of CsGeI -based perovskite solar cells (PSCs) was optimized through systematic optimisation of the absorber, hole and transport layer thickness and interface defects between different charge transport layers. The optimized device has power conversion efficiency of 44.04 %, an open-circuit voltage of 1.27 V, a current density of 2.06 mA/cm^2, and a fill factor of 87.14%, indicating its suitability for indoor light harvesting.

Keywords: Perovskite, Indoor Light harvesting, $CsGeI_3$.

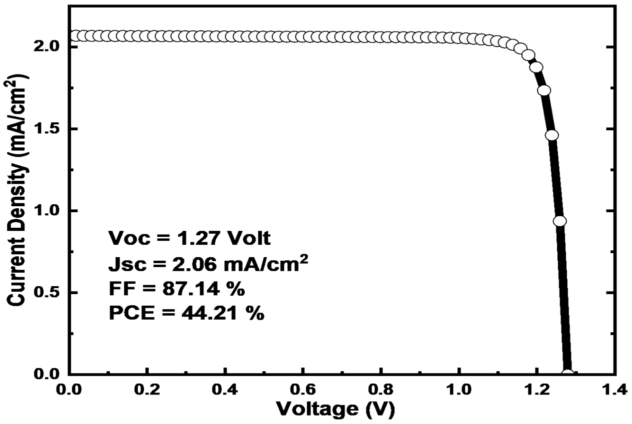

Fig: J-V curve of optimized device

Materials & coating for batteries, super-capacitors and fuel cells

Development of High Energy Density Room Temperature Na-S Batteries

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ABSTRACT

The growing need for large-scale energy storage has increased by the global shift to renewable energy and the electric based transport which results into increasing demand on lithium resources. Given lithium's finite reserves and geographically uneven distribution, it is essential to develop and investigate post-lithium battery chemistries and technologies to ensure sustainable, and low-cost energy storage solutions. Room temperature Na-S battery system is one of the promising candidates due to its high theoretical specific capacity ~840 mAh g^{-1} (at electrode level) and specific energy density of ~1230 Wh kg^{-1} [1]. Moreover, the abundance and low cost of sodium and sulfur make it a sustainable system for future battery technology. However, the sulfur cathode is electronically insulating and suffers from polysulfide dissolution leading to sluggish kinetics and severe shuttle effect [2].

Here we report a modified SPAN (sulfurized polyacrylonitrile) cathode material with a conductive element to boost the conductivity and nitrogen containing agent to reduce the polysulfide dissolution. The addition of conductive element increases the kinetics and results in a high specific capacity as compared to the reference electrode. For modified cathode a high initial discharge capacity of 2309 mAh g^{-1} is achieved in contrast to 1389 mAh g^{-1} of SPAN. Similarly, after 50th cycle, a higher discharge specific capacity was retained (1190 mA h g^{-1}) for modified cathode than that of reference SPAN (690 mA h g^{-1}). Owing to the high capacity the same amount of active material results in a higher specific energy density. We have explored the scaling up possibility by making a pouch cell with the modified electrode.

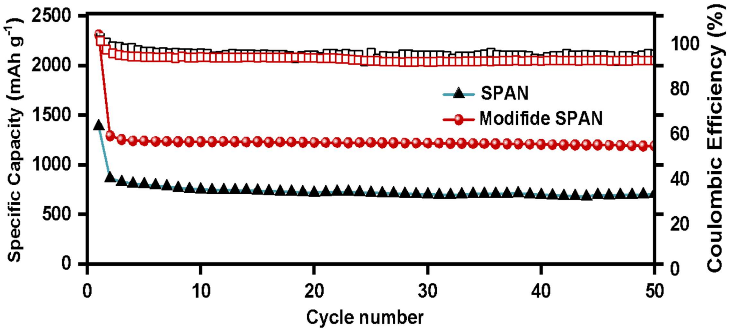

Figure: Specific capacity vs cycle life for the reference cathode and modified cathode.

1: Sungjemmenla, Soni, C. B., Vineeth, S. K. & Kumar, V.. *Mater. Adv.* **2**, 4165–4189 (2021). 2:Tang, W., Aslam, M. K. & Xu, M.. *J. Colloid Interface Sci.* **606**, 22–37 (2022).

Keywords: RT Na-S battery; High energy density; Pouch cell.

Insights into the areal loading optimization to realize the development of high-energy Na-ion Bipolar Batteries

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Abstract: Achieving higher energy density in sodium-ion batteries is challenging due to the lower specific capacity and average discharge voltage of the materials used. While connecting cells in series can increase the voltage, it also adds significant dead weight from casings and connectors, which ultimately reduces the overall energy density at the battery level. A more effective solution is the bipolar battery configuration, which increases the average voltage while minimizing dead mass compared to full cells connected in series. Recent applications have focused on combining this configuration with solid-state and gel electrolytes; however, these can hinder active material loading due to ion interactions, thereby increasing resistance. To improve energy density, a liquid electrolyte can enhance ion interactions within the cell, though careful management of electrolyte intermixing in a bipolar battery configuration is crucial to prevent cell failure. This work optimizes the carbon-coated sodium vanadium phosphate (NVP/C) slurry to achieve a material loading of 25 mg/cm². A monopolar coin cell configuration is used to optimize liquid electrolyte intake to 1 μL/mg, resulting in an energy density of 180.80 Wh/kg at the cathode. This further yields an energy density of 13.76 Wh/kg at the cell level in a single-layer bipolar battery with a pouch cell configuration.

Keywords: Li-ion, Sodium-ion, Full-Cell, Monopolar Cell, Bipolar Battery, Pouch Cell

(Abstract Domain: Computational modelling & simulations)

Improved Cavitation Characterization Using PANS on a Francis-Turbine Hydrofoil Section

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ABSTRACT

Accurate prediction of cavitation dynamics on turbomachinery blades is essential for improving the efficiency, reliability, and lifetime of hydraulic turbines operating over extended ranges. Traditional Reynolds averaged Navier Stokes (RANS) turbulence models often oversimplify unsteady vortical structures and cavitation shedding mechanisms, while fully resolved large eddy simulation (LES) remains computationally expensive for practical engineering applications. In this study, a hybrid Partially-Averaged Navier–Stokes (PANS) turbulence model is employed to numerically investigate cavitating flow over a NACA 65-021 hydrofoil, representative of Francis turbine blade sections, at an incidence angle of 9°. Schneer Saur mass-transfer model, while the interface dynamics are resolved using the Volume-of-Fluid (VOF) method.

The PANS approach demonstrates enhanced capability in resolving unsteady vortex structures and re-entrant jet behaviour compared to conventional RANS modelling, providing improved predictions. Results indicate that at 9° angle of attack, the hydrofoil experiences intensified suction-side cavitation associated with strong flow separation and vortex shedding near the trailing edge. The numerical predictions align well with experimentally reported trends, confirming the model's reliability.

This study highlights the potential of PANS as an effective compromise between RANS and LES for cavitation prediction in hydro-turbine environments, offering improved physical fidelity at moderate computational cost. The approach enables better characterization of unsteady cavitation mechanisms and hydrodynamic instabilities relevant to turbine blade erosion, vibration, and performance degradation. The findings support the integration of scale-resolving turbulence models in turbine design and optimization workflows, particularly under off-design conditions where cavitation effects are most severe.

Keywords: Cavitation; Turbulence Modelling; Hydrofoil

Exploring the Role of Fe-Doping in Enhancing the Stability and Optoelectronic Properties of Lead-Free $MASnI_3$ Perovskite Thin Films

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Abstract:

Lead-free perovskite materials such as methylammonium tin iodide ($MASnI_3$) have emerged as promising candidates for next-generation photovoltaic applications due to their narrow bandgap, high carrier mobility, and strong light absorption. However, their practical deployment is severely limited by the oxidation of Sn^{2+} to Sn^{4+}, which deteriorates structural and electronic stability. In this study, we investigate the effect of transition metal (Fe) doping on the structural, electronic, and stability characteristics of $MASnI_3$ perovskite thin films. Fe incorporation is hypothesized to modulate the local lattice environment, suppress Sn oxidation, and enhance charge transport dynamics by introducing defect tolerance within the perovskite framework. Density Functional Theory (DFT)-based simulations were employed to analyse the changes in band structure, density of states, and defect formation energies upon Fe substitution. Theoretical insights indicate that Fe doping can potentially reduce the bandgap and stabilize the Sn–I lattice network. The results aim to establish Fe doping as an intrinsic strategy to improve the air stability and device efficiency of tin-based perovskites.

Keywords: **L**ead-free perovskite, $MASnI_3$, Fe doping, Tin oxidation**,** Density Functional Theory (DFT)**,** Band structure Stability enhancement.

(Abstract Domain: 5. Perovskite, Silicon, and CdTe thin films solar cells)

Controlling Ion Flux via Substrate Biasing during ITO deposition: A Key to Preserving Passivation Quality in Silicon Heterojunction Solar Cells

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Silicon heterojunction (SHJ) solar cells leverage the excellent surface passivation properties of hydrogenated amorphous silicon (a-Si:H) to achieve high power conversion efficiencies. However, the deposition of transparent conducting oxides (TCOs), such as indium tin oxide (ITO), via sputtering often results in degradation of these passivation layers due to energetic ion bombardment. This sputter-induced damage increases interface defect densities and recombination velocities, ultimately reducing cell performance. A critical yet often overlooked process parameter influencing ion flux is the electrical potential of the substrate during TCO deposition. When the substrate is left electrically floating, uncontrolled surface charging leads to enhanced ion acceleration and higher energy ion flux onto the passivated layers. In contrast, grounding the substrate provides control over the stability of its surface potential and reduces ion energy impact, significantly preserving the passivation quality.

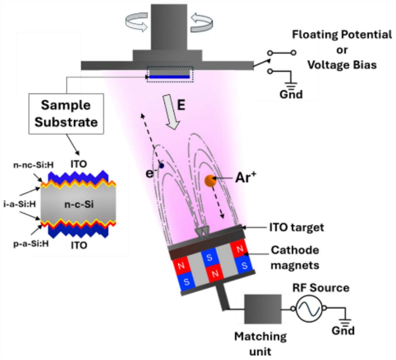

Figure 1: Schematic diagram of the sputtering system incorporating the substrate bias

This study investigates how grounding the substrate during ITO sputtering in SHJ solar cells reduces local plasma ionization and weakens sheath potential near the substrate surface, thereby lowering both ion flux and secondary ion energy incident on the passivation layer and effectively mitigating sputter-induced damage. Quantitative analysis reveals that under floating substrate conditions, effective carrier lifetime drops from 2.3 ms to 1.1 ms, with a slight decline in iVoc from 739.5 mV to 733.0 mV, and iFF falling from 85.7% to 83.9% after ITO deposition. In contrast, grounding the substrate during sputtering leads to superior preservation of device performance, with carrier lifetime decreasing only marginally from 2.3 ms to 2.0 ms. At the same time, iVoc slightly improves from 738.8 mV to 742.5 mV, and iFF remains stable at 85.9%. These results underscore the effectiveness of substrate grounding in mitigating sputter-induced passivation damage, offering a robust and scalable approach for high-efficiency SHJ solar cell fabrication.

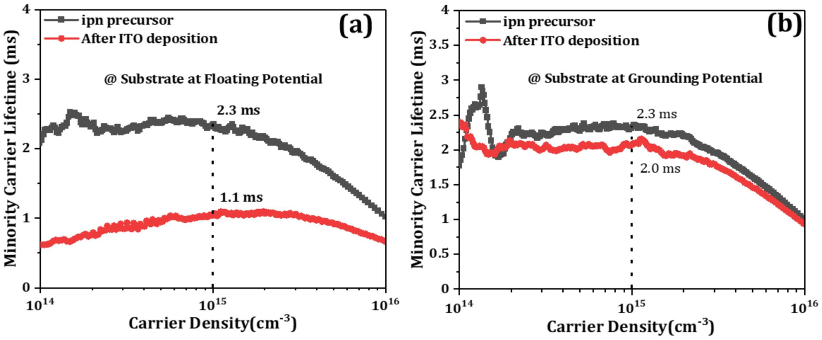

Figure 2: Reduction in minority carrier lifetime (a) under floating potential (b) under grounding potential

Keywords: Silicon heterojunction solar cell, sputter-induced damage, transparent conducting oxides

Tailoring the electronic structure and morphology of TiO_2 nanoparticle using glycerol: Magnetic field enhanced photocatalysis

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Metal oxides play a major role in photocatalytic applications due to their tunable electronic, optical properties, chemical and thermal stability. Titanium dioxide (TiO_2) has drawn a lot of interest from the past 70 decades due to its affordability, cost-effectiveness, excellent oxidising capability, and low toxicity. TiO_2 generates the electron-hole pairs under illumination, and the rapid recombination reduces the efficiency of the sample, which is a great challenge for TiO_2 as a photocatalyst. To overcome this challenge, glycerol treatment was introduced to TiO_2 to improve surface reactions, enhance electron-hole pair lifetime, and facilitate more efficient charge transfer. Furthermore, the application of an external magnetic field was used to promote the photocatalytic efficiency.

Glycerol-modified TiO_2 was synthesised using the solvothermal method. The glycerol modification induces the morphology transformation from spheres to nanorod flowers, which enhances the surface reactivity. Further, the electrochemical measurements, including Cyclic voltammetry, Electrochemical Impedance Spectroscopy (EIS), Nyquist plot and Mott-Schottky measurements, show that the glycerol-modified sample exhibited higher peak current responses, lower charge transfer resistance, and good linearity across varying scan rates and lower flat band potential. Among the synthesised samples, the glycerol-modified sample achieved an 80% degradation efficiency under combined magnetic field assistance and light irradiation.

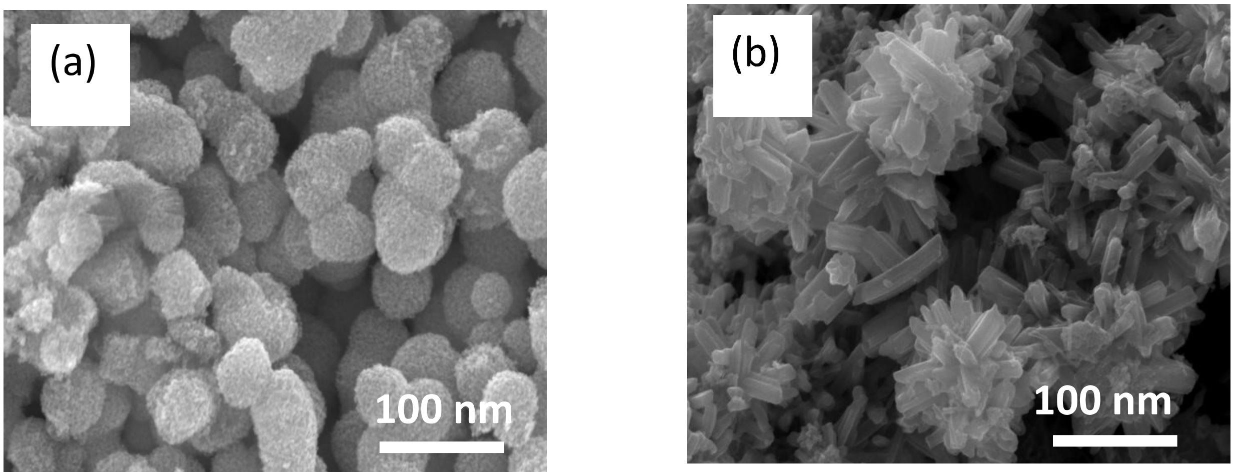

Figure: HR-SEM images of (a) untreated TiO_2 spheres, (b) glycerol-modified TiO_2 nanorods flowers

(Abstract Domain : Perovskite, Silicon, and CdTe thin films solar cells)

Performance of mixed cation-mixed halide perovskite solar cell under Indoor Illumination

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ABSTRACT

Highly efficient mixed cation perovskites have shown good stability but usually it contains methylammonium (MA) cation which is not thermally stable. FA and Cs-based perovskites are recently in focus as they perform well, exhibit excellent thermal stability, and easy bandgap tunability achieved by adjusting the halide content. Recently, indoor perovskite solar cells (IPSCs) have emerged as a promising candidate for powering low-power electronic devices and IoT sensors. Here, a mixed-cation mixed-halide perovskite $FA_{0.75}Cs_{0.25}Pb(I_{0.8}Br_{0.2})_3$ has been optimized under air ambient conditions as a potential absorber for IPSCs. The perovskite films were deposited using a three-step spin-coating process with an antisolvent treatment by a green antisolvent, anisole, followed by annealing at different temperatures (100 °C, 120 °C, 140 °C, and 160 °C) to optimize the film properties. The optimized perovskite film, annealed at 140 °C, exhibiting a bandgap of ~1.68 eV, making it suitable for indoor light harvesting and as a potential top cell absorber in tandem PSCs. With increasing annealing temperature, a PbI_2 peak emerges at 12.7°, prominently observed in the 160 °C-annealed sample. An increase in annealing temperature leads to a shift of XRD peaks toward lower 2θ angles. The 140 °C-annealed sample shows the highest peak intensity, confirming superior crystallinity at the optimal annealing condition. In place of the conventional HTM spiro-OMeTAD, a low-cost and more stable alternative, TOP-3, was utilized in the device. Furthermore, the conventional HTM solvent chlorobenzene was substituted with a less toxic and more environmentally benign alternative, anisole. The optimized device exhibited a power conversion efficiency (PCE) of 13.18% under standard AM1.5G illumination. The device containing the 140 °C-annealed perovskite exhibited a PCE of 25.44% under cool white LED illumination (6500 K), confirming excellent performance under indoor illumination.

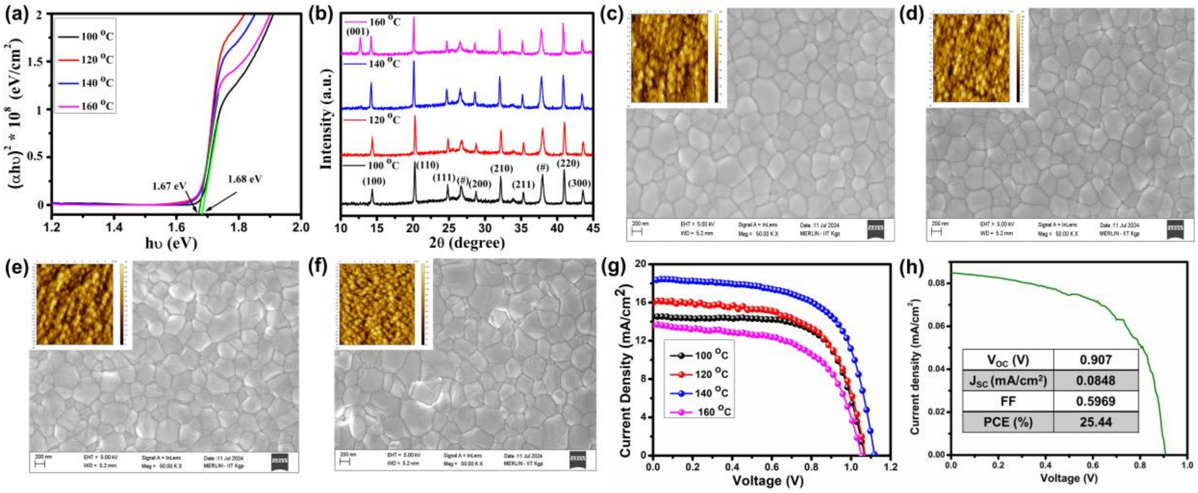

Figure 1: (a) Tauc plots and (b) XRD patterns of $FA_{0.75}Cs_{0.25}Pb(I_{0.8}Br_{0.2})_3$ films annealed at different temperatures. (c–f) SEM images with AFM insets of films annealed at 100 °C, 120 °C, 140 °C, and 160 °C. (g) *J–V* characteristics under 1 Sun for all temperatures. (h) Indoor J–V curve under 6500 K LED for the optimized (140 °C) device.

Bibliography

Mishra, S., Ghosh, S., Boro, B., Kumar, D., Porwal, S., Paul, M., ... & Singh, T. (2022). Solution-processed next generation thin film solar cells for indoor light applications. Energy Advances, 1(11), 761-792.

Boro, B. *et al.* Thermal Stability Analysis of Formamidinium–Cesium-Based Lead Halide Perovskite Solar

Cells Fabricated under Air Ambient Conditions. *Energy Technol.* **n/a**, 2400034

Nishimura, H. *et al.* Additive-free, Cost-Effective Hole-Transporting Materials for Perovskite Solar Cells Based on Vinyl Triarylamines. *ACS Appl. Mater. Interfaces* **12**, 32994–33003 (2020).

Keywords: Perovskite Solar Cell; Indoor Photovoltaics; Thin film; Green Solvent;

Materials & coating for batteries, super-capacitors and fuel cells

Tailoring the solvation through molecular engineering in a blend quasi-solid polymer electrolyte for a high-performance sodium metal battery

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ABSTRACT

The quest for quasi-solid polymer electrolytes (QSPEs) for high-performance sodium metal batteries is considered promising. However, poor electrode-electrolyte interface with low ionic conductivity and transference number limits its employment in sodium metal batteries. To overcome this limitation, poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) based QSPE is developed. Molecular engineering is enabled by introducing electron-withdrawing groups in the system. This directly enhanced the room-temperature ionic conductivity (~1.01 mS cm^{-1}), and transference number (0.78), and widened the electrochemical stability window to ~5 V. Furthermore, the developed system favoured aggregate ion pairs, which are decisive for the formation of inorganic-rich interphase. Symmetric cells based on sodium stably functioned over 200 hrs at a high current density of 1 mA cm^{-2}. Moreover, the SMB based on an in-house fabricated Prussian blue cathode demonstrated performance over 500 cycles, with a high initial capacity of 159 mAh g-1 at 0.5 C, and exhibited an average Coulombic efficiency of ~98%. Overall, the concept of molecular engineering strategy was shown to be an effective solution to catalyse the growth of various QSPE-based high-performance SMB systems.

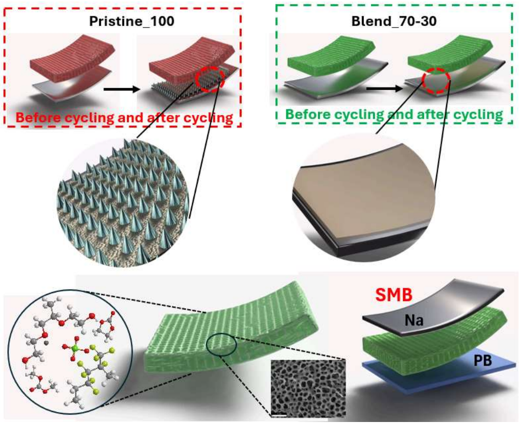

Figure: Schematic representation of molecular engineered blend QSPE for SMB application

Keywords: Quasi-solid Polymer Electrolytes • Electrode- Electrolyte Interface • Sodium Metal battery

(Abstract Domain: Computational modelling & simulations)

Wind Resource Assessment and Energy Potential in the Rann of Kutch, India, Using WAsP Software

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ABSTRACT

The Rann of Kutch, located in western India, is identified as a potential region for large-scale wind energy development in support of India's renewable energy goals for 2030. This study presents a numerical assessment of wind resource characteristics and energy potential using the Wind Atlas Analysis and Application Program (WAsP). A long-period dataset of near-surface wind parameters from the ERA5 Global Wind Atlas was analyzed to establish the regional wind climatology. Key parameters including mean wind speed, prevailing wind direction, wind shear, turbulence intensity, and wind ramp characteristics were evaluated. WAsP was employed to generate site-specific wind atlases and energy maps. The workflow involved transforming ERA5 reanalysis data into generalized wind climates, applying terrain and roughness corrections using digital elevation and land cover inputs, and simulating microscale flow patterns through the WAsP linear flow model. Energy yield estimations were then performed by integrating turbine power curves, wake effects, and long-term wind statistics to calculate the Annual Energy Production (AEP). The findings suggest that the Rann of Kutch exhibits significant wind energy potential suitable for future utility-scale projects. The study demonstrates the effectiveness of WAsP-based numerical modeling as a reliable pre-feasibility tool for wind resource evaluation, site selection, and investment planning in India's expanding wind energy sector.

Keywords: Wind Resource Assessment; WAsP Software; Rann of Kutch; Annual Energy Production.

(Abstract Domain: Thin Films Growth, Novel techniques and concepts)

Enhancement of Anomalous Hall Angle in Cr-rich Cr_xTe_y

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ABSTRACT

Over the past years, 2D materials like graphene, transition metal dichalcogenides (TMDs) and silicene provided a promising platform for advancing spintronics research. These materials possess spin-dependent properties such as prolonged spin relaxation time, Rashba spin-orbit coupling, spin-valley locking, and quantum Hall effect. The recent discovery of intrinsic 2D ferromagnetism in CrI_3 and $Cr_2Ge_2Te_6$ led to the exploration of transition metal chalcogenides (TMCs) for they provide an approach to modulate their properties in the 2D-regime. The TMCs have the chemical formula M_mX_n (where M could be any transition metal like Fe, Co, Cr, Mn, etc. & X could be any chalcogens like O, S, Se, and Te). The 2D TMCs thin films have emerged as a new avenue for exploring exotic electronic, magnetic, and topological behaviors by controlling their composition, layer thickness, doping, strain, and proximity effect [1]. Among the TMCs, Chromium Tellurides (Cr_xTe_y) have drawn significant attention due to their tunable Curie temperature (T_c), anomalous Hall effect, and magnetic anisotropy which can be manipulated by varying composition of Te, film strain, growth temperature, and film thickness. The Cr_xTe_y family offers a range of stable compositions, like CrTe, $CrTe_2$, Cr_2Te_3, Cr_3Te_4, and Cr_7Te_8 which exhibit intrinsic ferromagnetism with T_c that can be scaled up to room temperature and their ferromagnetism can persist with decreasing thickness down to monolayer limit [2]. However, intercalation of Cr-atom within the unit cell of a particular phase of Cr_xTe_y affect the overall magnetic properties of that phase and consequently, alter T_c and magneto-transport properties.

In this study, we present the successful synthesis of Cr-rich Cr_xTe_y via DC-magnetron co-sputtering and their structural, morphological and magnetic characterizations. To see the effect of composition, we have varied the composition of Te by changing sputtering power of Te at the same growth conditions. Analysis of glancing incidence X-ray diffraction patterns reveal the monoclinic crystal structure of these films. The magnetization vs. temperature measurement shows the T_c of the grown films close to room temperature (300K). Furthermore, we have concluded from Hall effect measurements that the anomalous Hall angle is enhanced from **1.25%** to **3.35%** as we move towards higher Cr:Te ratio. This study provides the critical information on the tunning of anomalous Hall angle in Cr_xTe_y family.

Keywords: Transition metal chalcogenides, Ferromagnet, Anomalous Hall angle.

References:

[1] B. Zhao, D. Shen, Z. Zhang, P. Lu, M. Hossain, J. Li, B. Li, X. Duan, 2D Metallic Transition-Metal Dichalcogenides: Structures, Synthesis, Properties, and Applications, Adv Funct Mater 31 (2021).

[2] L. Meng, Z. Zhou, M. Xu, S. Yang, K. Si, L. Liu, X. Wang, H. Jiang, B. Li, P. Qin, P. Zhang, J. Wang, Z. Liu, P. Tang, Y. Ye, W. Zhou, L. Bao, H.J. Gao, Y. Gong, Anomalous thickness dependence of Curie temperature in air-stable two-dimensional ferromagnetic 1T-CrTe2 grown by chemical vapor deposition, Nat Commun 12 (2021).

(Abstract Domain: Coating materials for wind and hydro turbine blades)

Characterization of HVOF-sprayed Co-NiCrAlY-Al_2O_3 coatings with variable ceramic fraction for erosion behaviour evaluation of hydraulic turbine steel

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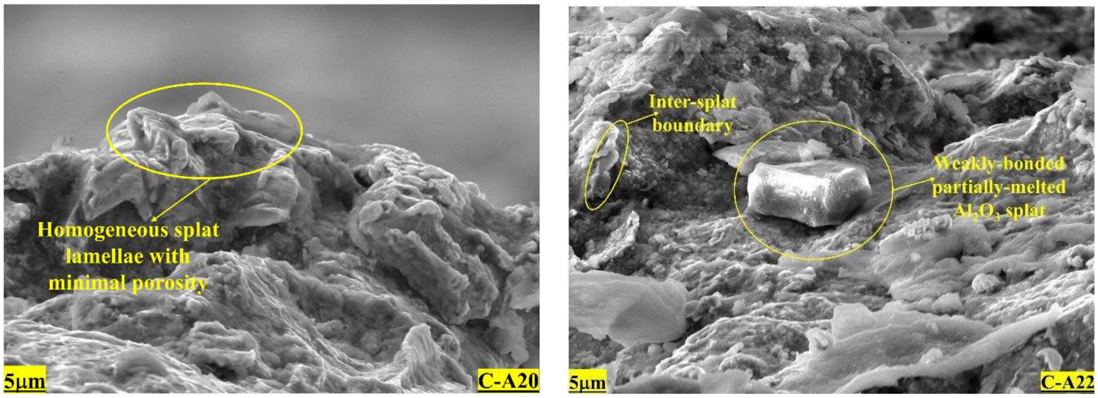
ABSTRACT

Erosion of hydraulic turbine components remains a critical issue in sediment-laden hydropower plants, primarily caused by the continuous impingement of hard silt particles suspended in the water flow. This erosive wear leads to a gradual loss of material, surface roughening, and efficiency deterioration of the turbine. To minimize this problem, the present work investigates the development and characterization of CoNiCrAlY-Al_2O_3 composite coatings, to improve the erosion resistance and surface reliability of turbine steel operating in sediment-laden environments. The HVOF technique is employed to deposit the coatings on 18Cr8Ni turbine-grade stainless steel substrates, yielding strongly bonded coatings with stable metallurgical characteristics. Two different coating compositions (C-A20 and C-A22) are developed by varying the Al_2O_3 percentage within the CoNiCrAlY matrix to attain an optimal combination of hardness, ductility, and interfacial bonding characteristics.

Comprehensive microstructural and metallurgical characterizations are performed using scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD) to assess particle morphology, splat bonding, porosity distribution, and phase stability. Mechanical characterization involves Vickers microhardness and contact angle measurements to evaluate surface hardness and wettability. Slurry erosion experiments are carried out to examine the effect of impact angle and velocity on the erosion performance of both bare and coated specimens. The tests were conducted at impact angles of 30°, 45°, 60°, and 90°, and velocities ranging from 6 to 12 m/s under controlled conditions using a slurry erosion tester.

Results indicate that the HVOF-sprayed coatings significantly enhanced erosion resistance compared to the uncoated turbine steel. Between both the compositions and bare substrate, coating containing 20% Al_2O_3 (C-A20) shows the best erosion-resistive performance. This improvement is attributed to an effective balance of mechanical properties, wherein the hard ceramic phase provides surface protection against abrasive wear, while the ductile CoNiCrAlY matrix absorbs impact energy and suppresses crack propagation. The combined action of these two phases results in reduced material loss and enhanced surface stability under slurry erosion conditions.



(a) (b)

Keywords: CoNiCrAlY; Al_2O_3; HVOF; Erosion

(Abstract Domain: Computational modelling & simulations)

Influence of a Wind-Lens on the Aerodynamic Performance and Flow Behaviour of a Horizontal Axis Wind Turbine

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ABSTRACT

The influence of a wind-lens on the aerodynamic performance of a horizontal axis wind turbine is investigated using two-dimensional computational fluid dynamics simulations. The study focuses on analysing the flow behaviour and pressure distribution around a cycloidal-profile diffuser equipped with a circular brim to understand its role in enhancing flow acceleration and power augmentation. The unsteady Reynolds-Averaged Navier–Stokes equations, coupled with the SST k–ω turbulence model, are employed to capture unsteady aerodynamic phenomena such as vortex formation and low-pressure region development behind the brim. The computational domain is sufficiently extended to minimize blockage effects, and a refined structured mesh is employed near the shroud and throat regions. Simulations are performed for multiple geometric configurations to examine the influence of brim height on flow acceleration, pressure distribution, and potential power augmentation relative to a bare wind turbine. The preliminary results shows that wind lens effectively enhanced suction at the diffuser exit and significantly increased the axial velocity and mass flow rate through the throat compared to the baseline turbine condition. Stable vortices formed near the brim generated a sustained low-pressure region downstream, strengthening the suction effect and accelerating the incoming airflow. Further increase in the brim height amplified flow entrainment, leading to greater velocity augmentation and improved aerodynamic performance. These findings provide valuable insights for the design and optimization of compact, high efficiency wind lens turbines suitable for distributed and urban renewable energy applications.

Keywords: Wind lens, Flow acceleration; Power augmentation

(Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts)

Large anomalous Hall effect in sputtered Iron Silicon alloy thin films

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The control and creation of pure spin current are critical for the evolution of next-generation spintronics technologies, such as Magnetic Random-Access Memories (MRAMs) and neuromorphic devices. Rare earth elements, particularly when combined with expensive heavy metals, exhibit novel spin phenomena such as the topological Hall effect and spin Hall effect, which are essential for these applications. However, the growing need for increased data storage capacity, along with the scarcity of crucial rare-earth elements, underscores the urgent requirement to develop novel magnetic materials that are free of rare-earth and other expensive components while still exhibiting exotic spin phenomena. This crucial need encourages research and innovation to discover new magnetic materials that utilize abundant and economically feasible resources, ensuring long-term technological growth.

The binary iron silicide alloy, a rare earth-free material system, hosts a rich gamut of compounds such as Fe_3Si, Fe_5Si_3, Fe_2Si, FeSi and $FeSi_2$, which showcase exotic magnetic phenomena ranging from excellent soft magnetic properties and half metallicity to unusual magnetic characteristics, which makes them potentially interesting for their fundamental understanding as well as their technological applications. For a considerable period, Fe_5Si_3 was regarded as a weakly ferromagnetic bulk material characterised by low magnetisation, rendering it unsuitable for practical applications. However, recent studies have significantly heightened interest in this material, demonstrating its *diverse topological spin textures*[1] and a *high spin Hall angle*[2] in nanostructured form. These findings have revitalised the potential of Fe_5Si_3 for advanced spintronic applications, warranting further investigation into its properties and potential uses.

In this study, we investigate the structural and magnetotransport properties of direct current magnetron-sputtered Fe_5Si_3 thin films with thicknesses ranging from 100 nm to 20 nm. The electrical transport measurements confirm the metallic nature of these Fe_5Si_3 thin films. Glancing incidence X-ray diffraction (XRD) patterns revealed the hexagonal structure of these films. The temperature dependency of differential magnetization (dM/dT) in the Fe_5Si_3 samples corroborates a Curie temperature (T_c) of **365 K**, consistent with the previously reported values[1]. Additionally, the coercive field and saturation magnetization for in-plane orientation of the applied magnetic field are determined to be **80 Oe** and **7.9 μ_B/f.u.** at 300 K, respectively. A *remarkably high value of anomalous Hall resistivity* of **3.47 μΩ·cm** is observed at 300 K in 50 nm thin Fe_5Si_3 films. These findings are crucial for understanding the properties of Fe_5Si_3 and are expected to stimulate further research into rare-earth-free innovative materials within the field of spintronics.

References:

[1] X. Feng, S. Yan, X. Zhang, L. Yin, H. Wang, Y. Wen, J. Yao, H. Wang, R. Cheng, Z. Li, J. He, Spontaneous Skyrmion Bubbles in an Iron-Silicon Alloy with Uniaxial Magnetic Anisotropy, ACS Nano (2024). https://doi.org/10.1021/acsnano.4c00658.

[2] K.D. Belashchenko, Exchange-driven spin Hall effect in anisotropic ferromagnets, Phys Rev B 109 (2024) 1–9. https://doi.org/10.1103/PhysRevB.109.054409.

Keywords: Spintronics, Iron Silicon alloy, Anomalous Hall Resistivity

(Abstract Domain: Computational modelling and simulations)

Investigation of the deposition parameters for simulating the growth dynamics of vanadium carbide nanosheet in plasma enhanced chemical vapour deposition system

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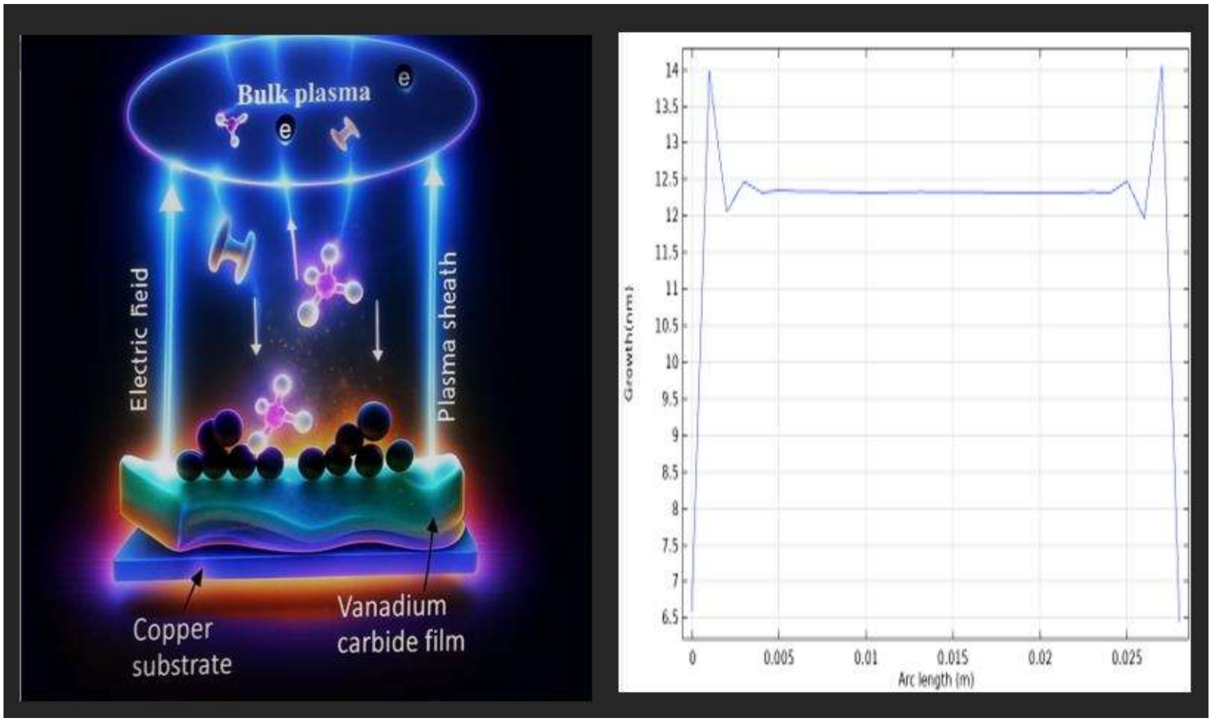
ABSTRACT

The aim of the present study is to develop a computational model to investigate the influence of process parameters on the growth kinetics of vanadium carbide nanosheet in the reactive plasma environment consisting of hydrogen, argon, methane gas mixture. A two dimensional axisymmetric inductively coupled plasma module in COMSOL Multiphysics simulation software was utilized for the simulation. The simulation results indicates that process parameters have direct impact on both the plasma characteristics and growth aspects of the nanosheet. The effect of gas pressure was examined and the results reveal that the electron density and electron temperature decreases with increasing gas pressure while neutral number density increases. Furthermore, the growth of vanadium carbide nanosheet was found to increase with increasing the gas pressure. These findings align well with the experimental observations, thereby validating the developed model.

Keywords: PECVD ; COMSOL; Vanadium carbide nanosheet; Gas pressure.



Electrodeposition and Characterization of galfenol (Fe$_{80}$Ga$_{20}$)

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ABSTRACT

FeGa (Galfenol) is a promising functional material owing to its exceptional magnetic and mechanical properties. It exhibits a magnetostrictive constant of approximately 400 ppm, which is significantly higher than that of conventional magnetostrictive materials such as Fe, Co, or Ni alloys. Furthermore it possesses superior mechanical resilience and a lower saturation magnetization compared to Terfenol-D which is another giant magnetostrictive material known for its brittleness. This unique combination of properties makes it highly suitable for sensor and actuator applications, particularly in MEMS-based devices.Electrodeposition of FeGa (Galfenol) thin films offers distinct advantages over conventional vacuum-based techniques, including low cost, high deposition rate, and the ability to uniformly coat large or non-planar surfaces. Additionally, electrodeposition is a non-line-of-sight process that enables *in situ* growth of active layers, facilitating efficient device integration.In this study, FeGa (Galfenol) thin films were synthesized via electrodeposition using an electrolytic bath containing 0.5 M gallium sulphate, 0.5 M boric acid, 0.15 M sodium citrate, 0.3 M ferrous sulphate, and 0.2 M sodium sulphate in a 20 mL solution. The solution was stirred at 100 rpm for 20 minutes to ensure homogeneity. A platinum mesh served as the anode, while the cathode was a Si/Ti/Ag substrate prepared via electron-beam deposition and diced into 1 cm × 1.5 cm pieces, with an active deposition area of 1 cm × 1 cm. Electrodeposition was carried out at current densities of 15, 30, 45, and 60 mA/cm^2 for 30 minutes each.A noticeable increase in film thickness was observed with increasing current density, demonstrating effective control of film growth through current modulation. At a current density of 45 mA/cm^2, the measured film thickness was approximately 5 µm after 30 minutes of deposition, corresponding to a deposition rate of about 0.1667 µm per minute. Significant variations in magnetic parameters were also recorded, indicating a strong dependence of the structural and magnetic properties of FeGa (Galfenol) thin films on the applied current density.

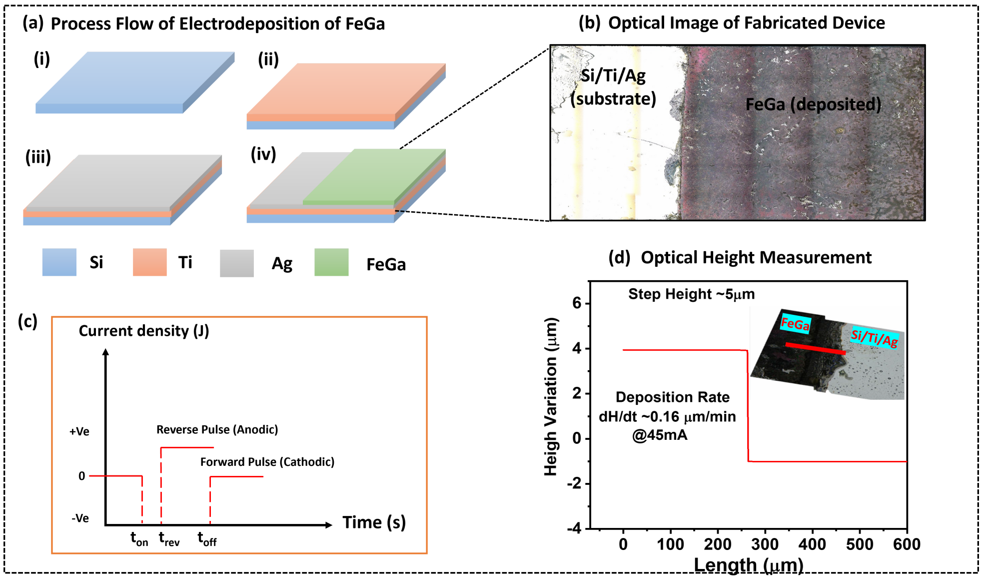

Figure 1: Process Flow of Electrodeposition of FeGa

(Abstract Domain 1: Thin films/Nano-materials Growth, Novel techniques and concepts)

Type II Based Tise$_2$/Tio$_2$ Heterostructures for Hydrogen Evolution Reactions (HER)

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ABSTRACT

The hydrogen evolution reaction (HER) confers a sustainable method for producing hydrogen. The main goal of this work is to create a type-II heterostructure based on titanium diselenide/titanium dioxide ($TiSe_2/TiO_2$). For $TiSe_2$, selenium and titanium oxide powder were used via Chemical vapour deposition (CVD) on silicon and for TiO_2, hydrothermal synthesis in order to increase HER control. TiO_2 nanorods are combined with transition metal dichalcogenides, such as $TiSe_2$, which are renowned for their exceptional qualities, to create a potent photocatalytic system. Field-emission scanning electron microscopy (FE-SEM), Raman spectroscopy, and X-ray diffraction (XRD) were among the characterization methods used. Both ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS) provide a broad understanding of charge transport kinetics and electronic interactions. The UPS experiments demonstrate that an improvement in catalytic active sites is defined by a shift in peak positions in XPS spectra. It was confirmed that the heterostructure's enhanced energy environment to start the charge transfer strengthened the creation of hydrogen. According to the UPS research, the heterostructure minimum work function ($TiSe_2$) calls for improvement in charge transfer. $TiSe_2/TiO_2$ heterostructure is therefore deemed a likely material for sustainable hydrogen generation.

Keywords: $TiSe_2/TiO_2$ heterostructure; Chemical vapour deposition; Hydrothermal synthesis.

References:

[1] Dawood F, Anda M, Shafiullah GM. Hydrogen production for energy: an overview. Int J Hydrogen Energy Feb. 07, 2020;45(7):3847–69. https://doi.org/10.1016/j. ijhydene.2019.12.059. Elsevier Ltd.

[2] Lasia A. Mechanism and kinetics of the hydrogen evolution reaction. Int J Hydrogen Energy Jul. 26, 2019;44(36):19484–518.https://doi.org/10.1016/j. ijhydene.2019.05.183. Elsevier Ltd.

[3] Dincer I, Acar C. Review and evaluation of hydrogen production methods for better sustainability. Int J Hydrogen Energy Aug. 2014;40(34):11094–111.https://doi. org/10.1016/j.ijhydene.2014.12.035.

Avaada Electro's Vision for Next-Generation Solar Cell Efficiency: Advancing from Industrial TOPCon to Next-Generation Tandem Architectures

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ABSTRACT

Avaada Electro Pvt. Ltd. is actively advancing high-efficiency crystalline-silicon solar cell technologies to support India's accelerating renewable-energy expansion and global competitiveness in PV cell manufacturing. This presentation outlines Avaada Electro's multi-stage R&D roadmap aimed at continuous solar-cell efficiency enhancement, beginning with industrial TOPCon (Tunnel Oxide Passivated Contact) development and extending toward emerging tandem solar-cell architectures.

Our current focus includes optimizing Edge-Passivation Deposition (EPD) TOPCon cells, implementing poly-finger and exploring bi-poly for reducing the optical losses, and zero-busbar (ZBB) metallization schemes to enable higher current collection and improved module-level aesthetics. These technology upgrades are being designed to align with scalable, cost-effective industrial production.

As part of Avaada's long-term innovation strategy, we are establishing a collaborative framework with national and international academic institutions to advance materials research, device modelling, advanced characterization, and pilot-scale prototyping. The roadmap culminates in the development of high-efficiency tandem solar cells, targeting >28% efficiency for next-generation manufacturing lines.

Through this presentation, Avaada Electro seeks to showcase its R&D capabilities, highlight ongoing and future innovation programs, and explore collaborative opportunities to accelerate India's leadership in advanced solar photovoltaic technologies.

Keywords: Industrial TOPCon Solar Cells, Silicon-Perovskite Tandem, Avaada Electro's R&D vision

References:

1. *International Technology Roadmap for Photovoltaics (ITRPV), 2024 Edition.*
2. *Fraunhofer ISE, "Photovoltaics Report," 2023.*
3. *NREL, "Best Research-Cell Efficiency Chart," National Renewable Energy Laboratory, updated 2024.*
4. *J. Werner et al., "Tandem photovoltaics efficiency roadmap and trends," Nature Energy, 2022.*
5. *K. A. Bush et al., "Perovskite-silicon tandem solar cells: device design and scaling challenges," Nature Reviews Materials, 2023*

(Abstract Domain : Coating materials for wind and hydro turbine blades)

Comprehensive Investigation of Erosion–Corrosion Behaviour of CF8M Stainless Steel for Hydro Turbine Application

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ABSTRACT

In a hydro power plant, especially located in hilly region of north India, the phenomenon of erosion and corrosion plays an important role in material degradation and performance deterioration of hydraulic turbines components. The high slurry content in river water, combined with high velocity impacts of suspended particles, causes significant erosive and corrosive wear on hydro turbine parts. The erosive and corrosive factors are areas of severe concern as they are affecting the service life and performance of hydro turbines. In the present study, erosion and corrosion behaviour of CF8M material is investigated using a slurry erosion tester under controlled operating conditions. CF8M (AISI 316 equivalent stainless steel) is being widely preferred for hydro turbine components due to its excellent corrosion resistance, mechanical strength and reasonable cost; however, despite its good erosion and corrosion properties, CF8M is susceptible to slurry erosion under high impact conditions which necessitates its evaluation for corrosion and erosion behaviour. Our study focuses on the effect and influence of impact velocity at varying impact angles. Experiments are performed at different impact angles ranging from 30° to 90° degree with impact velocities ranging from 6 m/s to 12 m/s. The slurry medium consisted of water mixed with sand particles of known size distribution to replicate the natural sediment process. The eroded surfaces were further characterised using advanced characterisation techniques such as X-ray diffraction, Scanning Electron microscopy technique to identify the dominant wear mechanism and microstructural changes. The result significantly states that micro cutting, ploughing and selective material removal are primary erosion behaviour mechanisms. Corrosion studies suggests that oxidation reactions accelerate the material loss in the presence of slurry medium, establishing a relation between erosion and corrosion. The empirical correlation between erosion rate and corrosion rate is established for understanding the material degradation under combined operating condition and emphasizes the importance of selecting appropriate surface coating for turbine components. The outcome of this research can help in the optimisation of material selection and surface engineering strategies for improving the surface life and operational durability of CF8M hydro turbine parts operating in erosive-corrosive environment.

Keywords: Hydro turbine; Erosion; Corrosion; Slurry Erosion tester.

(Abstract Domain: Computational modelling and simulations)

Surface-Based Passive Mitigation Effects on Wake Structure and Aerodynamic Performance of an H-Rotor Vertical Axis Wind Turbine

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ABSTRACT

The aerodynamic influence of surface-based passive mitigation approaches on the wake development of a two-straight-bladed H-type vertical axis wind turbine is investigated utilising two-dimensional unsteady computational fluid dynamics. The near-wake and early far-wake regions are analysed to evaluate the impact of blade-surface and shaft-surface modifications on velocity deficit, turbulence formation, and coherent vortex structures. Structured meshes are generated throughout the computational domain to ensure accurate resolution of boundary-layer evolution and wake characteristics. Baseline rotor predictions are validated against experimental data, and wake regions are identified based on the location of maximum velocity deficit. The baseline rotor exhibits a pronounced velocity deficit and strong unsteady vortex shedding within the near-wake region. In contrast, the modified rotor, incorporating surface-based passive mitigation, demonstrates reduced vortex roll-up, enhanced flow attachment over the blades, and a measurable reduction in both the width and intensity of the shaft-dominated deficit zone. These improvements contribute to smoother downstream velocity recovery and reduced asymmetry in the developing wake. Additional analysis of boundary-layer transition, vortex evolution, and interaction between blade-induced and shaft-induced structures highlights the potential of passive mitigation strategies for effective wake control in small-scale vertical axis wind turbines.

Keywords: Vertical Axis Wind Turbine (VAWT); Wake recovery; CFD; Mitigation technique.

Materials & coating for batteries, super-capacitors and fuel cells

Dip-Coated PS-PANI-Based Nanocomposites for Efficient Electron Transfer in Microbial Fuel Cells

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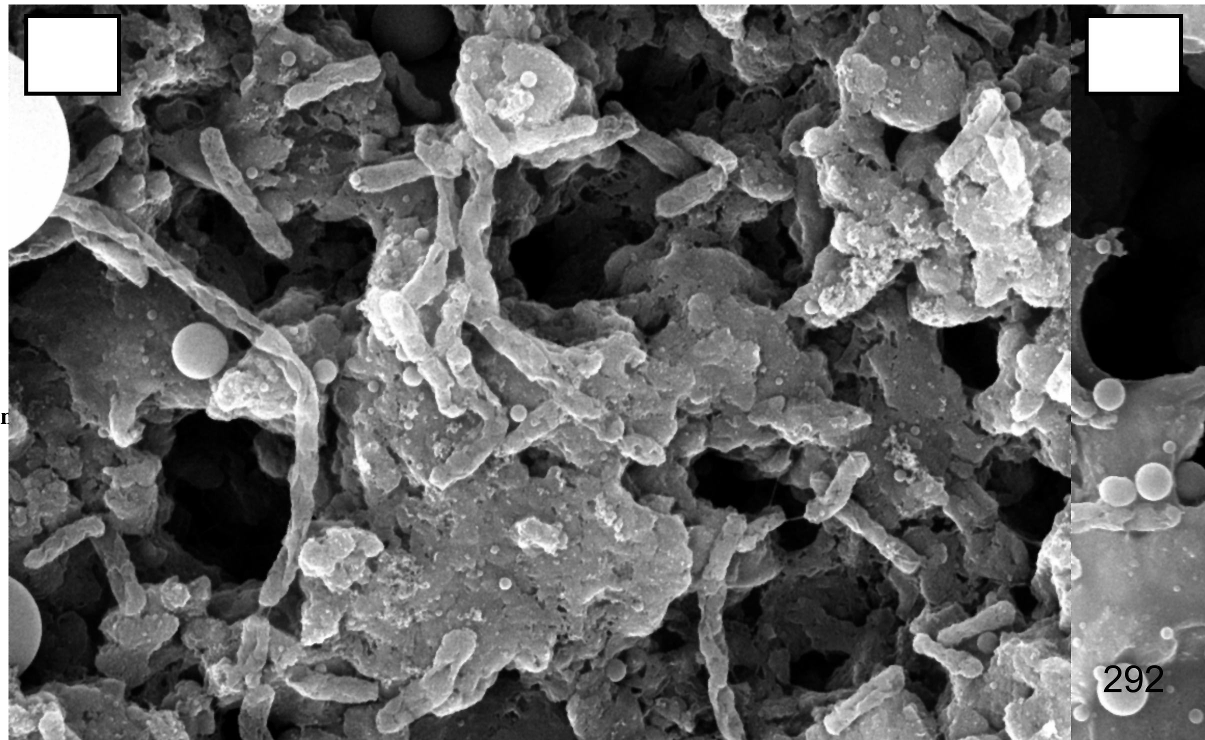
ABSTRACT

This study concentrates on the fabrication and performance optimization of polymer composite electrodes for microbial fuel cells (MFCs). Indium tin oxide (ITO) glass substrates were modified by dip-coating with a cheap blend of polystyrene and polyaniline (PS–PANI) to prepare the electrodes. We used Shewanella cultures in a three-electrode setup to test the modified electrochemical activity of these electrodes. Cyclic voltammetry (CV), chronoamperometry (CA), and chronocoulometry (CC) analyses demonstrated a consistent rise in current density and charge accumulation with an increasing number of coating dips. A peak current density of approximately 140 µA/cm² were achieved after four dips. Adding nanoparticles like carbon nanotubes (CNT) and graphene oxide (GO) to double-sided ITO electrodes made extracellular electron transfer much better than that found on electrodes with one sided coating. GO-coated electrodes displayed a peak current density of about 200 µA/cm² and could store up to 40 C/cm² of charge. The FESEM analysis showed that the PS–PANI morphology and the addition of nanoparticles made the biofilms have much increased surface area which was found to be conducive for microbial interaction and increased electron transfer efficiency, indicating the strong potential of these electrodes for sustainable energy generation in bio-electrochemical systems.

Keywords: Microbial Fuel Cell, Dip coating, PS-PANI electrode, nanocomposite

Fig. 1 **Biofilm forr**
electron transfer



Abstract Domain: Supercapacitors

Synthesis, characterization and performance study of biomass derived activated carbon from mustard husk as a high-performance supercapacitor electrode

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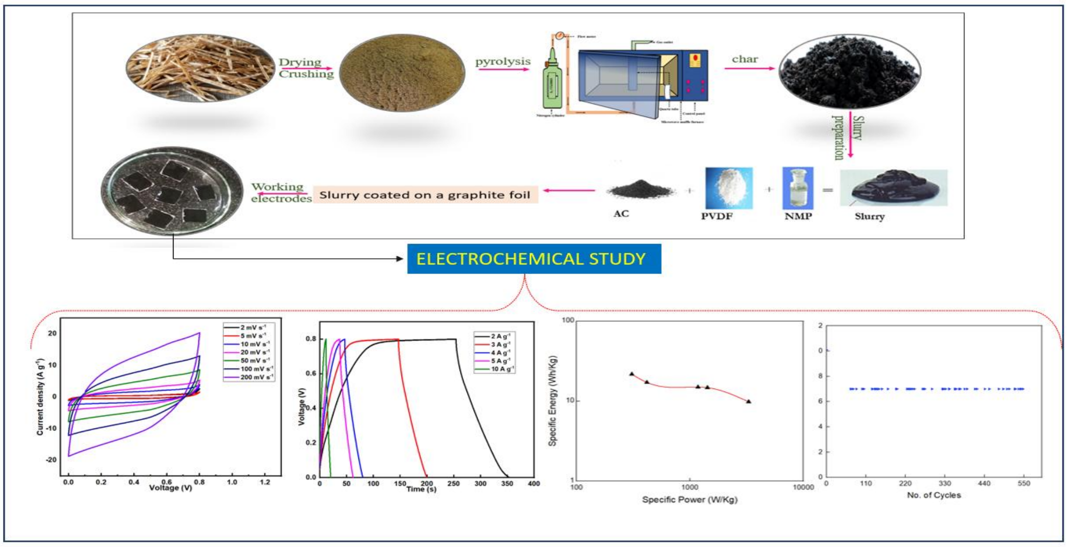
ABSTRACT: The capabilities of biomass derived supercapacitor electrodes and their use in the field of energy storage is a promising area of research. Commercial (industrial) based activated carbon are highly expensive and has adverse effect on the environment. Switching from industry based activated carbon to biomass derived activated carbon is a cleaner approach without altering the performance of biomass derived supercapacitor electrode significantly. The present work includes electrochemical study of MSH-derived electrode. MSH was converted in mustard husk char (MSHC) through microwave pyrolysis. Characterization of MSH and MSHC is done using ultimate and proximate analysis, SEM, FTIR, TGA-DTG. Ultimate and proximate analysis confirms that the carbon content in MSHC is 58.55% while MSH contains 44.45 % carbon which conclude high carbonaceous properties of MSHC as compared to MSH. TGA data of MSH and MSHC shows that MSHC was thermally stable at 280 °C while MSH at 232 °C which shows high thermal stability of MSHC over MSH. SEM observations reveal substantial morphological transformations in MSH upon exposure to microwave radiation. FTIR analysis is used to identify functional groups and surface properties that contribute to improve electrochemical performance. Electro-chemical study on MSHC electrode is conducted using three electrode system with the potential window of 0.0- 0.8 V. 2M- KOH was used as an electrolyte. Specific capacitance of MSHC derived electrode was calculated as 244.50 F g−1. Charging-discharging cycle lowered the specific capacitance from 244.50 F g−1 to 110.62 F g-1 when a current density increases from 2 Ag-1 to 10 Ag-1. The drop is less significant at lower scan rate. This is because of the accumulation of charge on uneven surface of electrode. The present study suggested that MSH has the potential to be used as a supercapacitor electrode.

Keywords: Charging- discharging cycle, Biomass, Specific capacitance, Supercapacitor electrode



(Perovskite, Silicon and CdTe thin films solar cells)

"Electrochemical Impedance Spectroscopy Analysis of Interfacial Layer Effects in $FAPbI_3$ Perovskite Solar Cells"

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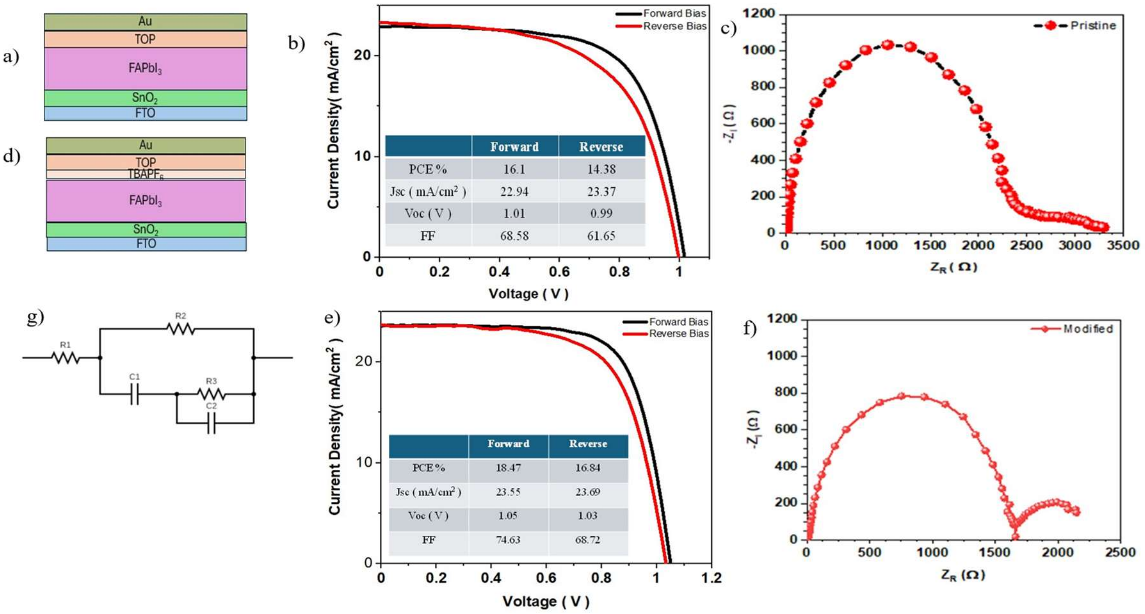
Abstract

This work investigates the impact of an engineered interfacial layer on charge transport and recombination in perovskite solar cells. Devices with FTO/SnO_2/$FAPbI_3$/TOP/Au (pristine) and FTO/SnO_2/$FAPbI_3$/$TBAPF_6$/TOP/Au (modified) structures were characterized using electrochemical impedance spectroscopy (EIS) and J-V measurements. Pristine cells exhibited a power conversion efficiency (PCE) of 16%, with fast electronic charge movement at high frequencies but notable ionic migration and charge build-up at the perovskite/hole transport layer (HTL) interface, contributing to charge trapping and performance losses.

Incorporation of the $TBAPF_6$ interfacial layer increased device efficiency to 18%. EIS data suggest passivation by $TBAPF_6$ reduces defect states, benefiting surface uniformity, band alignment, hole extraction, and lowering charge-transfer resistance. Enhanced carrier lifetime, fill factor, and open-circuit voltage were observed, indicating suppressed interfacial accumulation and trap states.

Overall, the $TBAPF_6$ interfacial layer improves charge transport and stability, leading to more reliable, high-performance perovskite solar cells.

Keywords: Perovskite solar cells, Electrochemical impedance spectroscopy, Ionic migration, Device stability



	Forward	Reverse
PCE %	16.1	14.38
Jsc (mA/cm²)	22.94	23.37
Voc (V)	1.01	0.99
FF	68.58	61.65

	Forward	Reverse
PCE %	18.47	16.84
Jsc (mA/cm²)	23.55	23.69
Voc (V)	1.05	1.03
FF	74.63	68.72

Fig. 1 a) *n-i-p* structured device of pristine b) J-V curve of pristine c) Nyquist plot of pristine d) *n-i-p* structured of modified e) J-V curve of modified f) Nyquist plot of modified g) Equivalent circuit

A Scalable Dopant-Free Spiro-OMeTAD: P3HT composite HTL Strategy for Stable, High-Efficiency Perovskite Optoelectronics

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Abstract

Spiro-OMeTAD remains the benchmark hole transport material (HTM) in high-performance perovskite solar cells (PSCs), yet its reliance on dopants and vulnerability to moisture-induced degradation limit long-term stability and scalability. We report a dopant-free composite HTM comprising Spiro-OMeTAD and low-concentration poly(3-hexylthiophene) (P3HT, 8 mg/mL), systematically optimized across five blend ratios. The optimal composition, Spiro-OMeTAD$_{0.94}$: P3HT$_{0.06}$ (2SP) achieves a power conversion efficiency of 20%, with a fill factor of 71.4% and an open-circuit voltage of 1.05 V—surpassing pristine Spiro controls. Time-resolved and steady-state photoluminescence reveal enhanced hole extraction and reduced carrier lifetimes. Photoresponse measurements under zero bias show a 43% (λ=532nm) and 38.2% (λ=655nm) increase in responsivity (A/W) for 2SP compared to pristine Spiro. X-ray diffraction of perovskite/HTM heterojunction films under 80% relative humidity confirms suppressed δ-phase evolution. Unencapsulated devices retain over 80% of initial efficiency after 700 hours in ambient conditions. This work presents a reproducible and scalable HTM strategy for stable, high-efficiency PSCs, highlighting its potential for integration into perovskite-based photodetectors.

Keywords: *Composite HTM, Moisture Stability, Dopant-Free , Perovskite Solar cells*

[‡] These authors contributed equally.

Development and Characterization of ZnO Thin Films for Surface Acoustic Wave Magnetoelectric Antennas

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ABSTRACT: This work presents the development of Zinc Oxide (ZnO) thin films deposited on Si/SiO$_2$ substrates for application in surface acoustic wave (SAW) magnetoelectric (ME) antennas. ZnO is chosen due to its high piezoelectric coupling coefficient, chemical stability, and compatibility with microfabrication processes, making it an ideal material for efficient acoustic wave generation in SAW resonator. The ZnO thin films were synthesized via a 0.2 M sol-gel process followed by spin coating, offering a cost-effective, controllable, and reproducible deposition method that ensures good film uniformity and surface quality. Interdigital transducers (IDTs) with 10 µm finger width were fabricated on top of the ZnO layer for acoustic excitation. Structural characterization of ZnO thin film by X-ray diffraction (XRD) revealed preferential C-axis oriented growth along the (002) plane with polycrystalline film. Atomic force microscopy (AFM) showed smooth film morphology with a root mean square roughness of 16.14 nm ideal for SAW ME antenna. Finite element simulations (FEA) based on admittance analysis predicted a resonant frequency of approximately 67.2 MHz corresponding to a 40 µm SAW wavelength, aligning well with the target operating frequency range for ME antennas. These results establish a robust foundation for optimizing ZnO-based piezoelectric layers in SAW-ME devices intended for advanced wireless applications. A notable aspect of this study is the fabrication of ME antennas using sol-gel deposited ZnO thin films through a simple and scalable approach. Additionally, the sol-gel process allows for easy doping of ZnO, enabling tailored functional properties and enhanced versatility for device optimization.

Keywords: ZnO thin film; Sol-gel; SAW; Magnetoelectric antenna.

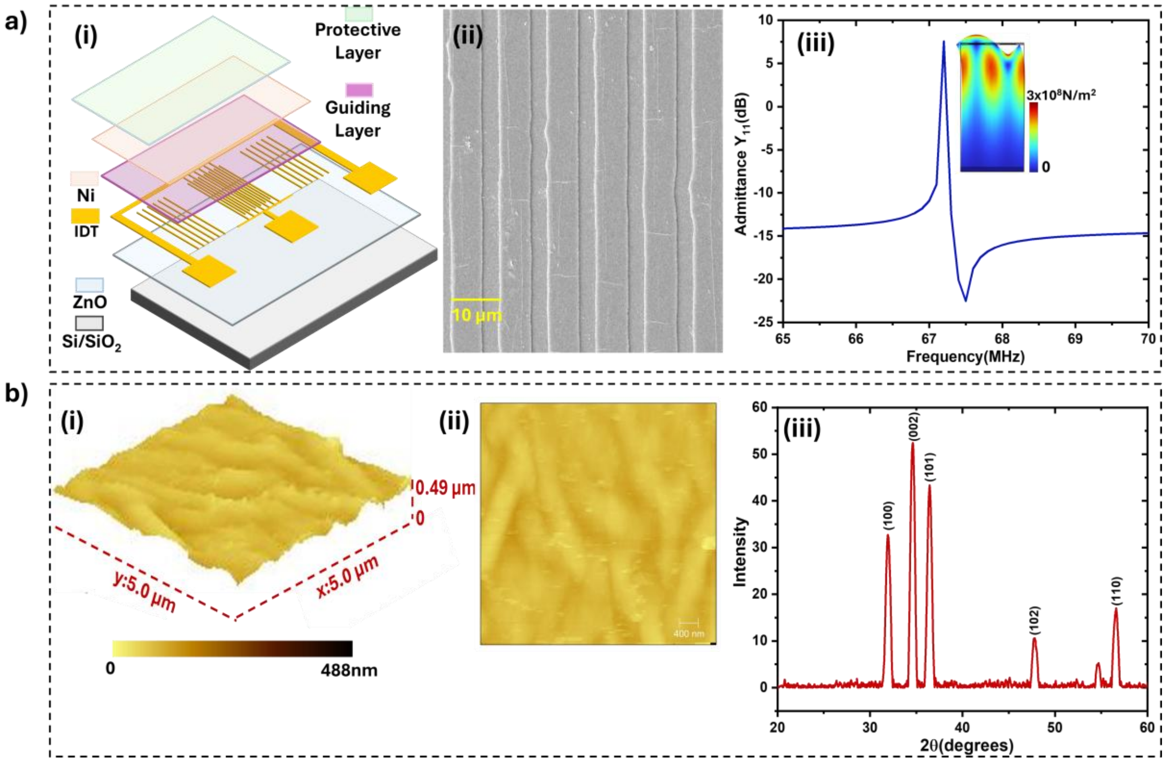

Figure 1: (a) ME antenna design and simulation: (i) Schematic illustration of the multilayer thin-film stack used for ME antenna fabrication, (ii) FESEM image of the fabricated SAW resonator structure, and (iii) admittance response obtained from COMSOL finite element analysis (FEA). (b) ZnO thin-film optimization and characterization: (i) 3D and (ii) 2D AFM surface topography of the ZnO thin film, and (iii) XRD pattern of the 0.2 M sol–gel derived ZnO film confirming its crystalline quality.

Perovskite, Silicon and CdTe thin films solar cells

Pivotal role of piranha cleaning in optimizing silicon surface morphology and enhancing solar cells performance

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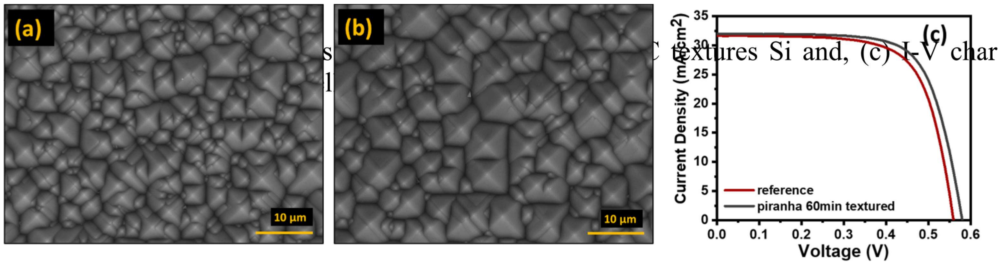
ABSTRACT

The present study investigates the key role of piranha cleaning (PC) treatment in tailoring the surface properties, morphology for enhanced performance of the PEDOT:PSS/n-type silicon (Si) based solar cell. The de-ionized water (DI), iso-propyl alcohol (IPA) and acetone based simple cleaning (SC) is substituted by PC of Si wafers. The measured contact angle (θ_c) on SC and PC Si surfaces are 5.49° and 2° respectively. The decrement in θ_c on PC surface suggest the increased wettability on PC compared to SC Si surfaces. The reaction rate of potassium hydroxide (KOH) and IPA aq. solution is also investigated on different wettability Si surfaces. Further, the etching of Si surfaces under identical parameters is studied by varying etching time (30 min, 45 min and 60 min) on PC samples and the results are compared with SC 60 min textured Si surface. FESEM micrographs analysis, shown in Fig. 1(a and b), concludes that the reaction rate of aq. KOH solution is fast on PC Si surface which is well supported by the increased pyramids dimension ~1.45 folds on optimized 60 min PC Si surface compared to SC Si surfaces. Further, the surface passivation study is done by PEDOT:PSS on different textured Si surfaces by the minority carrier lifetime measurements. The lifetime enhanced ~1.17 folds on optimized PC 60 min textured surface compared to SC textured Si indicates improved passivation. The calculated solar weighted reflectance (SWR) for optimized 60 min PC textured surface and SC 60 min textured Si with and without PEDOT:PSS coating are 13.94%, 12.93% and 8.70%, 8.38% respectively. However, there are minimal to negligible changes observed in optical properties. Nevertheless, the overall device (Ag/PEDOT:PSS/n-Si/In:Ga) performance as shown in (Fig. 1(c)) of the solar cells fabricated on the PC textured Si surface exhibits significant enhancement in open circuit voltage (V_{oc}) ~20mV and in power conversion efficiency (PCE) ~1.06 fold due to improved active junction quality. Thus, the minor optimization in cleaning process can yield more aligned morphology and favourable interface for enhanced PCE of solar cells.

Keywords: piranha; micro-texturing; PEDOT:PSS; hybrid silicon solar cells.



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(Abstract Domain :1 Thin films/Nano-materials Growth, Novel techniques and concepts)

Structural and Conformational Analysis of Ultra-Thin P(VDF–TrFE) Ferroelectric Films Using XRD and FTIR

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ABSTRACT

Ferroelectric copolymers such as poly(vinylidene fluoride-trifluoroethylene) [P(VDF-TrFE)] have attracted significant attention for their potential use in flexible sensors, transducers, and non-volatile memory devices. The crystallinity and phase composition of these polymers play a critical role in determining their ferroelectric and piezoelectric behaviour.

In this study, ultra-thin P(VDF-TrFE) films were prepared by spin coating using dimethylformamide (DMF) as solvent and subsequently annealed at controlled temperatures below the melting point (~152 °C). The structural and conformational phase transitions were systematically examined using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). FTIR spectra exhibited strong absorption bands at 840, 506, and 468 cm^{-1}, characteristic of the all-trans β-phase conformation associated with ferroelectric activity. XRD analysis confirmed the presence of a dominant diffraction peak at $2\theta \approx 20.3°$, corresponding to the (110)/(200) planes of the β-phase crystal structure.

The combined XRD and FTIR results establish that suitable thermal treatment can promote a higher degree of β-phase crystallization even below the melting point, which is essential for achieving strong ferroelectric polarization in thin P(VDF–TrFE) layers. These findings provide valuable insights into process–structure relationships that guide the optimization of polymer ferroelectrics for future flexible and wearable electronic applications.

Keywords: P(VDF-TrFE); β-phase; XRD; FTIR

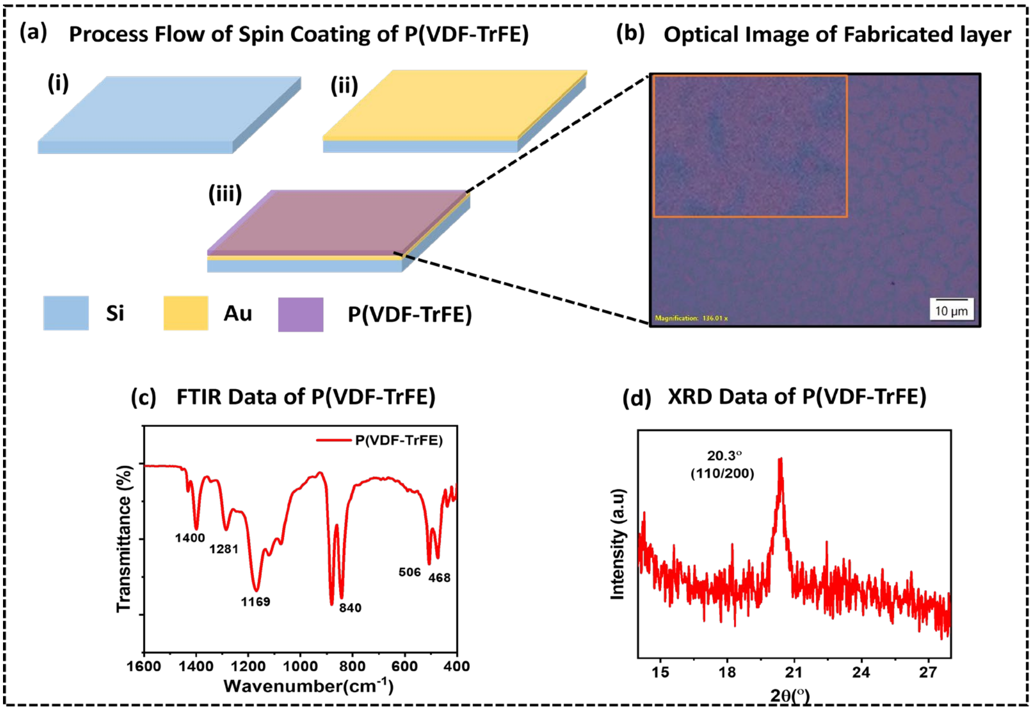

Figure1: Process Flow for Ultra-Thin Film And Characterization Of Thin Film P(VDF-TrFE)

Structural, Optical, Electrical, and Morphological Characterization of Sol Gel Spin Coated CZTS Thin Films

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ABSTRACT

The motivation of this study is to develop high-efficiency solar cells using Copper Zinc Tin Sulphide (CZTS) thin films, which are promising absorber materials due to their earth abundance, non toxicity, and suitable optoelectronic properties. Fabricating CZTS films through a cost-effective and scalable process like the sol-gel spin coating method is essential for advancing sustainable photovoltaic technologies. In this work, CZTS thin films were successfully fabricated on glass substrates using the sol-gel technique. The precursor solutions were meticulously prepared and spin-coated to achieve uniform thin films. Multiple coating cycles followed by controlled annealing ensured appropriate thickness and crystallinity of the films. This process allowed precise control over film composition and morphology, critical for solar cell applications. Comprehensive characterization was carried out to evaluate the structural, optical, electrical, and morphological properties of the fabricated films. X-ray diffraction (XRD) analysis confirmed the formation of a single-phase kesterite CZTS structure with predominant (112) plane orientation, which is key for efficient charge transport. UV-Visible spectroscopy measurements provided absorbance data, from which the absorption coefficient and optical band gap (1.35 eV) were derived; the films exhibited a direct band gap optimal for solar absorption. Electrical characterization using the four-probe method determined the resistivity of the films, essential for understanding charge carrier mobility. Surface morphology and roughness assessments by atomic force microscopy (AFM) and scanning electron microscopy (SEM) showed smooth and compact surfaces without cracks or pinholes, indicating high film quality, with average surface roughness value: 16 nm. SEM was also utilized for thickness (1.9 µm) measurement, confirming film uniformity. Energy-dispersive X-ray spectroscopy (EDAX) offered elemental analysis, verifying near-stoichiometric composition aligning with intended precursor ratios.

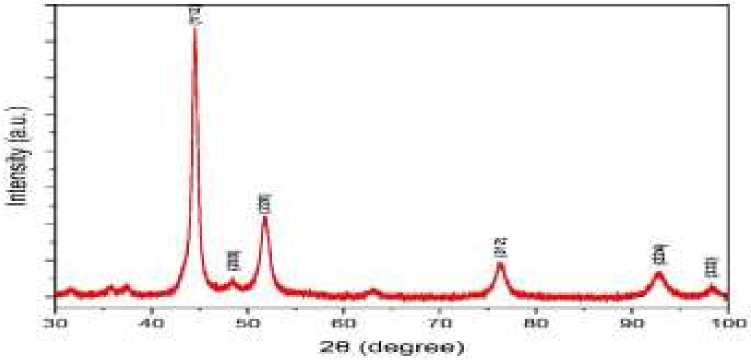

Fig. 1. XRD pattern of kesterite CZTS Thin film

Keywords: Cu_2ZnSnS_4, thin film, spin coating, morphology

(Abstract Domain: Perovskite, Silicon, and CdTe thin film solar cells)

Functional Layer Optimization and Tuning of Interfacial Dipole for Highly Stable Air-Ambient Fabricated Perovskite Solar Cells

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Perovskite solar cells (PSCs) have achieved remarkable power conversion efficiencies (PCEs); however, the simultaneous attainment of high performance and long-term operational stability under ambient processing conditions remains a critical challenge. Here, we report a synergistic strategy that integrates functional layer optimization of the electron transport layer (ETL) with interfacial dipole engineering using cyclohexylmethylammonium iodide (CHMAI) for stable air-ambient fabricated formamidinium lead iodide ($FAPbI_3$) PSCs. Moreover, we have used a less explored material, TOP-α3, as an HTL, which is cost-effective compared to conventional HTL materials.

Subsequent CHMAI treatment induced the formation of a low-dimensional 2D/3D perovskite heterostructure, evidenced by new X-ray diffraction peaks at 5.24° and 10.5°, corresponding to layered perovskite phases. UPS measurements confirmed that the CHMAI interlayer introduced an interfacial dipole, shifting the valence band maximum of the perovskite and facilitating improved energy-level alignment with the HTL TOP-α3. This dual modification reduced non-radiative recombination, suppressed interfacial defects, and enhanced moisture resistance, resulting in a champion PCE of 23.55 % with negligible hysteresis. Notably, CHMAI-modified unencapsulated devices retained nearly 90% of their initial efficiency after over 5000 hours of storage in the dark, demonstrating substantial device stability. This work highlights the critical role of interfacial dipole engineering in achieving simultaneously efficient and stable PSCs through scalable, ambient-compatible processes.

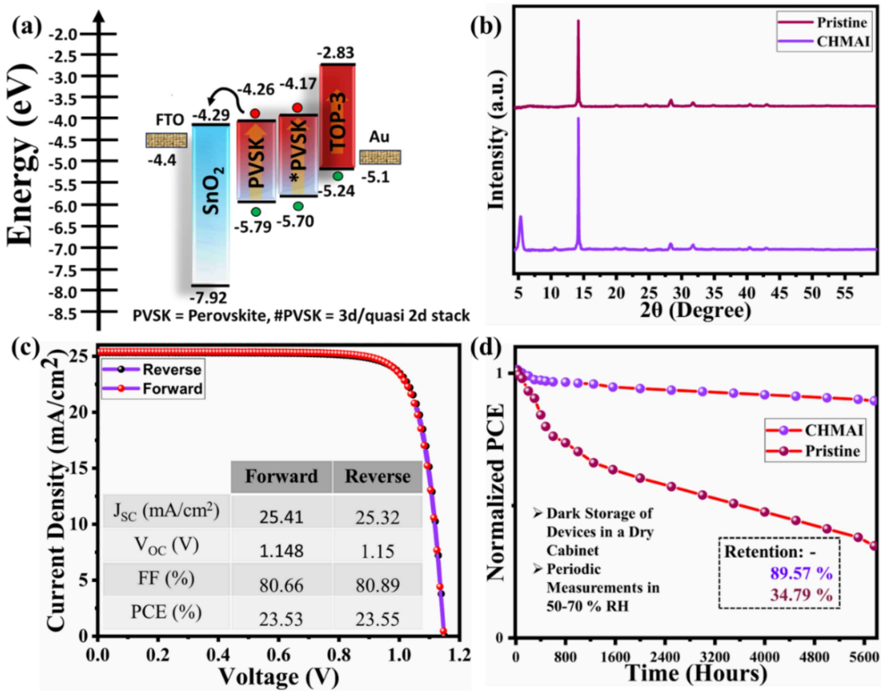

Figure 1: *The analysis of with and without treatment by CHMAI (a) the improved energy level alignment as confirmed by UPS, (b) XRD of both perovskite films, (c) J-V curve of the best-performing modified device, and (d) Long-term stability analysis of both devices.*

(Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts)

Diode Laser-Assisted Optimisation of Double-Sided Laser-Induced Graphene

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ABSTRACT

Laser-Induced Graphene (LIG) has emerged as a highly versatile, cost-effective, and lithography-free technique for directly transforming carbon-rich precursors into porous, electrically conductive graphene networks. Owing to its tunable nature, the LIG process enables modulation of microstructure and surface chemistry by adjusting laser parameters, rendering it ideal for flexible electronics, sensors, and energy storage devices. However, the fabrication of double-sided laser-induced graphene (D-LIG) structures can enhance surface area, electrical transport, and mechanical stability, but has not yet been thoroughly investigated. This study systematically investigates and optimises the diode-laser-assisted fabrication of D-LIG on commercial polyimide (PI) films, emphasising the correlation between laser parameters and the structural evolution of LIG on both sides.

A 60 W air-assisted diode laser (λ = 455 nm) was employed for laser direct writing, with the PI substrate firmly mounted on a solid aluminium base to ensure uniform heat dissipation and prevent thermal deformation. The laser power and scan speed were systematically varied while maintaining a constant DPI of 254. The optimisation revealed a distinct interdependence between laser power, scan speed, and the extent of graphitisation. At low powers (6–10%) and high scan speeds (>140 mm/s), the energy input was insufficient to trigger carbonisation, while excessive power (>24%) and low scan speeds (<100 mm/s) led to thermal degradation and surface ablation. The optimal processing window for uniform, defect-minimised LIG formation was identified as laser power 26–30% and scan speed 130–140 mm/s. Furthermore, the laser power was found to significantly influence the thickness of both the LIG layer and the underlying PI substrate. Lower powers (<20%) failed to induce graphitisation, while excessive power caused ablation and substrate thinning. Optimal double-sided processing at 28–30% on one side and 24–26% on the other yielded uniform, defect-free D-LIG with minimal substrate damage. Higher power enhanced localised heating and photothermal decomposition, increasing LIG thickness, whereas excessive energy led to unwanted ablation. A custom-designed mould was used to ensure precise alignment, enabling symmetric exposure and uniform LIG thickness on both sides. Re-optimisation of the second-side parameters prevented over-carbonisation and thermal distortion induced by heat conduction through the pre-patterned opposite layer.

Structural and spectroscopic analyses confirmed the successful formation of high-quality D-LIG. FESEM imaging revealed a porous, foam-like morphology conducive to high surface area and charge transport. XRD patterns exhibited broad peaks at 25.1° and 43.1° (2θ), corresponding to the (002) and (100) planes of graphitic carbon, confirming the development of turbostratic graphene domains. Raman spectra displayed characteristic D (1350 cm^{-1}), G (1575 cm^{-1}), and 2D (2690 cm^{-1}) bands, with a low I_D/I_G ratio ~ 0.57 indicating limited disorder and an I_{2D}/I_G ratio ~ 0.62 suggesting few-layer graphene with good crystallinity. Overall, the optimised diode-laser parameters enabled symmetric and controllable graphitisation of both sides of PI, achieving uniform LIG thickness, structural integrity, and minimal substrate degradation. This work establishes a sustainable, energy-efficient, and material-effective route for the fabrication of high-quality D-LIG, offering strong potential for applications in flexible electronics, electrochemical energy devices, and multifunctional sensing

systems.

Keywords: LIG; Diode laser; Flexible electronics; multimodal sensors.

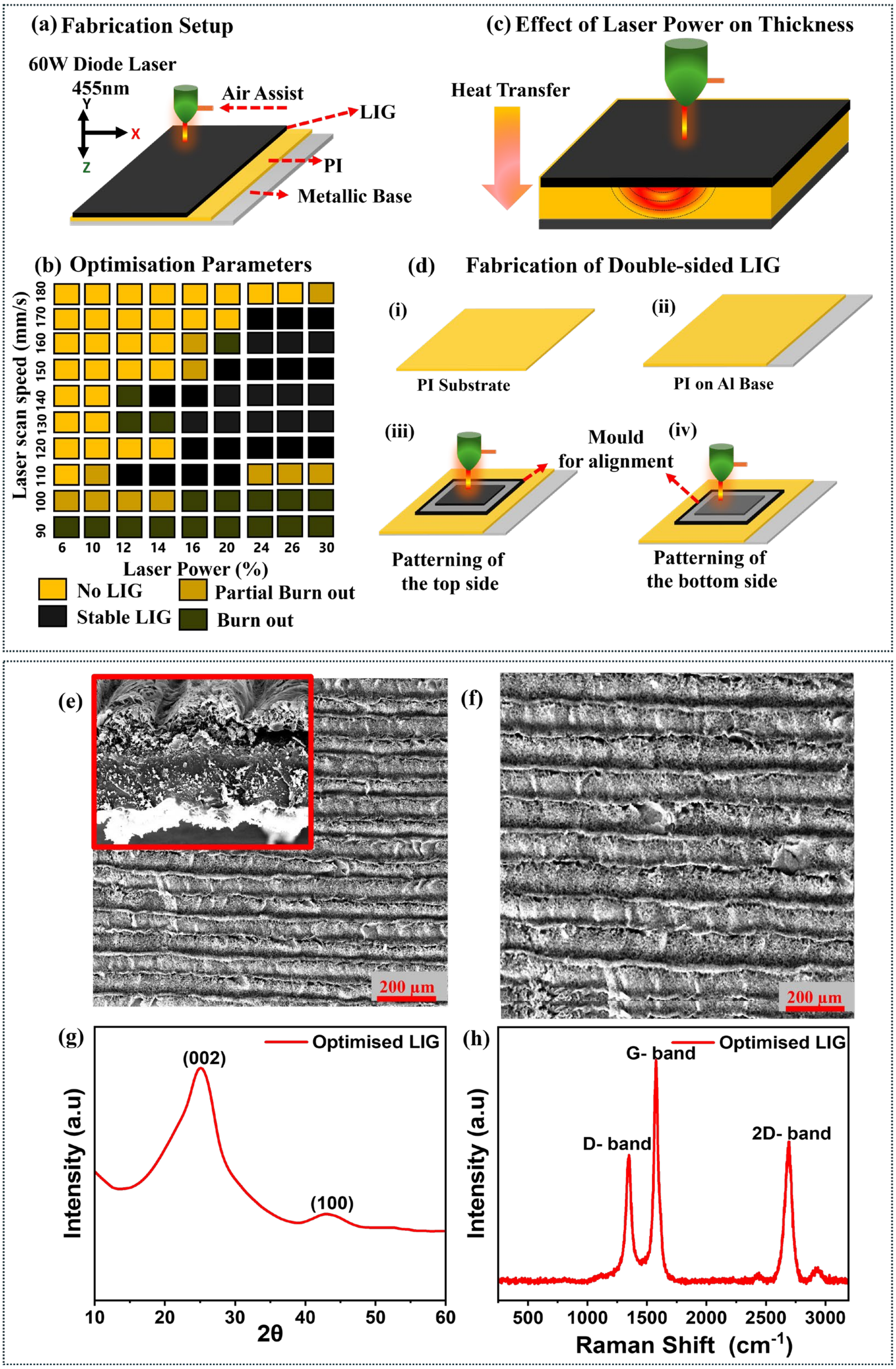

Figure 1. (a) Schematic of diode laser setup; (b) Optimisation parameters (c) Effect of laser power on D-LIG and substrate thickness; (d) Fabrication process of D-LIG; (e) SEM image of the top-side LIG (inset showing cross-section of D-LIG); (f) SEM image of the bottom-side LIG; (g) XRD pattern and (f) Raman spectrum of optimised LIG.

Synergistic NiCo/MgAl Layered Double Hydroxide Composites for High-Performance Supercapacitors

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In the pursuit of sustainable and high performance energy storage systems, supercapacitors have emerged as promising devices owing to their superior power density and long cycle life. Layered double hydroxides (LDHs) based materials offering tunable interlayer structures and high electrochemical activity, making them ideal for supercapacitor electrodes. However, the limited electrical conductivity and restricted redox activity of pristine MgAl layered double hydroxides (LDHs) often hinder their practical applicability. To overcome these drawbacks, NiCo LDH was introduced into MgAl LDH to form a composite via hydrothermal route to enhance its electrochemical performance. The remarkable electrochemical performance of the NiCo/MgAl LDH composite can be attributed to the synergistic coupling between the redox-active Ni/Co layers and the structurally stable MgAl LDH. While Ni^{2+}/Ni^{3+} and Co^{2+}/Co^{3+} couples contribute to reversible faradaic reactions, the MgAl structure enhances ion diffusion and prevents structural degradation during continuous cycling, resulting in superior specific capacitance and long term stability. The optimized electrode exhibited a high specific capacitance of 1144 F g^{-1} at 1 A g^{-1}, with excellent rate capability, Owing to its synergistic layered structure, the composite achieved a remarkable energy density of 128.6 Wh kg^{-1} at power density of 1123 W kg^{-1}.

Keywords: Supercapacitor, layered double hydroxides, electrochemical activity, specific capacitance

(Supercapacitors)

V_2O_5 nanorods embedded Polymer for Enhanced Electrochemical Performance

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ABSTRACT

The growing global demand for sustainable energy storage has intensified the pursuit of materials that combine high energy density, long cycle life, and rapid charge–discharge capability. Supercapacitors have emerged as efficient energy storage devices, bridging the gap between batteries and traditional capacitors. In this study, a vanadium pentoxide (V_2O_5) and polypyrrole (PPy) nanocomposite was synthesised and evaluated as a high-performance electrode material. The nanocomposite was fabricated using thermal decomposition route. The hybrid design integrates the redox activity of V_2O_5 with the superior conductivity and flexibility of PPy, enabling a balanced combination of stability and capacitance. Various analytical techniques were employed to comprehensively characterise the synthesised material. Structural and morphological analyses through X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Field emission scanning electron microscopy (FESEM) ensure uniform nanorod growth and homogeneous polymer distribution. Thermogravimetric analysis (TGA) and contact angle measurements verified the material's stability and surface compatibility. Electrochemical analyses—cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS)—demonstrated superior specific capacitance in aqueous electrolytes, where proton mobility accelerated redox kinetics. The synergistic interplay between V_2O_5's pseudo-capacitance and PPy's electronic conductivity enhanced ion diffusion and reduced internal resistance, leading to improved electrochemical efficiency. Overall, the synthesis route is straightforward, low-cost, and environmentally friendly, underscoring its potential for scalable fabrication. The V_2O_5/PPy nanocomposite exhibits high stability, mechanical flexibility, and excellent energy-storage behaviour, establishing it as a strong candidate for next-generation, commercially viable, and sustainable supercapacitor systems.

Keywords: V_2O_5, Polypyrrole, Supercapacitor, Electrochemical Performance

Mxene/Activated Carbon Composite based electrode for High Performance Supercapacitor

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Abstract

MXene have emerged as promising electrode materials for supercapacitors owing to their exceptional electrical conductivity, abundant surface terminations, and remarkable pseudocapacitive behavior. In this study, a MXene/Activated carbon nanocomposite electrode was synthesized via physical blending method to enhance the overall supercapacitor performance. The fabricated MXene/Activated Carbon nanocomposite electrode demonstrated exceptional electrochemical performance, achieving a specific capacitance of 576 F g^{-1} at a scan rate of 10 mV s^{-1}, from cyclic voltammetry measurements. Galvanostatic charge-discharge profiling further validated the superior electrochemical attributes, yielding a specific capacitance of 564 F g^{-1} at a current density of 2 A g^{-1}, substantially surpassing pristine MXene and establishing the composite as a favorable candidate for electrode material in supercapacitor devices. These superior electrochemical traits are attributed to the synergistic contribution of pseudo-capacitance from MXene and the Electric Double Layer capacitance from the Activated Carbon.

Optimizing Vacancy Ordered Perovskite Solar Cells (Cs_2SnI_6) Using SCAPS-1D Simulations

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Perovskite solar cells (PSCs) have emerged as promising candidates for next-generation photovoltaic technology due to their high power conversion efficiency (PCE), tunable bandgap, and low-cost fabrication. However, the toxicity and instability of lead-based perovskites have driven the search for lead-free alternatives. This study investigates vacancy ordered double perovskite (VODP) Cs_2SnI_6 as a stable, non-toxic absorber material using SCAPS-1D numerical simulations. The device was modeled in an n–i–p configuration with the structure ITO/ZnO/Cs_2SnI_6/$SrCuO_2$/Au. The optimized device achieved a PCE of 23.86%, with an open-circuit voltage (Voc) of 1.0322 V, short-circuit current density (Jsc) of 27.77 mA cm^{-2}, and fill factor (FF) of 83.22%. Further, the variation of absorber layer thickness, acceptor (Na) density, and defect density was systematically studied to understand their effect on photovoltaic performance and internal resistances. The results reveal that moderate Na doping enhances charge extraction, while lower defect density minimizes recombination losses. Variations in absorber thickness were found to influence charge generation and recombination balance, whereas changes in series and shunt resistance significantly affected carrier transport and fill factor. The copper-based hole transport layer ($SrCuO_2$) also exhibited excellent performance, contributing to the overall device efficiency. These findings highlight the potential of Cs_2SnI_6 based VODPs as stable, lead-free absorber materials with tunable optoelectronic properties suitable for high-efficiency single-junction and tandem solar cell applications.

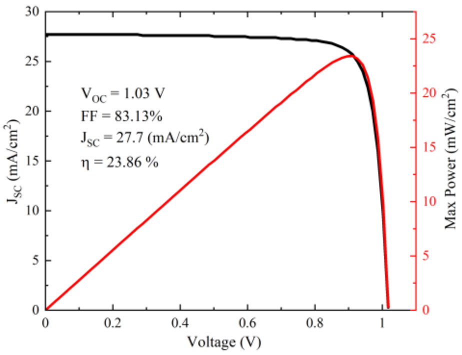

Figure 1: J-V curve of the optimized solar cell.

Keywords: Perovskite, Efficiency, Recombination, SCAPS-1D

Process Optimization of Sub-5 μm MEMS-Based SAW Resonators on LiNbO$_3$ for Biomedical Sensing Applications

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ABSTRACT- The advancement of wearable health monitoring and point-of-care diagnostic systems depends on the development of miniaturized, highly sensitive, and reliable biosensors. Surface Acoustic Wave (SAW) resonators have emerged as a promising technology for such biomedical applications due to their exceptional sensitivity to surface-mass loading and capability for real-time, label-free detection of biomolecules, pathogens, and biomarkers. However, fabricating high-quality SAW resonators with sub-5 μm interdigital transducer (IDT) features on piezoelectric substrates creates significant challenges. Issues such as weak resist adhesion, poor electrode lift-off, and the line-of-sight nature of deposition often result in discontinuous metal patterns and degraded device performance. Therefore, optimizing the fabrication process is crucial for achieving consistent device characteristics such as high-quality factor (Q), low insertion loss, and stable resonance frequency, which are key metrics for biomedical sensing.

This work presents an optimized fabrication process for SAW resonators on single-side polished 128° Y-cut lithium niobate (LiNbO$_3$), selected for its high electromechanical coupling and low acoustic propagation loss. The resonators, designed for operation at 200 MHz, utilize Ti/Au (40 nm/40 nm) IDT electrodes with sub-5 μm finger widths. A comparative lithography study was conducted using positive resist S1813 and image reversal resist AZ5214E. While S1813 produced tapered sidewalls that caused partial bridging, AZ5214E formed a well-defined undercut profile, enabling clean lift-off and sharply defined IDTs. Metal deposition via electron-beam evaporation followed by lift-off in heated Remover PG resulted in smooth, uniform electrode structures.

The addition of a biocompatible sensing layer on the SAW surface enhances biomedical functionality by improving molecular selectivity. The layer selectively interacts with specific biomolecules or analytes, causing localized mass loading that shifts the resonance frequency, enabling precise, real-time, and label-free detection. The optimized AZ5214E process provided superior lithographic control and device reproducibility, directly enhancing sensing performance for advanced biomedical diagnostic applications.

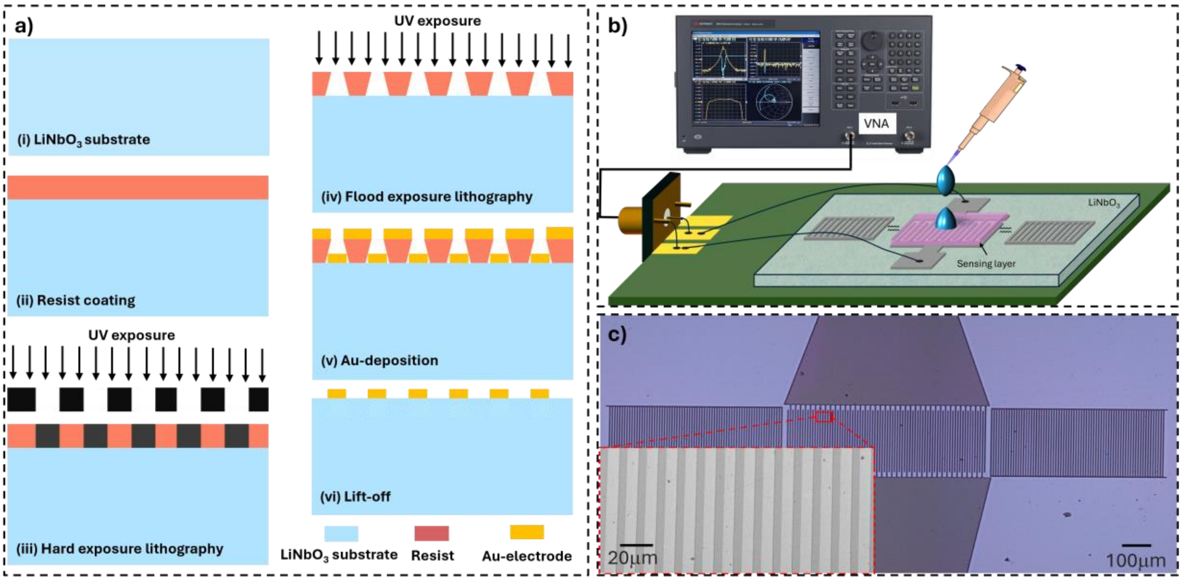

Fig. 1. (a) Fabrication schematic of IDTs on LiNbO$_3$: (i) cleaning, (ii) AZ5214E coating, (iii) UV exposure and reversal bake, (iv) flood exposure, (v) Ti/Au deposition, and (vi) lift-off. (b) Experimental set-up for testing sensor response. (c) Fabricated SAW resonator.

Keywords: SAW Resonator; IDT; Lift-off; Lithium niobate.

(Computational Modeling & Simulations)

Designing and analysis of D–π–A–π–D and A–D–A structured π-conjugated organic compounds for utilization as field effect transistors

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ABSTRACT

In this work, a series of novel organic semiconducting molecules were computationally designed and analyzed for utilization as potential candidates for high-performance organic field effect transistors (OFETs). The studied molecular systems are based on two different electronic architectures viz. D–π–A–π–D and A–D–A. Here, D, π and A represent electron donor, π bridge and electron acceptor moieties respectively. Indacenodithiophene (IDT) and benzodithiophene (BDT) were used as electron donor units, and perylenediimide (PDI) and naphthalenediimide (NDI) were used as electron accepting units. Geometry optimization and electronic structure analyses were carried out using *Gaussian* and GaussView softwares. All calculations were performed using density Functional theory (DFT). Key charge transport parameters, namely adiabatic and vertical ionization potentials (IP_a and IP_v), adiabatic and vertical electron affinities (EA_a and EA_v), and reorganization energies for holes (λ_h) and electrons (λ_e), were evaluated to determine their suitability as efficient OFET materials. The results reveal that the D–π–A–π–D systems exhibit lower λ_h values and higher IP values, suggesting strong hole transport characteristics suitable for *p*-type semiconducting behaviour, whereas A–D–A systems demonstrate lower λ_e and higher EA values, indicative of *n*-type transport properties. The balanced λ_h/λ_e ratios and tunable frontier molecular orbital energies in both architectures underscore their potential for ambipolar OFET performance. Overall, this study establishes the reliability of *Gaussian*-based DFT analysis in predicting charge transport efficiency and provides a rational molecular design pathway for developing next-generation organic semiconductors with tailored electronic properties.

Keywords: OFET; IDT; BDT; NDI.

Abstract Domain: Materials & coating for batteries, super-capacitors and fuel cells.

Development of anode materials for Sodium Dual-Ion Batteries

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ABSTRACT

The transition away from Lithium-Ion Batteries(LIBs) and exploration in other alternatives comes as a need for today considering scarcity of Lithium in the crust and rising price to import and manufacture a LIB. Sodium Dual-Ion Batteries comes forward as a suitable alternative that can offer higher operating voltages and better ionic conductivity, Transition metal layered oxides are identified as suitable electrode candidate for SDIBs, and Molybdenum dioxide (MoO_2) has emerged as a promising anode material owing to its unique combination of metallic conductivity, structural stability, and shallow-intercalation charge storage behaviour. In lithium-ion batteries (LIBs), MoO exhibits high theoretical capacity (~838 mAh g ^{1}), faster chemical kinetics, and better rate capability. MoO_2 exists in nano-particle range which enables it to better control the surface intercalation properties. Recognizing the larger ionic radius of Na , our approach focuses on exploiting the shallow-intercalating nature of MoO to facilitate surface intercalation rather than deep bulk insertion, thereby ensuring faster kinetics and structural reversibility. The synthesised MoO_2 indicates successful phase reduction and desirable features that align with shallow-intercalation charge storage mechanisms which directly tie to future exploration of the material that involves electrochemical testing and optimising the material for Na-based anode chemistry to evaluate capacity retention, rate capability, and cycling stability bridging the gap between high energy density and rapid charge-discharge capability.

Keywords: High Capacity Anode, Sodium Dual-Ion Batteries, Transition Metal Oxides, Nanostructured Material.

(Abstract Domain: Thin films/Nano-materials Growth, Novel techniques and concepts)

Exploring the memristive behaviour in spray pyrolyzed Cerium Oxide thin film.

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Abstract

The rapid development of information technology has led to the efficient use of energy storage device. ReRAM is a non-volatile memory device which stores data in the form of resistance. Cerium oxide becomes the material of choice because of it has the ability to switch back and forth between two oxidation states +3, +4. When a voltage is applied, cerium switches between these two states either by undergoing oxidation or reduction. Cerium Oxide is not much explored material. Cerium is a rare earth metal. This work aims to the development of FTO/CeO_2/Ag thin film memristor device using spray pyrolysis. Ag and FTO are used as top and bottom electrode. CeO_2 thin film of three different concentrations of 0.01M, 0.03M, 0.05M of precursor solution was coated on FTO. Structural studies were carried out using X ray diffraction. The peaks corresponding to the (111), (200), (220) and (311) plane confirms the presence of Cerium Oxide. Morphological studies were carried out using scanning electron microscopy. Optical properties were analysed using UV-Visible spectroscopy and photoluminescence. The band gap is found to be decreasing with increase in concentration from 3.05eV to 2.91eV. The absorbance peak is found to be around 300 nm. Photoluminescence, reveals a peak formed around 350nm that corresponds to cerium oxide and a peak at 470 nm shows the formation of oxygen vacancy. I-V characteristics were studied using Keysight B2901A. It shows memristor property of the deposited material. The On/Off ratio is 4 for the device fabricated with thin films deposited using 0.03M concentration precursor.

Keywords: Cerium Oxide; Spray Pyrolysis; Memristor

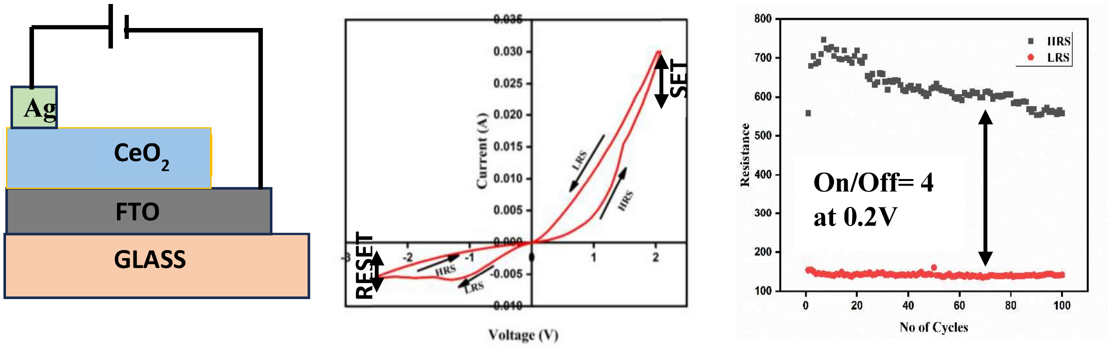

Fig:(a) **Fig: (b)** **Fig:(c)**

Fig:(a) Schematic of <FTO/CeO_2/Ag> Memristor, Fig:(b) I-V curve characteristics of thin film deposited using 0.03M concentration precursor, Fig:(c) endurance cycle of the former graph

Understanding Charge Transport across defects in TMDs

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Abstract

Defects in transition metal dichalcogenide can be classified as point defects (vacancies) and line defects (grain boundaries) [1], Understanding charge carrier dynamics in the presence of defects and engineering them for improved performance is imperative. With recent development of single crystal large area MoS_2 growth techniques understanding the influence of point defects on the charge transport is crucial [2]. We here fabricated Field effect transistor using single crystal sulphur vacancy rich CVD grown monolayer MoS_2 as channel material. We observed an intrinsic n-type conductivity with significant hysteresis suggesting sulphur vacancy defect induced trapping. To engineer sulphur vacancy a careful defect passivation technique involving F4TCNQ as the molecular dopant was developed and a concurrent increase in photoluminescence, reduced carrier concentration and reduced hysteresis was observed all attributed to sulphur vacancy passivation. To understand the influence of vacancy defects on optoelectronic properties, photodetection measurement were performed and a significantly large fall time was observed for the as-grown sample in vacuum conditions, this effect is known as persistent photoconductivity (PPC). To understand the main cause of PPC, sulphur vacancy was passivated using F4TCNQ and a significantly lower fall time was observed, the PPC mechanism was explained using rigorous first principles model. Capture rate was calculated for various point defects to understand the dominant electron capture defect. Our calculation revealed that the sulphur bi-vacancy presents significant lattice deformation and large barrier for carrier capture in its ionised state explaining PPC.

References:

1.Zhou, Wu, et al. "Intrinsic structural defects in monolayer molybdenum disulfide." *Nano letters* 13.6 (2013): 2615-2622.

2. Li, Lu, et al. "Epitaxy of wafer-scale single-crystal MoS2 monolayer via buffer layer control." *Nature Communications* 15.1 (2024): 1825.

Computational Modelling & Simulations

Tuning Hot Carrier Dynamics in Vacancy-Ordered Halide Perovskites through Lattice Compression: Insight from *ab initio* Quantum Dynamics and Machine Learning

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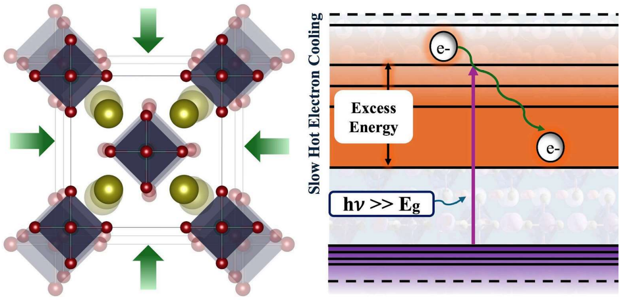
ABSTRACT



The efficient harvesting of hot carriers (HCs) from high-energy photons can significantly enhance optoelectronic performances. However, ultrafast HC cooling through intra-band transitions poses a significant challenge for extraction using traditional semiconductor absorbers. The stable and compressible vacancy-ordered halide perovskites with isolated octahedra exhibit discrete electronic states at the conduction band edge, indicating possible slow cooling of hot electrons (HE). Using state-of-the-art ab initio quantum dynamics simulations and unsupervised machine learning (ML), we investigate the effect of lattice stress on HE dynamics in vacancy-ordered Cs_2SnBr_6. The moderate stress enhances structural rigidity and weakens dynamic electron-phonon interactions at the conduction bands. Such modifications and the widened energy gap at the conduction band edge partially suppress intra-band non-adiabatic transitions, eventually elongating the HE lifetime. The pairwise mutual information extracts hard-to-find highly non-linear dynamic structure-excited state property correlations, offering the unique opportunity to strategically design efficient lead-free halide perovskites for HE-based optoelectronics.

Nanoscale Thermal Transport in 2D/3D Composites: xSThM Insights Toward High-ZT>2 Thermoelectrics

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Significant improvements in thermoelectric power factor have been demonstrated in Sb_2Te_3/MoS_2 multilayer systems and $Sb_2Te_3/AgSbTe_2$ composite structures through careful material design and optimization. To accurately assess anisotropic thermal transport in these nanoscale architectures, a novel technique—cross-sectional scanning thermal microscopy (xSThM)—was utilized. This method involves fabricating a shallow-angle wedge on the sample surface, enabling localized thermal conductance measurements across regions of varying thickness. Each point along the wedge effectively represents a distinct material cross-section, allowing simultaneous extraction of in-plane (k_{xy}) and out-of-plane (k_z) thermal conductivities. An analytical model complements the measurements by quantifying interfacial thermal resistance between the sample and substrate. By optimizing the number and thickness of MoS_2 layers, ultralow thermal conductivity values (0.7 ± 0.1 $W \cdot m^{-1} \cdot K^{-1}$) were achieved alongside high power factors ($(4.97 \pm 0.39) \times 10^{-3}$ $W \cdot m^{-1} \cdot K^{-2}$), resulting in an impressive figure of merit $ZT = 2.08 \pm 0.37$at 300 K. Similarly, tuning the Ag content in $Sb_2Te_3/AgSbTe_2$ composites led to optimal ZT values. This methodology offers a powerful framework for probing thermal transport in ultrathin films and layered materials, paving the way for the rational design of high-efficiency thermoelectric devices.

References:

1. M. Ahmad‡, K. Agarwal‡, S. G. Munoz, A. Ghosh, N. Kodan, O.V. Kolosov and B.R. Mehta. Engineering interfacial effects in electron and phonon transport of Sb2Te3/MoS2 multilayer for thermoelectric ZT above 2.0, Advanced Functional Materials 2206384 (2022) Impact Factor: 19.92. Page No. 1-13, DOI: 10.1002/adfm.202206384
2. Jean Spièce, Charalambos Evangeli, Alex J. Robson, Alexandros El Sachat, Linda Haenel, M. Isabel Alonso,○ Miquel Garriga,○ Benjamin J. Robinson, Michael Oehme, Jörg Schulz, Francesc Alzina, Clivia Sotomayor Torres, Oleg V. Kolosov, Nanoscale, 24, 10829 (2021).

(Abstract Domain: 5)

Compositional Engineering of Double-cation Single-halide Perovskite for Efficient Solar Cell fabrication under Air Ambient Conditions

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ABSTRACT

Metal halide perovskites offer excellent photovoltaic potential, but their instability under ambient conditions limits scalable fabrication. FA^+-based perovskites are especially prone to phase degradation due to volatile organic cations and strain-induced lattice distortion. In this work, we address these challenges through compositional engineering of $FA_{1-x}Cs_xPbI_3$ (x = 0.05-0.25), with all film deposition and device fabrication conducted in an air ambient (RH < 30%). Systematic incorporation of Cs^+ induces lattice contraction and strengthens the PbI_6 octahedral framework, enabling effective tuning of residual tensile stress, an important parameter governing phase stability and defect formation. Among all compositions, $FA_{0.9}Cs_{0.1}PbI_3$ exhibited optimal structural and optoelectronic properties. XRD showed a pronounced peak shift and reduced FWHM for the Cs 10% films, consistent with lower tensile stress and improved crystallinity. Ambient stability tests demonstrated that $FA_{0.9}Cs_{0.1}PbI_3$ preserved its dark perovskite phase with minimal degradation even after 30 days, outperforming both lower and higher Cs contents. SEM confirmed larger, well-connected grains with fewer grain boundaries, while optical measurements revealed enhanced absorbance and photoluminescence, indicating suppressed non-radiative recombination. For device fabrication, TOP-3 was employed as a cost-effective and stable hole-transport layer, replacing Spiro-OMeTAD. The resulting device ($FTO/TiO_2/FA_{0.9}Cs_{0.1}PbI_3$/TOP-3/Au) achieved an efficiency of 17.14%. Overall, this study highlights Cs-mediated residual stress modulation as a key strategy for improving ambient-processable perovskites and advancing scalable, low-cost photovoltaic technologies.

Keywords: perovskite solar cells; compositional engineering; ambient processing; lattice stress.

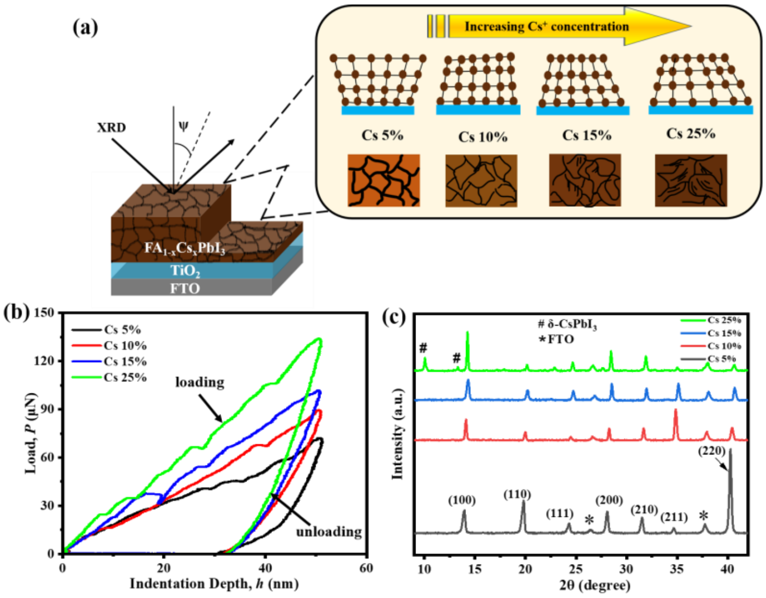

Figure 1. (a) $FA_{1-}Cs_xPbI_3$ perovskite film samples deposited on TiO_2-coated FTO substrate, (b) *P-h* curves, (c) XRD patterns of the perovskite films.

Smart Wireless Throttle Body in Automobile System

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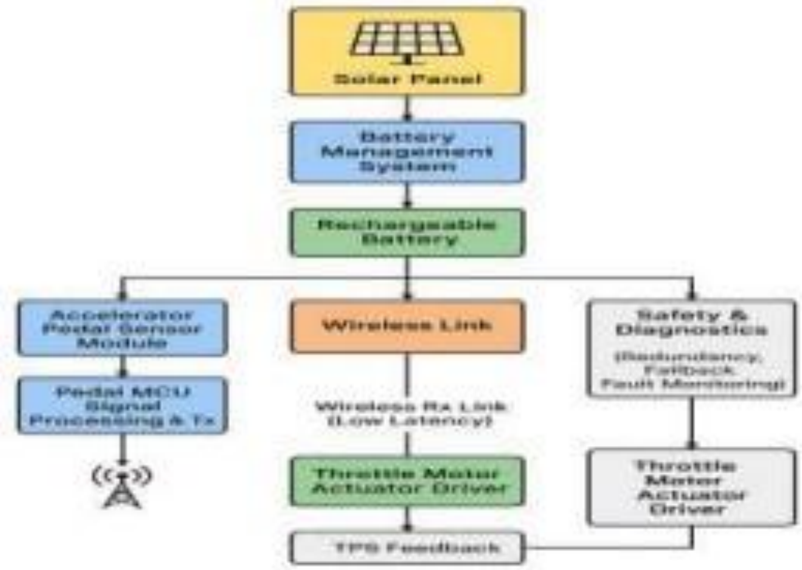
Abstract

The Wireless Throttle Body System (WTBS) is an innovative solution designed to replace the conventional wired throttle linkage between the accelerator pedal and the throttle body with a fully wireless control mechanism. This system enhances flexibility, reduces wiring complexity, and improves reliability in modern automotive applications.

In this modified design, solar energy is incorporated as a sustainable power source to charge the system's rechargeable battery, which in turn powers all modules involved in the throttle operation. The system consists of an Accelerator Pedal Sensor Module that measures the pedal position and transmits data wirelessly to the Throttle Controller Unit (ECU). The ECU interprets the signals and commands the Throttle Motor Actuator Driver to control the throttle plate position accurately. A wireless communication link ensures low latency, high reliability, and secure data transmission between the pedal and throttle modules. The inclusion of a Solar Charging unit with an intelligent Battery Management System (BMS) ensures continuous operation, even under varying sunlight conditions. Safety features such as sensor redundancy, link monitoring, and fault detection are integrated to maintain operational integrity. The system not only reduces wiring weight and installation complexity but also contributes to energy efficiency and environmental sustainability by utilizing renewable solar power for autonomous operation.

Keywords: Throttle body, Wireless transmission, Solar Battery and Management system.



Block Diagram: Wireless Throttle body System

(Abstract Domain: Computational modelling & simulations)

PANS Turbulence Model Based One-Way Fluid-Structure Interaction Analysis of a KP505 Propeller

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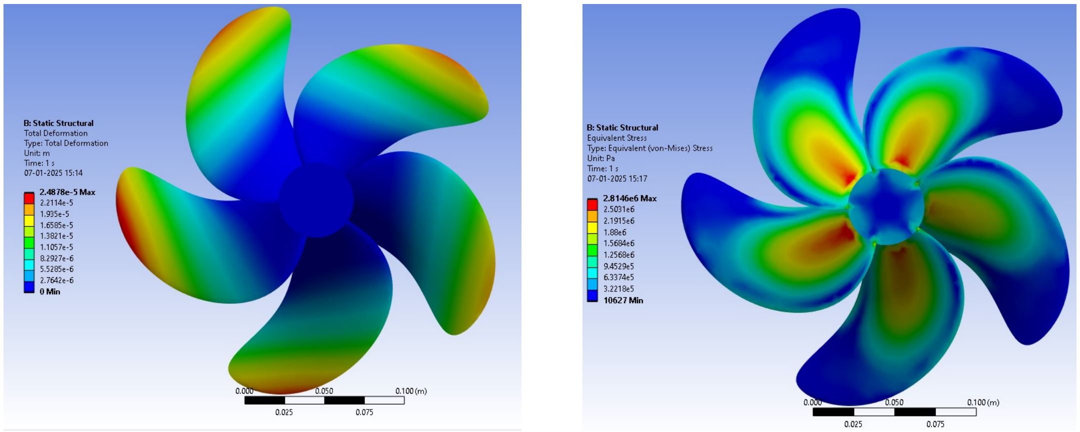
ABSTRACT

The accurate prediction of hydrodynamic performance and structural response of marine propellers is crucial for ensuring propulsion efficiency and fatigue resistance in ship design. In this study, a detailed numerical investigation of the KP505 propeller with KCS hull is carried out using the Partially Averaged Navier-Stokes (PANS) turbulence model for hydrodynamic analysis, followed by a one-way fluid-structure interaction (FSI) study to capture the structural response under the cyclic hydrodynamic loading. The PANS methodology, bridging Reynolds Averaged Navier-Stokes (RANS) and Direct Numerical Simulation (DNS), provides enhanced resolution of unsteady vortical structures and pressure fluctuations in the wake region, offering a more real-life flow field than conventional RANS models.

The hydrodynamic analysis is performed in ANSYS Fluent using the PANS turbulence model. The domain is discretized with Fluent meshing, applying inflation layers on the propeller and hull and refinement in the upstream and downstream regions to capture wake flow accurately. The maximum wall y^+ is kept at 5 for the propeller and 80 for the hull. The simulation is conducted at an advance ratio $J = 0.3$ and propeller speed $n = 14$ rps. As the full domain with 47.5 million cells is computationally expensive, it is truncated by introducing a section plane 0.5 m upstream, where the extracted velocity profile is applied as the inlet condition. The PANS model on the segmented domain captures finer turbulent structures and resolves wake features better than RANS, with thrust and torque coefficients closely matching experiments, confirming its accuracy in predicting hull-propeller flow dynamics.



(a) (b)

Figure 1. Distribution of (a) deformation and (b) equivalent stress on propeller surface

The one-way FSI analysis of the propeller is performed using static structural in ANSYS Workbench. Initially, the hydrodynamic pressure data from the CFD solver are imported in static structural and mapped onto the structural mesh of the KP505 propeller made of nickel-aluminum-bronze (NAB) alloy. The material properties considered are density of 7400 kg/m^3, Young's modulus of 1.24×10^5 MPa, Poisson's ratio of 0.33, and shear modulus of 46,617 MPa. The static structural solver computes deformation and von Mises stress distributions for different time steps CFD data. Figure 1 depicts deformation and equivalent stress contour on the propeller. The maximum total deformation is found to be 2.48×10^{-5} m, concentrated near the blade tips due to higher bending moments. The maximum von Mises stress is 2.84 MPa, occurring near the blade-hub junction where the pressure loading is highest. Stress gradually decreases toward the blade tips, consistent with the dissipation of hydrodynamic forces. Time-dependent analysis indicates that both deformation and stress reach steady periodic values after several time steps, following the transient fluid stabilization.

Keywords: Propeller; Wake dynamics; PANS; One-way FSI