

GLOW2024

Global Conference for Women Leaders and Emerging Researchers in Materials Science

GLObal Conference for Women Leaders and Emerging Researchers in Materials Science (GLOW 2024), held in Nanyang Technological University, Singapore from 9 to 11 July 2024, is a platform to shine a spotlight on the remarkable contributions of women talents in the field of Materials Science.

At this inaugural global conference, a series of oral presentations by the Travel Awardees from different parts of the world and our NTU Emerging Scientists, will be featured to share their achievements on the latest advancements and emerging trends in the areas of:

- Characterization
- Energy & Artificial Intelligence
- Healthcare
- Nanomaterials
- Sustainability

We have also lined up poster sessions and networking opportunities for researchers to showcase their research and participants to form meaningful connections within the field. Hope your participation at GLOW 2024 offers you new insights and opportunities in your Science and Engineering journey.



FROM LAB TO LEADERSHIP:

WOMEN SHAPING THE FUTURE OF SCIENCE

Tuesday, 9 July 2024

Day 1:

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| 08.30 - 10.00 | Registration with Light Refreshment |
| 10.00 - 10.15 | Opening and Welcome Speech <i>Professor Lee Pooi See</i> <i>Vice President (International Engagement)</i> <i>Nanyang Technological University</i> |
| 10.15 - 10.30 | Speech <i>Professor Tim White</i> <i>President, Materials Research Society, Singapore</i> <i>Professor, Nanyang Technological University</i> |
| HEALTHCARE (Chaired by Assoc Prof Terry Steele) | |
| 10.30 - 11.10 | Keynote Speech Bioactive Composites for Bone Replacement and Modelling <i>Professor Elizabeth Tanner</i> <i>Queen Mary University of London, UK</i> |
| 11.10 - 11.30 | Synergizing Mechanical Strength and Infection Control in Bone Cement Using Antibiotic Methacrylic Comonomers <i>Dr Juhi Singh</i> <i>Carnegie Mellon University, USA</i> |
| 11.30 - 11.50 | Bioresponsive materials as organelle-specific drug delivery systems for therapy of cancer and cardiovascular diseases <i>Dr Xuerui Chen</i> <i>Shanghai University, China</i> |
| 11.50 - 14.00 | Networking Lunch & Poster Session |
| SUSTAINABILITY (Chaired by Asst Prof Hortense Le Ferrand) | |
| 14.00 - 14.40 | Keynote Speech Towards Net Zero: Opportunities and Challenges from a Materials Scientist's Perspective <i>Professor Chen Li-Chyong</i> <i>National Taiwan University, Taiwan</i> |
| 14.40 - 15.00 | Lignin-Based Nanofertilizers for Controlled Release of Phosphorous <i>Dr Alice Boarino</i> <i>Università degli Studi di Torino, Italy</i> |

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| 15.00 - 15.20 | Image Analysis of Mycelium Growth on High-Content Spent Coffee Grounds for the Fabrication of Mycelium-Based Composites <i>Assistant Professor Pimpet Sratong-on</i> <i>Thai-Nichi Institute of Technology, Thailand</i> |
| 15.20 - 15.40 | Utilizing Lignin for a circular sustainable solution <i>Dr Sara T. R. Velasquez</i> <i>University of Twente, The Netherlands</i> |
| 15.40 - 16.00 | End-of-Life management of silicon photovoltaics: Recycling and Repurposing <i>Dr Ying Sim</i> <i>Nanyang Technological University, Singapore</i> |
| 16.00 - 16.20 | Tea break |
| 16.20 - 17.00 | Poster Session |
| 17.00 | - End of Day 1 - |

Wednesday, 10 July 2024

Day 2:

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|---------------|--|
| 08.30 - 09.30 | Light Refreshment |
| | NANOMATERIALS (Chaired by Prof Hng Huey Hoon) |
| 9.30 - 10.10 | Keynote Speech Electrical control in the chemical vapor deposition synthesis for electronics and separation applications <i>Professor Jing Kong</i> <i>Massachusetts Institute of Technology, USA</i> |
| 10.10 - 10.30 | Nanoscale Surface Chemistry for Next-Generation Energy and Optoelectronics Technologies <i>Dr Park Somin</i> <i>Northwestern University, USA</i> |
| 10.30 - 10.50 | Designing interfaces in thin films via atomic and molecular layer deposition <i>Assistant Professor Barbara Putz</i> <i>Montanuniversität Leoben, Austria</i> |

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| 10.50 - 11.10 | Atomistic modelling on the structural and electronic properties of advanced two-dimensional materials <i>Miss Yujia Tian</i> <i>Nanyang Technological University, Singapore</i> |
| 11.10 - 11.30 | Tuneable Optical Properties of Carbon-based Quantum Dots through Nitrogen Functionalization for Biomedical and Informatic Security Applications <i>Dr Fitri Aulia Permatasari</i> <i>Institut Teknologi Bandung, Indonesia</i> |
| 11.30 - 11.50 | Engineering Sustainable Nano-bio Interfaces for Environmental and Biomedical Applications <i>Dr Jieying Liang</i> <i>University of New South Wales, Australia</i> |
| NANOMATERIALS | |
| 11.50 - 12.30 | Keynote Speech Various Organic-Inorganic Hybrid Materials for Enhancing Biocompatibility of In Vitro Cell Culture and In Vivo Medical Implants <i>Professor Sung Yun Yang</i> <i>Chungnam National University, Korea</i> |
| 12.30 - 14.10 | Networking Lunch & Poster Session |
| 14.10 - 14.30 | Gender Equality in Research – 2024 Report <i>Mr Dominic Graham</i> <i>Elsevier</i> |
| PANEL DISCUSSION I (Facilitated by Prof Lam Yeng Ming) | |
| 14.30 - 15.30 | Building Success: Charting your roadmap towards rewarding career |
| 15.30 - 15.50 | Tea break |
| PANEL DISCUSSION II (Facilitated by Prof Lee Pooi See) | |
| 15.50 - 16.50 | Nurturing women leaders |
| 16.50 – 17.00 | Photo Session |
| 17.00 | - End of Day 2 - |



Thursday, 11 July 2024

Day 3:

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|---------------|--|
| 08.30 - 09.30 | Light Refreshment |
| | ENERGY & ARTIFICIAL INTELLIGENCE (Chaired by Assoc Prof Lydia Wong) |
| 09.30 - 10.10 | <p>Keynote Speech Harnessing Solar Energy through Catalysis for Fuel and Chemical Synthesis</p> <p><i>Professor Rose Amal</i> <i>University of New South Wales, Australia</i></p> |
| 10.10 - 10.30 | <p>Additively Manufacturing Smart Cellular Materials: Impact Energy Absorbers for Space Applications</p> <p><i>Dr Marlini Simoes</i> <i>California Institute of Technology, USA</i></p> |
| 10.30 - 10.50 | <p>Boosting Efficiency in Wide-Bandgap Pb-Free Perovskite Solar Cells with 4-Phenylthiosemicarbazide Additive: Achieving Over 12.2% Performance</p> <p><i>Dr Padmini Pandey</i> <i>Chung-Ang University, Korea</i></p> |
| 10.50 - 11.10 | <p>Phase behaviour and dynamics of organic cations in Formamidinium Lead Iodide (FAPbI₃) using machine-learned potentials</p> <p><i>Dr Sangita Dutta</i> <i>Chalmers University of Technology, Sweden</i></p> |
| 11.10 - 11.30 | <p>Harnessing AI for Advanced Nanomaterials Synthesis and Engineering</p> <p><i>Dr Bijun Tang</i> <i>Nanyang Technological University, Singapore</i></p> |
| 11.30 - 14.00 | Networking Lunch |
| | CHARACTERIZATION (Chaired by Asst Prof Wu Dongshuang) |
| 14.00 - 14.40 | <p>Keynote Speech High-throughput electron diffraction techniques accelerate the development of nanoporous materials</p> <p><i>Professor Zou Xiaodong</i> <i>Stockholm University, Sweden</i></p> |
| 14.40 - 15.00 | <p>High performance p-channel printed transistors on biodegradable PVA substrate for Transient Electronics</p> <p><i>Dr Devabharathi Nehru</i> <i>Aarhus University, Denmark</i></p> |

15.00 - 15.20 Resistive Switching in Hybrid Organic-Inorganic Halide Perovskite Memristors
Dr Jean Maria Fernandes
Indian Institute of Technology Madras, India

15.20 - 15.40 Optimization of chitosan-based membranes for in vitro permeability analysis of
trace elements from cosmetic and personal care products using inductively
coupled plasma mass spectrometry (ICP-MS)
Assistant Professor Nausheen W. Sadiq
Mount Royal University, Canada

15.40 - 16.10 Award Presentation & Closing Speech
Photo-Session

16.10 - 16.30 Tea break

SITE VISITS

16.30 - 18.00 A short tour of NTU Campus & Facilities

18.00 - End of Day 3 -

HEALTHCARE

Professor Elizabeth Tanner
Queen Mary University of London, UK

Bioactive Composites for Bone Replacement and Modelling

K. Elizabeth Tanner

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Abstract

At the simplest level bone is a ceramic filled polymer composite, giving mechanical properties below those of ceramics and metals and above those of polymers [1]. Furthermore the cells within bone are in direct contact and interact with the composite surfaces. To ensure good stress transfer when load bearing, similar moduli are required. Hence, to develop a bone replacement the use of ceramic filled polymer composites is attractive. The earliest such composites were high density polyethylene filled with hydroxyapatite (HA - $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$), a synthetic analogue of bone mineral, a substituted hydroxyapatite. These are effective in minor load bearing applications such as middle ear bone replacement, but do not have the strength for major load bearing applications [2].

For fracture fixation and tissue engineering scaffolds, a degradable composite is essential, with the all phases being either resorbed or incorporated in the newly formed bone. HA is only very slowly or never resorbed *in vivo*, hence tricalcium phosphate (TCP - $\text{Ca}_3(\text{PO}_4)_2$), which is degradable, has been used in some applications in combination with degradable polymers such as poly(lactic acid) and poly(hydroxybuterate).

The addition of bioactive fillers is beneficial. They increase the stiffness and potentially the strength of the composites [2]. They provide a surface texture which encourages bone cell attachment and proliferation. They can absorb and release bioactive moieties thereby increasing the response to the implant and allowing the local delivery of bone morphogenic proteins to accelerate bone growth and re-growth.

As with all composites the properties can be optimised using processing methods. Compounding extrusion can give stable composites but needs to be treated with caution when applied to degradable polymers. The use of fibre reinforcement can give mechanical properties similar to cortical bone with sufficient stiffness and strength to augment cortical bone. Electrospinning can be used to produce porous scaffolds for bone tissue engineering [3], using dual core to ensure the mineral phase is on the outer surface of the fibres and thus able to interact with the cells. Freeze drying (also known as lyophilisation), with or without the introduction of directional porosity, can be used to produce porous bioactive scaffolds or model surfaces for cell culture and modelling bone surfaces.

In summary, the technologies of conventional composites production can be applied to bioactive composites to produce bone analogues [2,3].

References

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**Towards Net Zero:
Opportunities and Challenges from a Materials Scientist's Perspective**

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Abstract

CO₂ emission is the primary driver of global climate change. Conversion of CO₂ to storable fuels or chemical products provides a carbon-neutral cycle that can mitigate the rapid consumption of fossil resources and the increasing CO₂ emission. In accordance with global CO₂ reduction regulations, carbon capture, utilization, and storage (CCUS) technologies for large-scale greenhouse gas reduction and conversion to high-value-added products have been intensively developed. Among the CCUS technologies, developing advanced catalytic materials is one of the key challenges. The discovery and development of materials for clean energy are essential to accelerate the transition towards a carbon-neutral economy. For instance, photocatalytic CO₂ conversion to hydrocarbon fuels, the so-called artificial photosynthesis, which makes possible simultaneous solar energy harvesting and CO₂ reduction reaction (CO₂RR), is considered a killing-two-birds-with-one-stone approach to solving the energy and environmental problems. However, the development of solar fuels has been hampered by the low photon-to-fuel conversion efficiency of the photocatalysts and lack of the product selectivity. Recent advancements in integrated nanostructured materials have offered unprecedented opportunities for photocatalytic CO₂RR [1]. Take 2D-layered nanomaterials as an example, a perfect planar layer structure is usually inactive. However, orders of magnitude enhancement in CO₂RR can be achieved with **defect engineering, surface modification, and heterostructures**. In this talk, a few cases in 2D-layered nanomaterials for enhancing CO₂RR will be illustrated [2-5]. Besides the challenges in the design and fabrication of materials, some key questions need to be addressed to make such energy conversion towards practical solutions. For instance: **Where does the reaction take place and what are the key steps for CO₂RR?** Advancements in scanning probe-based microscopies, *in situ* and *operando* synchrotron radiation-based spectroscopies, and vibrational spectroscopies have enabled scientists to probe the geometric, atomic, electronic, and bonding information of the catalyst and obtain atomic insights into the catalytic surfaces and reaction mechanisms. Moreover, some **theoretical frameworks** will also be illustrated on the guiding principles for CO₂RR.

References

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Electrical control in the chemical vapor deposition synthesis for electronics and separation applications

Jing Kong

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Abstract

Chemical vapor deposition (CVD) is widely used for the efficient growth of low dimensional materials. Typically, the synthesis parameters such as gas flow rate, temperature, pressure etc. are being optimized in order to achieve desirable results such as high-quality materials. Up to now, gas phase electro-chemical reactions have not been widely considered in CVD. In this talk, our explorations of using applied voltages to control the CVD synthesis results will be presented. We have found that applying an electric field between the copper substrate and a counter electrode has significant impacts on the growth of graphene. Electrochemical effect and ionic collision effect are observed in different conditions. We have developed a “cascaded compression” method via controlled electric field pulses during CVD process to synthesis nanoporous graphene membrane for separation applications [1]. Switching electric field can also be used to twist the chirality of carbon nanotubes [2]. It is anticipated that electrical control during CVD synthesis could open up new ways to assist the synthesis of low dimensional materials in the future.

References

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Various Organic-Inorganic Hybrid Materials for Enhancing Biocompatibility of In Vitro Cell Culture and In Vivo Medical ImplantsSung Yun Yang^{1,2*}¹*Department of Organic Materials Engineering, Chungnam National University,*²*Department of New Materials Engineering (Polymer Engineering Major), Graduate School of Chungnam National University, Daejeon 34134, Korea***Abstract**

In biomedical applications, polymers play a crucial role, yet challenges persist in optimizing their efficacy for high-performance, in vivo medical implants, applicable to both soft and hard materials. Silicone and titanium (Ti) implants are widely utilized in reconstructive surgery and orthopedics; however, their bio-inert characteristics hinder tissue integration, necessitating surface modifications to enhance biocompatibility. This study employs Layer-by-Layer (LbL) deposition to develop polyelectrolyte multilayer films on various implant surfaces. Various thin film coatings fabricated using the LbL method are examined, integrating hydrogel nanofiber coatings as soft matrices that mimic biological tissues to create biomimetic systems guiding cellular functions. Furthermore, pseudo-three-dimensional structures made from photo-curable resins explore effects on cellular morphology and motility. The investigation underscores the influence of chemical and physical properties of polymer or hybrid materials on cellular responses, crucial for advancing medical device technologies via surface modification and coatings to enhance medical implants. Additionally, this research introduces advancements in surface modification techniques for diagnostic biochips.

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Harnessing Solar Energy through Catalysis for Fuel and Chemical Synthesis

Rose Amal

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Abstract

In this presentation, I will explore the role of advanced catalysts in harnessing solar energy for the sustainable synthesis of chemicals and fuels. These catalysts, due to their unique intrinsic properties—including modified optical and electronic behaviours—greatly enhance the efficiency and selectivity of solar-driven chemical processes.

Our research leverages the entire solar spectrum, utilising UV and visible light for photocatalytic reactions and infrared radiation for thermal catalysis. These processes drive crucial reactions such as water splitting to generate H₂, CO₂ reduction, NO_x reduction, and CO₂ hydrogenation. I will highlight recent advancements in our work, particularly how we use advanced catalysis to enhance both the efficiency and selectivity of these solar-driven processes.

Our study has led to significant developments in photocatalysis, where we've engineered systems to concurrently produce hydrogen and selectively oxidise organics. Our investigations into Zn_xIn₂S_{3+x} photocatalysts have provided insights into the relationship between structure, activity, and selectivity optimising the reforming of furfuryl alcohol into hydrogen and hydrofuroin, a jet fuel candidate.

The integration of a solar-thermal reactor with a PV-electrolyser has enabled us to optimise the solar-driven reduction of CO₂ with hydrogen to methane. This innovative system, installed atop our building, exemplifies the practical application of our research.

Overall, our findings demonstrate the versatility and potential of solar energy in the production of clean fuels and the value-added transformation of organics, signifying a leap forward in the application of nano-engineered materials for solar energy conversion. This body of work contributes to global energy sustainability by providing alternatives to fossil fuels and advancing nano-catalysis technologies.

High-throughput electron diffraction techniques accelerate the development of nanoporous materials

X. Zou

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Abstract

Nanoporous materials such as zeolites, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs) have a wide range of applications in catalysis, storage, and separation. These materials have uniform pore sizes, large surface areas, and adjustable chemical functionality. To understand the functions of these materials and develop new porous materials, it is essential to know their 3D atomic structures. However, many zeolites, MOFs, and COFs are synthesized as polycrystalline materials and multiphasic mixtures, which are too difficult to study by conventional single crystal and powder X-ray diffraction. During the past decade, various new electron crystallographic techniques, i.e. three-dimensional electron diffraction (3D ED) and serial electron diffraction (SerialED) have been developed for studying such materials, which have made important breakthroughs in the development of nanoporous materials [1-2].

In this talk, I will present the 3D ED and SerialED techniques developed in my group and demonstrate their applications for the structure characterization of novel nanoporous materials [3-5]. Today, the structure determination of zeolites, MOFs, and COFs by 3D ED is as feasible and accurate as that by single crystal X-ray diffraction. A complete 3D ED dataset can be obtained on a standard TEM in less than a minute [6]. The refined structural models can reach better than 0.05 Å in accuracy for all non-H atoms and in many cases, H-atoms could also be located. Detailed structural features such as disorders and linker motions in MOFs could be identified [7]. To further speed up and automate data collection, we have developed high-throughput automated data collection and data analysis for 3D electron diffraction [5]. SerialED makes it possible not only to study extremely beam-sensitive crystals but also for phase analysis and detection of minor phases invisible by X-ray diffraction [8]. The developments of new 3D ED and SerialED techniques have revolutionized crystallography and provided new opportunities for discovering novel structures and new materials and exploring their properties and applications.

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Synergizing Mechanical Strength and Infection Control in Bone Cement Using Antibiotic Methacrylic Comonomers

J. Singh¹, J.C. Kadir¹, W.B. Ribnick¹, S.A. Sydlík¹

¹Department of Chemistry, Carnegie Mellon University, 4400 Fifth Avenue, Pittsburgh, PA, 15213, United States

Abstract

Periprosthetic joint infections present a significant challenge in total joint arthroplasty, leading to high rates of revision surgeries and substantial morbidity.^[1,2] Standard treatments including systemic antibiotic administration often fail due to the resilient nature of biofilms and reduced antibiotic efficacy.^[3] Existing antibiotic-loaded bone cements (ALBCs) used for localized delivery face limitations in mechanical strength and inefficient antibiotic release, which restricts their effectiveness.^[4] To address these issues, we developed therapeutic gentamicin methacrylic comonomers (gMAs) that incorporate antibiotics in to poly(methyl methacrylate) (PMMA) bone cement through covalent bonds. This innovation ensures controlled drug release via hydrolysis of the methacrylic carbonyl bond and enhances the mechanical properties of the cement. Our study investigates the structure-property relationships of gMA-loaded cements, focusing on variables such as tether bond type (amide vs. ester), gMA loading percentage (3-10%), and formulation type (standard PMMA vs. commercially available SmartSet MV). The results demonstrate that gMA-loaded cements achieve clinical strength standards even at higher antibiotic loadings and exhibit significantly improved drug release profiles compared to conventional ALBCs. In vitro assays show effective biofilm inhibition against *E. coli* and *B. subtilis* over a 7-day period. Preliminary in vivo testing against methicillin-resistant *S. aureus* reveals a notable reduction in bacterial counts on implant surfaces and in femur homogenates, surpassing the efficacy of standard antibiotic treatments. This novel approach offers a promising solution for the treatment of implant-associated infections, providing bone cements that are both mechanically robust and capable of sustained, controlled antibiotic release.

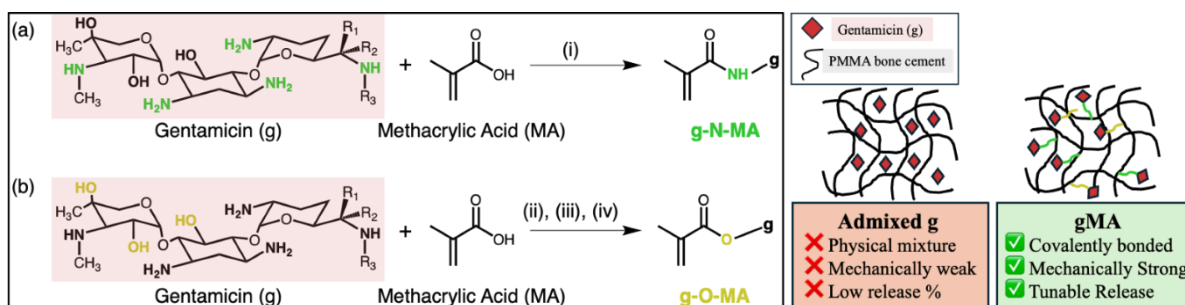


Figure 1: Design on antibiotic methacrylic comonomers for incorporation in PMMA bone cements to combat prosthetic joint infections.

References

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Bioresponsive materials as organelle-specific drug delivery systems for therapy of cancer and cardiovascular diseases

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Abstract

Bioresponsive materials have been applied in clinical drug delivery since the 1990s. They are sensitive to biological signals or to pathological abnormalities, and interact with or are actuated by them. Nano delivery strategies can be designed to control the spatial and temporal distribution of therapeutic agents in the body, which decreases side effects and increases therapeutic efficacy in the treatment of various diseases. In fact, several nanomedicines have received clinical approval due to equivalent efficacy but improved safety compared with freely administered small molecules. It awaits implementation of more complex multifunctional designs to enhance a drug's pharmacokinetics, stability, absorption and targeted exposure.

My works mainly revolve around bioresponsive materials as organelle-specific drug delivery systems for the therapy of cancer and cardiovascular diseases. Recently, only a small fraction of therapeutic payloads successfully reaches the organelle-specific point. I would like to dedicate efforts to direct delivery to subcellular organelles, finally tackling the high dosage requirements and systemic toxicities caused by the lack of specificity.

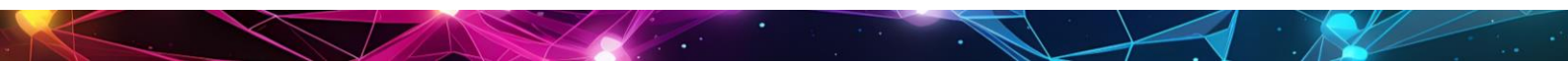
Mitochondria generate ATP as intracellular powerhouse, and are associated with multiple aspects of tumorigenesis and tumor development. We designed a mitochondrial-anchored biomimetic nanoplatfrom and studied its reversal of tumor hypoxia microenvironment underlying the mitochondria-located chemo-photothermal therapy. After shuttling into cancer cells, therapeutic payloads including cisplatin and Au nanozymes are controllably released in the ATP-overexpressed mitochondria. Cisplatin generates $O_2^{\bullet-}$, forms H_2O_2 for chemical fuels in the next reaction, and damages mitochondrial DNA. Catalase-like Au nanozymes catalyze the produced hydrogen peroxide for oxygen supply to relieve hypoxic tumor microenvironment, offering cytotoxic singlet oxygen against cancer cells under NIR treatment. These findings reinforce the synergistic effect of organelle-specific navigation and in situ oxygen self-sufficiency for combinational chemo-photothermal therapy of cancer.

microRNAs (miRNAs) are expected as genetic tools to rescue damaged myocardium, while therapeutic efficiencies of liposomes and viral vectors delivery have struggled with inefficient intracellular delivery, susceptible inactivation, or immunogenicity. Our work established a nanoparticle-patch system for lysosome-specific delivery of miRNAs in the murine myocardial ischemia-reperfusion injury model. Loaded with miRNAs, ZIF-8 nanoparticles leveraging proton sponge effect enable miR-30d to escape endocytic pathway, thus avoiding premature degradation in lysosomes. Meanwhile, the conductive microneedle patch offers a distinct advantage by intramyocardial administration for localized, effective, and sustained miRNAs delivery, and it simultaneously releases Au nanoparticles to reconstruct electrical impulses within the infarcted myocardium. Consequently, our work incorporated the conductive microneedle patch and miRNA nano delivery systems to synergistically transcend the limitations of common RNA transfection methods.

The two works mentioned above are my recent publications, and my efforts in designing organelle-specific delivery systems are ongoing. We aim to continue integrating insights from the materials chemistry of nano delivery systems with the biological processes of organelle-targeted drug delivery, thus addressing unmet clinical needs and fully realizing the potential of nanoparticle technologies for patients.

References

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Lignin-Based Nanofertilizers for Controlled Release of Phosphorous

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Abstract

One of the main challenges imposed by the rapid growth of the global population is the increase in food production, and therefore in crop yields. To do this, the amount of agrochemicals applied to our fields must also increase. A smarter and more sustainable way to address this challenge is to improve the efficiency of our agricultural technologies. Currently only a small part of the huge amount of nitrogen and phosphorous we supply to the soil is absorbed by crops (50% of N and 15% of P),^[1] while the rest is lost in the environment due to run-off, leaching and evaporation. This is not only a massive waste of resources, but also has terrible effects on the environment, such as water eutrophication and other forms of ecosystem pollution.^[2] Nanotechnology can play a key role in improving the effectiveness of fertilization.^[3] However, most of the nanomaterials developed so far for agriculture are simple nanosized formulations of the plant nutrient, while much greater efforts can be made to optimize the release of the active ingredient.

Herein, lignin nanoparticles were synthesized to provide phosphorous to plants in a well-controlled manner. A nitrogen-enriched lignin was crosslinked with a phosphorous containing molecule to develop particles of 200 nm size. These particles were conceived to be degraded by an enzyme produced by the plant roots, so that they can release the nutrients mainly in the plant proximity. The nanofertilizers showed great efficiency in controlled phosphorous release both in laboratory experiments in aqueous solution and in pot tests on *Arabidopsis thaliana*. These nanoparticles are promising tools for supplying nitrogen and phosphorous to crops in a smart and controlled way, avoiding nutrient losses in the environment and enriching the soil organic matter with lignin.

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Image Analysis of Mycelium Growth on High-Content Spent Coffee Grounds for the Fabrication of Mycelium-Based Composites

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Abstract

Mycelium-based composite (MBC) can replace hydrocarbon-based packaging materials due to the network of mushroom mycelium grown on agricultural wastes [1-2]. MBC is a sustainable solution for recycling waste, low-carbon production to fulfill a circular economy. As urban organic wastes, spent coffee grounds (SCG) can be utilized as a supplement for growing mushrooms with a maximum content of up to 33% [3]. Nevertheless, there are few studies about the fabrication of MBC derived from SCG. This research studied the growth of *Pleurotus ostreatus* mycelium on the high-content SCG substrate mixing with rice husks (RH) using an image processing technique to serve as the preliminary information for the fabrication of MBC grown on SCG. The mycelium growth was simulated by tracking the growth of master spawn on three compositions of substrates: 100% SCG, 50%SCG – 50%RH, and 100%RH on Petri dishes. Figure 1 shows that although 100%RH contained the least initial master spawn, 5.24%, the mycelium grown on the rice husks was the fastest from day 7. The growth of mycelium on 50%SCG – 50%RH was faster than 100%SCG as the higher content of lignocellulose in rice husks. It was found that the mycelium growth on 100%SCG was constant from day 10 to 20, then, it grew rapidly but did not fully cover the Petri dish. The results provided beneficial information for fabricating MBC with high-content SCG for the efficient recycle in the line of zero-waste strategy.

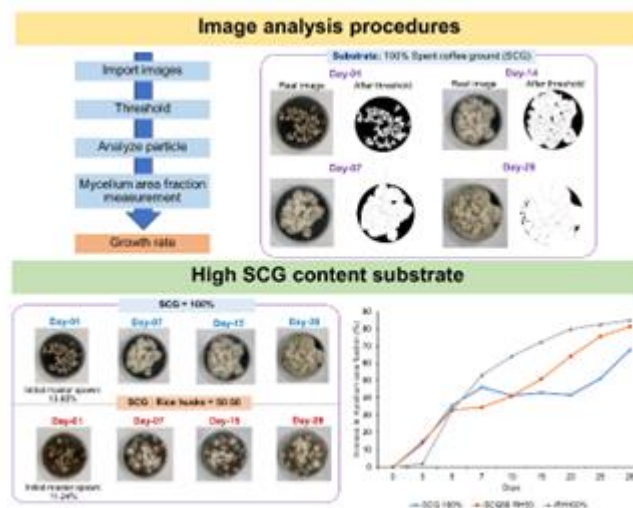


Figure 1. The image analysis procedures to track the mycelium growth rate on a high-content SCG and the growth rate mycelium on 100%SCG and 50%SCG – 50%RH

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Utilizing Lignin for a circular sustainable solution

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Abstract

Agricultural fungicide pollution is a huge environmental issue, which also has a negative impact on human health. Therefore, strategies to limit fungicide pollution are in high demand. Lignin is the second most abundant biopolymer on earth, mostly produced as a waste byproduct of paper production. Lignin biodegrades in the presence of laccase, which is present in some of the fungi that infect plants and agricultural produce, including *Fusarium*, which infects tomato plants. In this research we tested two plant protection approaches, layer-by-layer encapsulation of spores and lignin encapsulation of green Silver nanoparticles (AgNP). We relied on the degradation of the lignin by laccase to deliver plant protection when exposed to fungus.

The fungal strain *Trichoderma* is active against different pathogenic fungi making it a potential candidate for both improved and sustainable plant protection. However, using bio-control agents like *Trichoderma* create new challenges of instability upon exposure to physical stimuli and long-term storage, making it an inefficient solution. To overcome these drawbacks, we developed a mild and scalable encapsulation method of *Trichoderma* spores using a biopolymer layer-by-layer (LbL) approach. We prepared the encapsulated spores by applying alternate layers of cationic and anionic lignin polyelectrolytes implementing the promising protective properties of this polymer to the spores. We characterized the cationic and anionic lignin for naked- and encapsulated spores which were exposed to high (50°C) and low (-20°C) temperatures, UVC and UVB light, and long-term storage using germination tests to determine if spore stability was improved by encapsulation.[1]

AgNP are promising agents to improve agricultural crop growth and yield by enhancing seed germination, increasing water and fertilizer efficiency and providing antibacterial, antifungal, anti-inflammatory, and anti-angiogenic properties. However, their limited shelf life and need for repeated application are drawbacks. Therefore we encapsulated green AgNP, produced from grass waste or lignin capped AgNP, in lignin to provide targeted on-demand delivery of sustainable agrochemicals without chemical fungicides. The effectiveness of lignin-AgNP capsule in suppressing *Botryosphaeria dothidea* (Bot) and *Trichoderma* spores were tested in vitro.

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End-of-Life management of silicon photovoltaics: Recycling and Repurposing

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Abstract

The growth of photovoltaics (PV) has been fuelled by the global shift towards greener energy source, continuous technological advancements in module and cell designs, and increasing affordability of PV modules [1]. However, the growth inevitably brings about end-of-life (EOL) management challenges. A typical PV module is warranted to last 25 years before it gradually reaches its end-of-life (EOL) [1]. Other factors such as damage due to improper installation, damage during transportation and operational lifetime can result in failure of modules before their intended useful lifespan. These in turn leads to early-loss and contribute to EOL PV modules [1]. The cumulative waste volume of EOL PV modules is projected to rise to an alarming level of 60 and 78 million tonnes by 2050 in a regular-loss and an early-loss scenario respectively [1]. These modules contain valuable materials such as silver, silicon and copper which should not be buried in landfill and left idle [2]. Instead, the materials can be recovered through recycling, thereafter re-introduce into supply chain or re-purpose for other applications.

Current recycling strategies established for silicon photovoltaic mainly adapt high-temperature burning and/or mechanical treatments [3]. High-temperature burning not only consume large amount of energy, but also possibly emits noxious fluorinated by-products. Mechanical treatments reported to date generally focus on glass removal followed by thermal or mechanical processes to separate the different components. These approaches stop at this juncture and barely address metal extraction and recovery to achieve a more complete recycling process. Our team aims to (i) develop low-temperature techniques for delamination and liberation of embedded materials [4], (ii) design mechano-chemical/chemical processes for metal extraction and recovery [5] and (iii) demonstrate repurposing applications of recovered materials from silicon photovoltaics [6-8].

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Nanoscale Surface Chemistry for Next-Generation Energy and Optoelectronics Technologies

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Abstract

The research area of surface chemistry and optoelectronic devices focuses on the investigation and manipulation of chemical processes and interactions occurring at the interfaces of materials used in devices that convert light into electrical energy or vice versa. Achieving commercial viability in perovskite solar cells require enhanced stability, a multidisciplinary approach in material design, advanced characterization, device engineering, and in-depth mechanistic understanding. Surface chemistry plays a crucial role in solar technologies as it often dictates the optical and electronic properties of semiconductor materials and device interfaces. Here, I will discuss the work on the discovery of non-invasive ligands using surface-sensitive spectroscopy that stabilizes interfaces of perovskite solar cells at elevated operating temperatures. I will then describe the development of conformal self-assembled monolayers, aided by surface chemistry and molecular dynamics simulations, leading to low-loss hole-selective contacts for record solar cell performance. Finally, I will outline insights into material chemistry and strategies to address the current challenges in the field of emerging photovoltaics, highlighting the potential advancements for optoelectronic innovation.

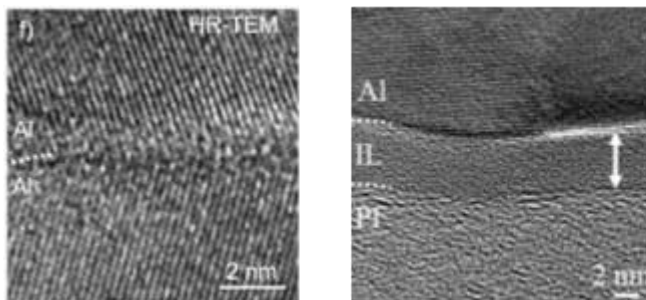
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Designing interfaces in thin films via atomic and molecular layer deposition

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Atomic and molecular layer deposition (ALD/MLD) hold enormous potential to design interfaces with tailored mechanical or functional properties, due to the unique way in which materials are built in an atomic layer-by-layer fashion and can reach deepest trenches and pores. When combined with other thin film techniques, such as magnetron sputtering (PVD), without breaking vacuum, the layer-by-layer nature of ALD/MLD can be harvested to design (sub)nanoscale interface and nanolaminates architectures with extremely good control over the layer thicknesses. For metal-oxide interfaces (Al/Al₂O₃), the minimum ALD layer thickness of one monolayer (nominal thickness 0.14 nm) far exceeds the thickness restrictions of natural oxidation of Al (2-10 nm [1]). High resolution TEM of a single Al₂O₃ ALD cycle (Figure 1, left) shows a distinct but very narrow interface between two adjacent Al sublayers, with atom rows of adjacent Al layers convening without interruption at the single-cycle ALD layer. Resulting Al/Al₂O₃ nanolaminates exhibit a brittle-to-ductile transition and strengthening mechanisms in their mechanical deformation behaviour.

**Figure 1**

left: Interface between two PVD Al layers modified by a monolayer of Al₂O₃. [2] right: Interface between polyimide (PI) and Al, showing a 5 nm amorphous interlayer (IL) [3].

Another interesting area for this combined deposition approach are metal-polymer interfaces, where it is known that thin amorphous interlayers between metal film and polymer substrate favor strong and thermally resistant interfaces [4]. Until now, interlayer formation is governed by the film and substrate chemistry [5] and the deposition method, preventing high interface quality for the majority of material combinations and fabrication routes. Since ultrathin ALD and MLD layers uniquely resemble natural ones in terms of structure and chemistry, interlayer formation can, for the first time, be mimicked artificially to clarify the role of these structures in thin film delamination and reveal underlying mechanisms as a function of thickness and chemistry. Going one step further, trigger mechanisms in artificial interlayers for controlled delamination in conditions beyond those of standard usage, can be investigated for ease-of-recycling opportunities.

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Atomistic modelling on the structural and electronic properties of advanced two-dimensional materials

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Abstract

Ever since the successful isolation of graphene in 2004, two-dimensional (2D) materials have garnered much attention due to their vast possibilities of property tuning, making them promising candidates for various applications. Employing atomistic modelling via first-principles calculations, we performed a series of studies examining the nuances of tuning the structural and electronic properties of 2D materials, providing insights into the novel design of related devices.

A prevalent approach to property modulation is strain engineering. However, rippling—a consequence of the intrinsic instability in free-standing 2D sheets—becomes prominent, especially during in-plane compression. In the literature, this rippling phenomenon has been proven to have a contrasting, remarkable impact on the properties of different 2D materials. Using antimonene (single-layer antimony) as an example, we demonstrate a systematic way of examining the effects of rippling by comparing the flat and rippled structures under uniaxial in-plane compression. Rippled antimonene is shown to exhibit highly stable properties like the work function and band gap upon structural relaxation at a range of compression levels, closely resembling its pristine state. Conversely, various changes are observed in its flat counterparts. To explain the differences, we then systematically analysed the deformation mechanisms of the two deformation modes and their effects on the materials properties with the results of the structural geometry and density of states. The identification of optimal ripple amplitudes under such in-plane mechanical deformation for which the properties of the pristine condition can be recovered will be highly significant in guiding the rational design of antimonene-based devices.

Further, we delved into the impact of out-of-plane compression. The Fermi level pinning (FLP) phenomenon at metal–2D semiconductor contact can hinder the tuning efficacy. We performed a detailed investigation of contact systems formed by common electrode materials and 2D tin monoxide (SnO), a promising transistor channel material. By analysing the geometry, bonding strength, charge transfer and tunnel barriers of charges, and electronic properties, we unearthed the mechanisms behind FLP. We also propose the insertion of a graphene buffer layer at the contact, which efficiently alleviates the metal-induced gap states and enhances the tuning efficiency of out-of-plane compression. This work scrutinises the possibilities of employing monolayer SnO in field effect transistors by systematically examining its contact with various electrode materials and methods of property tuning. The established atomistic model can be modified in the future to accommodate other factors to assess their impacts on the contact performance and mechanical behaviour of related devices.

Engineering Sustainable Nano-bio Interfaces for Environmental and Biomedical Applications

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Abstract

Biocatalysis has become an indispensable tool for modern organic synthesis, both in academia and across the pharmaceutical and chemical industries[1-2]. New materials chemistry strategies have been employed to modulate and enhance enzyme activity, uncovering new frontiers in natural enzyme catalysis. The applicant mainly focused on four strategies to enhance the activity of biocatalysts. Firstly, enzyme structure was modulated by ultrasound to obtain the optimal conformation. Metal-organic frameworks (MOFs) were then employed to rapidly “lock” the activated but more fragile enzyme conformations. This rapid locking and immobilization of enzyme conformations in MOFs opens up new possibilities for the exploitation of highly efficient biocatalysts for diverse applications[3]. Secondly, hierarchically porous MOFs were created through controlled structural etching to enhance multi-enzyme and cofactor-dependent enzyme biocatalysis. The ease, low cost, and potential scalability of this semi-confined strategy make these hierarchically porous biocatalytic MOF microreactors promising candidates for diverse biotechnological applications [4]. Thirdly, multi-enzyme cascades were programmed in MOFs via a novel peptide-induced MOF super-assembly process, providing a concept to facilitate the fabrication of next-generation smart materials based on precision chemistry[5]. Finally, highly active ferric-centered single-atom catalysts (Fe-SACs) were successfully developed via a biomineralization strategy. This strategy enables the homogeneous encapsulation of metalloproteins within MOFs, followed by pyrolysis. The results demonstrate that the constructed metalloprotein-MOF-templated Fe-SACs achieve up to 23-fold and 47-fold higher activity compared to those using metal ions as the single-atom source and those with large mesopores induced by Zn evaporation, respectively, as well as up to 25-fold and 1900-fold higher catalytic efficiency compared to natural enzymes and natural enzyme-immobilized MOFs [6]. We expect that continued ingenuity in materials development, along with the growing power and complexity of protein engineering techniques, will provide boundless surprises in the field of biocatalysis.

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Tuneable Optical Properties of Carbon-based Quantum Dots through Nitrogen Functionalization for Biomedical and Informatic Security Applications

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Abstract

Carbon-based quantum dots (QDs) are versatile nanomaterials with superior optical and electrical properties, making them ideal for optoelectronics, sensors, catalysts, and biomedical applications. This study focuses on the tuneable optical properties of carbon-based QDs achieved through nitrogen functionalization, targeting both biomedical and informatic security applications.

A rational design approach was employed with a facile synthesis method and in-situ functionalization to tailor the photoluminescence and absorption properties of carbon QDs. Experimental and computational studies elucidated the underlying role of nitrogen functionalization, demonstrating the successful tuning of QD emission from blue to yellow emission and a tuned absorption spectra from the UV to the first NIR window region (650-900 nm), ideally for biomedical applications, including biolabeling and photothermal cancer therapy.

For informatic security, a room-temperature phosphorescent (RTP) QDs was synthesized and optimized using machine learning. These QDs showed blue emission under UV light and a green afterglow lasting up to 7 seconds, useful for dynamic, time-dependent displays in high-level information encryption. This study provides a comprehensive understanding of nitrogen functionalization's role in tuning the optical properties of carbon-based QDs, advancing their applications in biomedical and security technologies.

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**Additively Manufacturing Smart Cellular Materials:
Impact Energy Absorbers for Space Applications**

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Abstract

Metallic cellular materials, such as lattices and honeycombs, are of interest in the design of lightweight and impact-resistant structures (high energy absorption capacity). However, the use of cellular materials in engineering applications has been hindered due to the challenges associated with the fabrication of such complex geometries. Additive manufacturing (AM) technologies have enabled the fabrication of geometries of significant complexity. Nevertheless, the design optimization of AM cellular materials for high strain rate loading scenarios remains relatively underdeveloped. Furthermore, even if those material structures dissipate energy efficiently during dynamic crushing, they do not recover their shape after impact. It is, therefore, necessary to understand the relationship between the AM process parameters, cellular material structures and dynamic performance, but also to develop the recovery of those structures after suffering an impact.

In this work, the opportunities created by additive manufacturing processes have been explored by: (1) studying the process-geometry-property interactions of metallic cellular materials, and (2) manufacturing cellular structures which can exhibit a functionality through shape memory effect. Firstly, quasi-static and dynamic mechanical testing on stainless steel 316L cellular geometries is combined with a wide range of material characterization techniques to understand the interplay between AM process parameters, geometry and high strain rate performance. Five cellular structures were investigated, finding that the geometry played a dominant role, relative to the Laser Powder Bed Fusion (LPBF) AM process [1]. Secondly, bulk and complex cellular structures that exhibit shape memory effect have been successfully manufactured. A diamond lattice structure and a new auxetic structure obtained through topology optimization recovered up to 70% their shape after impact. The main motivation and focus are on space applications to mitigate against impacts but this research is of relevance to a wide range of sectors: e.g., automotive crashworthiness, structural defence, and civil blast protection [2, 3].

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Boosting Efficiency in Wide-Bandgap Pb-Free Perovskite Solar Cells with 4-Phenylthiosemicarbazide Additive: Achieving Over 12.2% Performance

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Abstract

The utilization of wide-bandgap (WBG) tin halide perovskites (Sn-HPs) presents an eco-friendly alternative for multi-junction Sn-HP photovoltaics. However, their rapid crystallization results in suboptimal film morphology and the creation of defect states, compromising device efficiency. This study introduces 4-Phenylthiosemicarbazide (4PTSC) as an additive to achieve densely packed Sn-HP films with fewer imperfections. The strong chemical coordination between SnI_2 and the functional groups $\text{S}=\text{C}-\text{N}$ ($\text{Sn}\cdots\text{S}=\text{C}-\text{N}$), $-\text{NH}_2$, and phenyl conjugation enhances solution stability and delays perovskite crystallization through adduct formation. This process yields a pinhole-free film with preferred grain growth. 4PTSC acts as both a strong coordination complex and a reducing agent, passivating uncoordinated Sn^{2+} and halide ions while reducing SnI_4 formation, thereby minimizing defect formation. The π -conjugated phenyl ring in 4PTSC promotes the preferred crystal growth orientation of perovskite grains. Additionally, the hydrophobic nature of 4PTSC mitigates Sn^{2+} oxidation by repelling moisture, enhancing stability. A notable increase in open-circuit voltage was observed, rising from 0.78 V to 0.94 V with the 4PTSC-1.0 additive. The 4PTSC-1.0 enhanced device demonstrated a peak efficiency of 12.22%, surpassing all previously reported efficiencies for WBG Sn halide perovskite solar cells. Furthermore, the unencapsulated 4PTSC-1.0 device maintained outstanding stability for over 1200 hours under ambient atmospheric conditions.

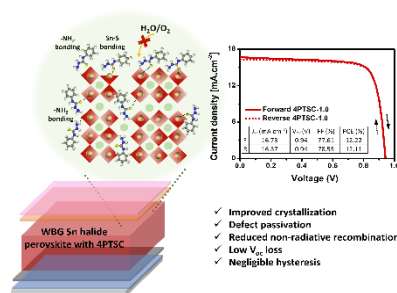


Figure caption. Plausible schematic illustration of the chemical coordination of 4PTSC additive with the perovskite defect passivation, and stabilization of the perovskite phase through Sn^{2+} coordination. Current density vs voltage (J-V) curves of 4PTSC-1.0 champion device in forward and reverse scans.

Post-Mortem Failure Analysis of Metal Halide Perovskite Modules

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Abstract

Metal halide perovskites are an emerging photovoltaic technology projected to play an important role in the clean energy transition due to their unprecedented solar cell efficiency rise to a record 26.1% for single-junction and 33.9% for Si/perovskite tandem in less than 15 years of research [1]. However, their lack of long-term operational stability in outdoor environments is a major hurdle to commercialization.

Perovskites are inherently sensitive to oxygen, moisture, heat, and light [2]. The degradation mechanisms have been extensively studied on a small area solar cell, however, scaling-up the technology reveals additional weaknesses, including processing heterogeneities, new interfaces from cell interconnection, and mechanical stresses during encapsulation. While various mitigation strategies are being developed to overcome chemical and thermo-mechanical stability issues [2], there is an urgent need to develop standardized and realistic accelerated stress testing protocols to objectively assess module performance and deepen our understanding of underlying degradation mechanisms. Only limited studies are currently available on module-level testing, with Perovskite PV Accelerator for Commercializing Technologies (PACT) center being in the forefront of this effort [3]. To date PACT has received and tested over 300 modules from 4 universities and 5 industry providers.

In the presentation I will show results of a post-mortem failure analysis of outdoor and indoor stress-tested perovskite modules. Tested modules were encapsulated with different encapsulation schemes (i.e., edge seal only, polymer-encapsulated). Depending on the type of encapsulation, field performance of tested modules varied from a few days to several months, with a current record of over 250 days above T80 (80% of module efficiency on day 1). Indoor testing applying light and elevated temperatures was found to most closely replicate the degradation seen outdoors. Chemical degradation in the scribe-line region interconnecting individual cells, void formation, and interfacial delamination were identified by post-mortem analysis as possible causes of the power loss observed in both outdoor and indoor testing, with the light at 75°C test condition significantly accelerating the degradation. Full encapsulation with a polymer in addition to an edge seal provides not only good barrier against moisture, but also mechanical support preventing premature interfacial delamination and suppressing outgassing of perovskite degradation biproducts. However, mechanical properties of the selected encapsulant were seen to play a crucial role in the product lifetime.

References

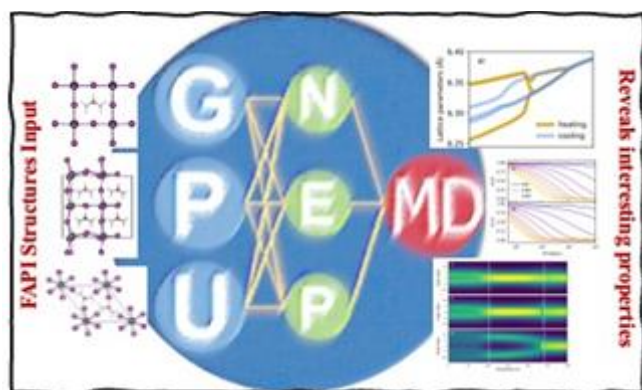
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Phase behaviour and dynamics of organic cations in Formamidinium Lead Iodide (FAPbI₃) using machine-learned potentials

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Abstract



Hybrid halide perovskites have received tremendous attention due to their promising applications in photovoltaics and optoelectronics, with FAPbI₃ emerging as one of the most interesting compounds, due to its tuneable stability. While it has already been extensively studied, there are remaining questions about its atomic structure and dynamics of FA cations, especially at low temperatures. In this context,

molecular dynamics simulations can bring insights into the unanswered questions. However, due to the chemical complexity, it is not trivial to construct a model for atomistic simulations of perovskites. Recently, the promise of machine learning has been demonstrated in simulating finite-temperature dynamics of complex materials using completely atomistic approaches with precision comparable to first-principles.

In the present study, we generate a machine-learned potential for FAPbI₃ using the Graphics Processing Units Molecular Dynamics (GPUMD) package [1] to study the phase behaviour and dynamics of FA molecules in FAPbI₃. We carry out MD simulations to understand the structural phase space of the material. Our machine-learned potential successfully captures all the phase transitions reported in the literature [2,3]. Additionally, we analyse the octahedral tilting and preferred FA orientations in each phase, which further sheds light on understanding the nature of the low-temperature phase of the material. Further, to understand the local symmetry we study the rotational dynamics of the FA molecules, leading to the discovery of a disordered glassy state at low temperature.

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Harnessing AI for Advanced Nanomaterials Synthesis and Engineering

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Nanomaterials, with their unique properties and immense potential, are at the forefront of technological advancements across various fields, from electronics to biomedicine. However, the synthesis of nanomaterials involves complex and multi-parameter processes that present significant challenges. Traditional trial-and-error approaches to optimizing synthesis conditions are time-consuming, resource-intensive, and often inefficient, necessitating a more innovative and systematic solution.

In this poster presentation, we explore the transformative role of artificial intelligence (AI), particularly machine learning (ML), in addressing these challenges. By leveraging ML's ability to uncover complex relationships within data, we can significantly enhance the efficiency and yield of nanomaterials synthesis [1-2]. We will highlight our recent achievements in ML-guided synthesis of nanomaterials through two representative case studies. The first case demonstrates the successful implementation of supervised ML for the chemical vapor deposition synthesis of high-quality few-layered WTe₂ [3]. This approach has enabled precise control over the formability and morphology of WTe₂, leading to breakthroughs in fabricating 1D WTe₂ nanoribbons. The second case illustrates the application of ML for multi-objective optimization in the hydrothermal synthesis of carbon quantum dots (CQDs). By optimizing various synthesis parameters simultaneously, we achieved superior optical properties in CQDs, including full-colour emission and high photoluminescence quantum yield, surpassing traditional synthesis methods [4].

This poster presentation aims to demonstrate how integrating AI with materials science not only accelerates the development of nanomaterials but also opens new avenues for innovation. By refining the synthesis process, we can unlock the full potential of nanomaterials and drive advancements in various technological fields.

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High performance p-channel printed transistors on biodegradable PVA substrate for Transient Electronics

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Abstract

The future electronics demands for a biodegradable, flexible, wearable, durable, cutting-edge transient electronics with superior performance using innovative fabrication techniques on green substrates.¹ In a way, electronics on degradable substrates alleviate the major challenge of electronic waste (e-waste). On the other hand, in transistors technology, currently the lack of stable p-type semiconductors with high hole mobility severely restricted their usage entering the electronic industries.² Herein, we try to address both the challenges by introducing an emerging tellurium material for the fabrication of transistors on a completely biodegradable PVA substrate using an electrolytic double layer insulator with top gated geometry via a high throughput inkjet printing method. The fabricated transistors demonstrate high hole mobility of $30 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, On/Off ratio of $>10^5$ with the excellent on-state conductance alongside having negligible hysteresis value all achieved at near room temperature. Finally, we studied the device degradability test by storing them in DI water and found that the samples start to degrade within 2 hours and completely vanishes by the end of 7 days. These results demonstrate the potential of printed electronics for high-performance transient electronics and as the new avenue toward zero e-waste. Also, the TFTs on biodegradable green substrates one may foresee their applications in use-and-throw electronic devices.

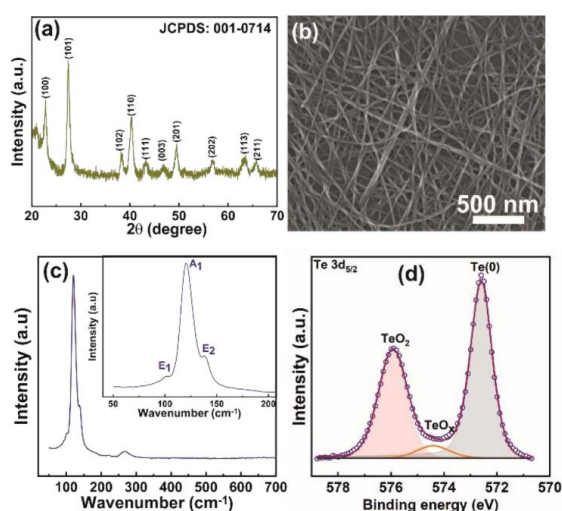


Figure 1: (a) XRD pattern of the as-synthesized Te nanowires synthesized in water via hydrothermal method. (b) SEM of the Te nanowire (c) Raman spectrum of the same sample showing the E₁, A₁ and E₂ vibrational modes (d) XPS Te 3d_{5/2} spectra of a Te nanowire sample obtained in water after purification and drying at 50°C in air.

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Resistive Switching in Hybrid Organic-Inorganic Halide Perovskite Memristors

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Abstract

Resistive switching property in hybrid organic-inorganic halide perovskites has garnered significant interest in recent years due to their mixed ionic-electronic conductivity, promising advancements in next-generation memristors for neuromorphic computing applications [1]. Ion migration, inherent to these perovskites, results in mobile ion redistribution and the formation of vacancies and interstitials, impacting charge transport under an electric field [2]. Memristors leverage this ion migration dynamics to modulate memory windows, offering versatile functionalities crucial for in-memory computing [3]. While halide perovskite materials are prone to degradation in humid and oxygen-rich environments, their superiority over conventional oxide-based memristors lies in their facile fabrication process, flexibility, and low processing temperatures [4].

In this work, resistive switching characteristics of memristors based on the standard halide perovskite Methylammonium Lead Iodide ($\text{CH}_3\text{NH}_3\text{PbI}_3$) thin films are explored, and the ITO/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ /Au device performance is investigated for varied film thicknesses. Notably, the device with ≈ 400 nm exhibits higher ON/OFF current ratio, which can be attributed to a reduction in the high-resistance state current [4]. The X-ray diffraction pattern and morphology of the $\text{CH}_3\text{NH}_3\text{PbI}_3$ thin film corresponding to this device are shown in figures (a) and (b), respectively. These results strongly suggest that resistive switching properties of hybrid organic-inorganic halide perovskite memristors can be tuned for desirable ON/OFF ratio using facile deposition methods.

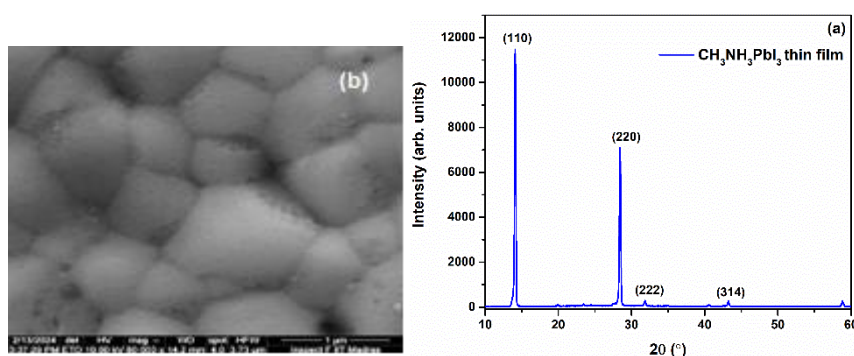


Fig. (a) X-ray diffraction pattern and (b) SEM image of the $\text{CH}_3\text{NH}_3\text{PbI}_3$ halide perovskite thin film

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Optimization of chitosan-based membranes for in vitro permeability analysis of trace elements from cosmetic and personal care products using inductively coupled plasma mass spectrometry (ICP-MS)

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Abstract

As cosmetic and personal care products are ubiquitous and often used daily, the determination of trace elements is imperative to ensure their safety. Through risk assessment studies, regulations to protect environmental and human health can be strengthened. Quantitative and qualitative risk assessments often involve in vitro and animal studies that evaluate exposure to individual elements. These studies may not account for real-world factors such as multi-elemental exposure, chemical interactions, and varying exposure frequency. The development of in vitro study models for risk assessment of trace elements, especially their permeation across the skin is important to address these shortcomings. Inductively coupled plasma – mass spectrometry (ICP-MS) was used to determine the concentration of trace elements (Al, V, Cr, Mn, Ni, Zn, As, Se, Cd, Hg, Pb) in commercially available cosmetics.

Using chitosan-based membranes, synthesized to mimic human skin, and 3D-printed diffusion cells, the concentrations of trace elements that permeate across the dermal layers were determined. This study further optimized the chitosan membrane to address the anatomical variations of skin relating to different body sites, age, sex, pigmentation, and health conditions. By understanding how a variety of products including hair, face, body and lip react to these various conditions, we can comprehensively evaluate the permeability of these heavy metals, using ICP-MS. The suitability of the membranes for this experiment in representing “real skin” will be assessed by comparing them with Strat-M® membranes which have been shown to resemble human skin through permeability in vitro experiments [1]. The chitosan membranes are designed to offer flexibility at low-cost while being biodegradable and helping to accurately determine the risk associated with cosmetic and personal care products in relation to human health.

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