GLOW2025

GLObal Conference for Women Leaders and Emerging Researchers in Materials Science

GLObal Conference for Women Leaders and Emerging Researchers in Materials Science, held in Nanyang Technological University, Singapore from 29 September to 1 October 2025, is a platform to shine a spotlight on the remarkable contributions of women talents in the field of Materials Science.

Participants will explore the latest advancements and emerging trends in materials science, spanning:

- Computational and Characterisation
- Future Electronics / Nanomaterials
- Healthcare
- Machine Learning & Artificial Intelligence
- Sustainability and Energy

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 2025 offers you new insights and opportunities in your Science and Engineering journey.

FROM LAB TO LEADERSHIP :

WOMEN SHAPING THE FUTURE OF SCIENCE

Monday, 29 September 2025

Day 1:

08.30 – 09.30	Registration
09.30 – 09.40	Opening Address *Professor Ernst Kuipers* *Vice President (Research) and Distinguished University Professor* *Nanyang Technological University, Singapore*
09.40 - 09.50	Welcome Speech *Professor Lee Pooi See* *Chair, GLOW2025 Committee* *Nanyang Technological University, Singapore*
	FUTURE ELECTRONICS / NANOMATERIALS
09.50 - 10.20	Keynote 2D Materials as Building Blocks for Next-Generation Advanced Materials *Professor Dr.-Ing. Suelen Barg* *University of Augsburg, Germany*
10.20 - 10.40	Transparent, Patternable and Stretchable Conducting Polymer Solid Electrode for Dielectric Elastomer Actuators *Miss Eunyoung Kim* *Stanford University, USA*
10.40 - 11.10	Tea break
11.10 - 11.30	Development of Screen-Printed Boron-doped Diamond Nanoparticle for Electrochemical Sensor Application *Assistant Professor Prastika K. Jiwanti* *Universitas Airlangga, Indonesia*
11.30 - 11.50	Design and Validation of Laser-based Vibrational Circular Dichroism Spectroscopy using Digitally Referenced Detection *Miss Ruo-Jing Ho* *University of Illinois at Urbana-Champaign, USA*
11.50 - 12.20	Keynote Advancing Sustainable Electronics: Design of Biodegradable Materials for Healthcare Applications *Associate Professor Shweta Agarwala* *Aarhus University, Denmark*

12.20 - 14.00	Networking Lunch & Poster Session (*Poster Award Judging: Shortlist for Finals*)
	SUSTAINABILITY & ENERGY
14.00 – 14.30	Keynote Materials Revolution: SMaRT Technologies and MICROfactories™ Creating Sustainable Materials and Products from Waste Resources *Professor Veena Sahajwalla* *University of New South Wales, Australia*
14.30 – 14.50	Ferroelectric Polarization for Enhanced Photoelectrochemical Reaction *Dr Cui Ying Toe* *The University of Newcastle, Australia*
14.50 – 15.10	Driving the Performance and Stability of Vapour-Deposited Perovskite Solar Cells via Composition and Interface Engineering *Miss Siyu Yan* *University of Oxford, UK*
15.10 – 15.40	Tea break
15.40 – 16.00	Synthesis and Characterization of Earth-Abundant Chalcogenide Perovskite $BaZrS_3$ for Photovoltaic Applications *Miss Kiruba Catherine Vincent* *Purdue University, USA*
16.00 – 16.30	Keynote Biomaterials for Sustainable Foods of the Future *Associate Professor Nicole Tichenor Blackstone* *Tufts University, USA*
16.30	Conference Ends

Tuesday, 30 September 2025

Day 2:

COMPUTATIONAL & CHARACTERISATION	
09.30 – 10.00	Keynote Operando 3D Imaging of Solid Materials Professor Mizuki Tada Nagoya University, Japan
10.00 – 10.20	Building Nanoscale Laboratory using In-situ Electron Microscopy: From Nanomaterials Dynamics to Computational Imaging *Dr Serin Lee* *Stanford University, USA*
10.20 – 10.40	Unveiling Novel Phases in van der Waals Layered Magnets *Dr Shiyu Deng* *Institut Laue-Langevin, France*
10.40 – 11.10	Tea break
11.10 – 11.30	Hyper-gap Transparent Conductor *Miss Zhengran Wu* *Institute of Physics, Chinese Academy of Sciences, China*
11.30 – 12.00	Keynote Electricity and Fuels from the Sun: Understanding and Controlling Electron and Energy Transfer Reactions in Solar Energy Conversion Materials *Professor Maria Abrahamsson* *Chalmers University of Technology, Sweden*
12.00 – 14.00	Networking Lunch & Poster Session (*Poster Award Judging: Finals*)
14.00 – 15.00	PANEL DISCUSSION: Innovation: Caught or Taught?
HEALTHCARE	
15.00 – 15.30	Keynote Multiphoton Microfabrication and Micropatterning (MMM) – A "Programmable" Cell Niche Engineering Technology *Professor Barbara Chan* *The Chinese University of Hong Kong, Hong Kong*
15.30 – 15.50	Skin-Interfaced Flexible Sensors *Dr Yichen Cai* *Nanjing Tech University, China*

15.50 – 16.20	Tea break
16.20 – 16.40	From 2D to 3D Electrochemical Microfabrication of Zinc Architectures: Synthesis, Microstructure, and Mechanical Properties Characterization *Dr Maria Watroba* *Empa Swiss Federal Laboratories for Materials Science and Technology, Switzerland*
16.40	Conference Ends

Wednesday, 1 October 2025

Day 3:

MACHINE LEARNING & ARTIFICIAL INTELLIGENCE	
09.30 – 10.00	Keynote Leveraging Experimental Data in Machine Learning and Screening to Get From Computational Model to Real World Materials Fast *Professor Heather J. Kulik* *Massachusetts Institute of Technology, USA*
10.00 – 10.20	Chalcogenide Perovskites: A New Class of Functional Materials? *Assistant Professor Lucy Whalley* *Northumbria University, UK*
10.20 – 10.40	Bridging Atomistic Simulations and Real-World Catalyst Behaviours: A Multiscale Approach *Dr Xiaoyan Li* *Northwestern University, USA*
10.40 – 11.10	Tea break
11.10 – 11.30	Tuning Metastability and Deformation Mechanisms in High Entropy Alloys using Genetic Algorithm Machine Learning Predictions of Gibbs Free Energy *Miss Swati Mahato* *Indian Institute of Technology Kanpur, India*
11.30 – 12.00	Keynote Learning from Nature, Mathematics, and Artificial Intelligence for Sustainable Materials Design and Manufacturing *Assistant Professor Grace Gu* *University of California, Berkeley, USA*
12.00 – 12.20	An Insider's View of Nature Journals *Dr Wenjie Sun* *Senior Editor, Nature Nanotechnology* *Springer Nature, China*
12.20 – 12.40	Travel & Poster Award Presentation
12.40 – 12.50	Conference Closing Remarks *Professor Ng Kee Woei* *Chair, GLOW2025 Committee* *Nanyang Technological University, Singapore*

12.50 – 14.00	Networking Lunch
14.00	Conference Ends

KEYNOTES

FUTURE ELECTRONICS / NANOMATERIALS

Professor Dr.-Ing. Suelen Barg
University of Augsburg, Germany

Suelen Barg is a professor at the Materials Resource Management Institute, University of Augsburg, leading a research group towards the development of advanced materials solutions based on ceramics and 2D Materials with a focus on sustainable and digital materials development. Prior to her current appointment, she was a senior lecturer and group leader at the University of Manchester, specializing on 2D Materials, particularly MXenes and their processing into functional devices. She has obtained a doctoral degree in ceramics colloidal processing from the University of Bremen, followed by postdoctoral trainings in the areas of graphene-related 2D materials and bio-inspired composites at Imperial College London.

2D Materials as Building Blocks for Next-Generation Advanced Materials

Suelen Barg

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Abstract

The integration of 2D materials into diverse substrates, matrices, and architectures opens new avenues for designing advanced materials with enhanced performance and scalability. Among them, graphene and MXenes stand out for their potential to address diverse energy, environmental, and manufacturing challenges. These materials offer exceptional electrical conductivity, surface functionalization capabilities, and compatibility with colloidal processing, making them ideal candidates for next-generation devices and systems.

In this talk, we focus on the use of $Ti_3C_2T_x$ MXene as a model 2D material for colloidal-based fabrication techniques, highlighting its additive-free aqueous processability and the elimination of reductive steps required by other 2D systems. We explore how such unique features enable the efficient design and manufacturing of advanced material systems through techniques such as freeze-assisted tape casting and extrusion-based 3D printing. The potential of these approaches is illustrated through selected case studies, including: fabrication of vertically aligned $Ti_3C_2T_x$ films and multi-material heterostructures ($Ti_3C_2T_x$–hBN–$Ti_3C_2T_x$) for flexible, high-performance supercapacitors; the development of $Ti_3C_2T_x$-based aerogel composites for efficient electrothermal heating; and the creation of MXene-based printable ceramic formulations, optimized via data-driven tuning to enable sustainable structural ceramics.

These examples highlight the role of 2D materials and colloidal processing in accelerating the development of next-generation technologies, while also supporting the transition toward sustainable, scalable, and multifunctional material platforms.

FUTURE ELECTRONICS / NANOMATERIALS
Associate Professor Shweta Agarwala
Aarhus University, Denmark

Shweta Agarwala is full Professor and Associate Dean at the School of Engineering and Applied Science at Ahmedabad University, India where she leads the pioneering Green Materials and Devices Laboratory. Her interdisciplinary work focuses on the development of sustainable electronic materials and devices, with a vision to drive environmental responsibility in electronics through the creation of fully biodegradable and flexible devices. She completed her Master's degree at Nanyang Technological University (Singapore) and earned her PhD from the National University of Singapore. She was a tenured professor at Aarhus University, Denmark. An active contributor to the scientific community, Shweta has authored over 70 peer-reviewed publications in prestigious journals, books, and conferences. She is co-founder of many ventures. She is a senior IEEE member and is dedicated to advancing gender diversity in engineering.

Advancing Sustainable Electronics: Design of Biodegradable Materials for Healthcare Applications

Shweta Agarwala

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Abstract

The electronics industry is a major contributor to global carbon emissions and e-waste, posing serious environmental and health challenges. As demand for electronic devices surges, aligning the sector with the United Nations Sustainable Development Goals (SDGs) is both urgent and essential. Our research addresses this challenge by developing a novel library of sustainable electronic materials through green chemistry principles. These materials are designed to replace conventional toxic, non-biodegradable components commonly found in electronic devices.

We employ multifaceted strategies- integrating fillers, fluoropolymers, interfacial engineering, and crystallinity enhancement to engineer materials that are not only biodegradable but also suitable for high-performance electronic applications. These materials are formulated into printable inks, enabling energy-efficient, scalable manufacturing through printing techniques. Our primary application focus is in the healthcare sector, where biocompatibility and controlled biodegradability are critical. To validate environmental impact and performance, we assess our materials using established biodegradability standards and conduct comprehensive end-of-life cycle assessments. Our research represents a significant step toward reducing the ecological footprint of electronics and fostering a circular economy aligned with sustainable development.

SUSTAINABLITY & ENERGY

Professor Veena Sahajwalla
University of New South Wales, Australia

Australian Research Council (ARC) Laureate Professor Veena Sahajwalla is an internationally recognised materials scientist, engineer and inventor revolutionising recycling science. She is renowned for pioneering the high temperature transformation of waste in the production of a new generation of 'green materials.' In 2018 Veena launched the world's first e-waste MICROfactorieTM and in 2019 she launched her plastics and green ceramics MICROfactoriesTM.

She was the founding Director of the Centre for Sustainable Materials Research and Technology (SMaRT@UNSW) and held directorships at the ARC Industrial Transformation Research Hub for 'green manufacturing', the ARC Microrecycling Hub, and NESP Sustainable Communities and Waste Hub. Professor Veena has won several awards and awarded the 'Office of the Order of Australia' (AO) for distinguished service to science, sustainable materials research and technology and waste management in 2025.

Materials Revolution: SMaRT Technologies and MICROfactories™ Creating Sustainable Materials and Products from Waste Resources

Veena Sahajwalla

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Abstract

Waste is a resource that is waiting to be harvested through innovative pathways — it marks the beginning of renewable materials that could be regenerated for green manufacturing. Buried in discarded products when they reach the end-of-life or become obsolete are metals, polymers, and ceramics which could be remanufactured into new products, which are currently being pursued for single streams of materials where they are converted back into the same. However, our products are complex and contain mixed materials and are deemed as too hard to recycle and considered as not economically viable due to limitations of existing approaches. True sustainability demands we harness this potential and transform waste into a resource stream for advanced manufacturing. Instead of relegating waste to landfills, incinerators, or stockpiles, we must reimagine it as the cornerstone of a circular economy — one that drives innovation, supports local industries, creates jobs, and delivers environmental and social benefits. This presentation explores how so-called "end-of-life" materials can be transformed into high-value resources for sustainable production. SMaRT Centre is pioneering advanced technologies that align recycling and manufacturing of materials and products to deliver real-world impact. Through our science of microrecycling, we are able to challenge the norm, and have demonstrated that we could transform materials in manufacturing processes themselves. Among its most groundbreaking innovations is Green Steel Polymer Injection Technology ™ (PIT) , which enables the release of in-situ hydrogen and solid carbon from waste tyres in the making of green steel — a sustainable alternative to coke and coal in steel production [1]. This approach reduces the carbon footprint of steelmaking [2]. The Centre's Green Steel™ Polymer Injection Technology (PIT) also enhances electric arc furnace (EAF) steelmaking efficiency, and lowering reliance on coal and coke which are typically used as sources of carbon [3][4][5].

Through its science of microrecycling, SMaRT has developed modular, innovative solutions including MICROfactories™ that address some of the world's most problematic waste streams — including plastics, textiles, glass. These systems are already delivering measurable impact, transforming low-value, nonmetallic waste into durable Green Ceramics™ used in the built environment [6][7].

One of the advancements is the selective thermal transformation of waste materials into nanomaterials, such as metal oxides, and carbons through innovative techniques that introduce disruptions to the original structures of materials by controlling in-situ materials reactions. These nanomaterials can be repurposed for high-value applications, particularly in energy storage and supercapacitors [8][9][10][11]. This not only presents a strong economic opportunity but also delivers significant environmental benefits, proving that sustainable innovation and industrial value can go hand in hand.

SMaRT technologies and MICROfactories™ could drive materials circularity which could lead to industrial transformations enabling green materials to become mainstream in manufacturing — where waste becomes a renewable resource, reshaping the landscape of green manufacturing. New green supply chains could be developed to become a part of the ecosystem for remanufacturing, by forging pathways towards more sustainable industries that are good for the planet and people.

References

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SUSTAINABLITY & ENERGY
Associate Professor Nicole Tichenor Blackstone
Tufts University, USA

Nicole Tichenor Blackstone is an Associate Professor at Tufts University, with appointments in the Division of Agriculture, Food, and Environment in the Friedman School of Nutrition Science and the Department of Biomedical Engineering in the School of Engineering. Dr. Blackstone is a sustainability scientist who studies the environmental and social impacts of food system innovations, interventions, and policies. She is a founding affiliated faculty member of the Tufts University Center for Cellular Agriculture and Co-Project Director for the U.S. Department of Agriculture-funded National Institute for Cellular Agriculture. Currently, she leads / co-leads several cellular agriculture projects and the Leading a Sustainability Transition in Nutrition Globally (LASTING) Project. Dr Blackstone also collaborates with colleagues across disciplines and institutions.

Her research has been published in high-impact journals, such as *Nature Reviews Materials* and the *Lancet Planetary Health* and has been supported by over $13M of federal, philanthropic, and private sector funding to date.

Biomaterials for Sustainable Foods of the Future

Nicole Tichenor Blackstone[1,2], Amin Nikkhah[1], Edward B. Gordon[2], Reza Ovissipour[3], and David L. Kaplan[2]

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Abstract

With population growth and economic development, global demand for meat is projected to double by mid-century. This is happening amidst increasing, coupled pressures on planetary systems and food systems – from a changing climate and resource degradation to disease risk and food shortages. To help address these complex challenges, there is considerable interest in 'future foods.' These are "…foods for which our ability to produce considerable volumes is rapidly developing as a result of technological developments that offer the potential to scale production levels up and/or reduce the production costs out of concern for the environment" [1]. Biomaterials are key components in cellular agriculture and plant-based future foods production, providing nutrients in culture media or enhancing taste, texture, and stability of final products [2]. Because future foods aim to help solve environmental and societal challenges, environmental sustainability should be integral to their commercialization, alongside taste, texture, cost, and an understanding of broader social implications.

This talk will focus on sustainability assessment and optimization of two biomaterial applications for future foods: culture media components and scaffolds for cultivated meat. This will include our research on life cycle assessment (LCA) of commercial scale culture media using protein isolates [3], plant-based scaffolds, and multi-objective optimization of culture media using artificial intelligence [4]. Because much work on future foods is small scale with low technology readiness, I will present a new framework [2] on the integration

of process simulation, LCA, and technoeconomic analyses to inform future research on sustainable biomaterials development for future foods.

References

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COMPUTATIONAL & CHARACTERISATION

Professor Mizuki Tada
Nagoya University, Japan

Professor Mizuki Tada was received her Ph.D. at the department of chemistry, the University of Tokyo in 2005. She took up an assistant professor position at the University of Tokyo and moved to Institute for Molecular Science as an associate professor in 2008. She is a full professor of chemistry at Nagoya University since 2013. She worked at RIKEN as the team leader of element visualization team at SPring-8 during 2014-2019.

Her research interests are the surface design of metal-complex catalysts, heterogeneous catalysis on oxygen storage materials, and operando XAFS-CT imaging of functional materials (heterogeneous catalysts, MOFs, and fuel cells).

Operando 3D Imaging of Solid Materials

Mizuki TADA[1,2]

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Abstract

The solid structures of functional materials are heterogeneous and it is essential to understand their heterogeneous structures and real states related to their functions. The use of hard X-rays is promising for visualizing the structures and chemical states under operating conditions. The variety of X-ray imaging techniques has been achieved the two- or three-dimensional structural imaging with high spatial resolution, but the three-dimensional imaging of chemical states of each element in solid materials has been limited.

We have developed operando hard X-ray spectroimaging (XAFS-CT), combining X-ray absorption fine structure (XAFS) spectroscopy and computed tomography (CT) using synchrotron hard X-rays. The XAFS-CT imaging provides three-dimensional images of solid materials under working conditions, such as heterogeneous catalysts, the membrane electrode assembly of polymer electrolyte fuel cells, and metal-organic framework for guest adsorption [1-7]. The operando spectroimaging is one of the useful platforms to provide the statistic numbers of data of not only structures but also chemical states and performances of materials, which open new data-driven material science. In this paper, our recent examples of solid materials using *operando* XAFS-CT imaging will be presented.

References

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COMPUTATIONAL & CHARACTERISATION

Professor Maria Abrahamsson
Chalmers University of Technology, Sweden

Maria Abrahamsson is a full professor of physical chemistry at Chalmers University of Technology in Gothenburg, Sweden since 2022. She obtained her PhD in physical chemistry from Uppsala University in 2006, did her postdoctoral work at Johns Hopkins University (USA) as a recipient of the Swedish Research Council scholarship and joined Chalmers as an associate professor in 2015. Her current work is centered around understanding and controlling electron and energy transfer processes in a range of solar energy conversion materials including studies on multielectron transfer reactions, photon manipulation strategies such as singlet fission and photon upconversion, and photocatalytic CO_2-reduction. Her main experimental technique is based on time-resolved and steady state spectroscopy covering wide timescales, electro-chemistry and photocatalytic measurements.

Abrahamsson was the director for Chalmers' strategic research area in materials science between 2019-2024. She is currently the director of the Graphene Flagship CSA, a representative in the Wallenberg Initiative Materials Science for Sustainability (WISE) and sitting on several boards and councils in Sweden. Maria has received research grants, extensive supervision experience with Ph.D. students and postdoctoral researchers and active in innovation and outreach activities, including popular science lectures, podcasts and articles.

Electricity and Fuels from the Sun: Understanding and Controlling Electron and Energy Transfer Reactions in Solar Energy Conversion Materials

M. Abrahamsson[1]

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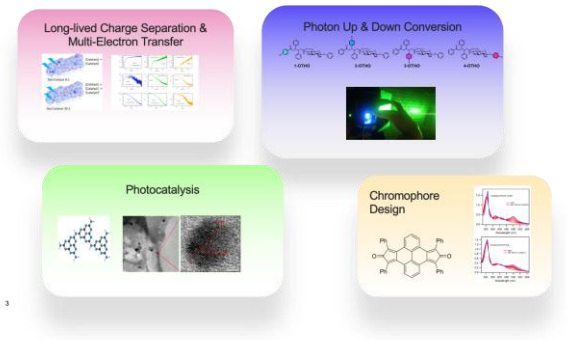
Abstract

Around 160 years ago, the first scientific article that showed that CO_2 is a greenhouse gas was published. Jump ahead to 1912 and the Italian photochemist Giacomo Ciamician stated that it would be wise to not use coal, but the sun, to satisfy our energy demands. Indeed, solar energy has tremendous potential to be a central part of the transition to a more sustainable society. If we can increase the efficiency of direct conversion of solar energy into useful forms by just 1%, it corresponds to more than the entire combined potential of all other types of renewable energy (nuclear not included). However, challenges remain, including how to better utilize all the solar irradiation and how to control light-induced multi-electron transfer reactions.

One of the avenues we are exploring concerns *singlet fission and photon upconversion materials* which can help overcome the thermodynamic efficiency limit of solar cell materials. Another branch of our research concerns how we can store solar energy in chemical bonds. This includes mechanistic studies of the *visible light-induced multi-electron transfer reactions with a focus on photocatalytic CO_2 transformation,* as well as fundamental mechanistic studies.



In the talk, I will give examples of how electron and energy transfer rates and yields in up- and down-conversion materials can be controlled. For example, we have shown that by changing the polarity of the surrounding solvent, we can control singlet fission dynamics on the femtosecond-picosecond timescales. To further understand the environmental effects, we have also studied well-known singlet fission and upconversion chromophores in gels, aiming at understanding of how self-assembly in the solid state can be used to achieve photon manipulation. I will also share some of our recent work on photocatalysis for efficient and selective CO_2 reduction in a fully aqueous solution using only benign elements, where we can produce CO with a turnover number (TON) exceeding 10^5 and selectivity ~96 % after 10 hours of visible light irradiation (400–700 nm).

The key to all research presented in this talk is the light-matter interactions and how we can control them.

HEALTHCARE
Professor Barbara Chan
The Chinese University of Hong Kong, Hong Kong

Prof. Barbara CHAN obtained her Bachelor degree in Biochemistry and PhD degree in Surgical Science from the Chinese University of Hong Kong. She received Postdoctoral Fellowship in Laser Medicine from the Massachusetts General Hospital in US. Prof. Chan served the Biomedical Engineering programme (University of Hong Kong) from 2003-2023 before serving School of Biomedical Sciences, Department of Biomedical Engineering, and Institute of Tissue Engineering and Regenerative Medicine at the Chinese University of Hong Kong. She established the Tissue Engineering Laboratory with the vision to improve patient's quality of life through bioengineering, biomaterials- and stem cell-based tissues for personalized therapies.

Her research interests covered tissue engineering and regenerative medicine, natural and biomimetic biomaterials, multi-cellular organoids and tumoroids, mechano-regulation, multiphoton microfabrication and micropatterning, cell niche engineering and laser medicine. Prof. Chan received her professional membership (Biomedical Engineering), has been a Chartered Engineer and Chartered Scientist from the Institute of Materials, Minerals and Mining IMMM) and a registered authorized person (AP) for advanced therapeutic products (ATPs) in Hong Kong. She has served both local and international professional communities in many aspects.

Multiphoton Microfabrication and Micropatterning (MMM) – A "programmable" cell niche engineering technology

B. CHAN

Au Chik Ko and Au Leung Shook Yin Professor in Biomedical Engineering
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Abstract

Cell culture is commonly used in research, pharmaceutical, biotechnology, biomaterial and tissue engineering industries. For decades, cells have been cultured on rigid, flat and plastic culture dishes, representing an artificial micro-environnement. In native tissues, cells reside in a complex and specialized niche, consisting of multiple niche factors including soluble signals, extracellular matrices, neighbour cells, topological features and mechanical cues. These cell niche factors orchestrate to maintain the native phenotype and normal function of cells and to determine their fate upon changes. Technologies able to recapitulate and reconstitute different cell niche factors *in vitro*, in a "programmable" manner, are useful platforms to "engineer" specific cell niches in achieving physiologically relevant culture conditions and hence cellular responses. Our lab has developed a multiphoton microfabrication and micropatterning (MMM) technology to reconstitute various cell niche factors (soluble signals, extracellular matrices, neighbouring cells, topological features and mechanical cues), individually or in combination, in a highly controllable and predictable manner. In this talk, the technical capabilities and the biomedical applications of the MMM platform will be discussed.

MACHINE LEARNING & ARTIFICIAL INTELLIGENCE

Professor Heather J. Kulik
Massachusetts Institute of Technology, USA

Professor Heather J. Kulik is the Lammot du Pont (1901) professor in the Departments of Chemical Engineering and Chemistry at MIT. She received her B.E. in Chemical Engineering from the Cooper Union in 2004 and her Ph.D. from the Department of Materials Science and Engineering at MIT in 2009. She completed postdoctoral training at Lawrence Livermore and Stanford, prior to joining MIT as a faculty member in November 2013. Her research has been recognized by an Office of Naval Research Young Investigator Award, DARPA Young Faculty Award and Director's fellowship, NSF CAREER Award, a Sloan Fellowship in chemistry, an AIChE Computational and Molecular Simulation Engineering Forum Impact Award, a Hans Fischer Senior Fellowship from the Technical University of Munich, and a Presidential Early Career Award for Scientist and Engineers, among others.

Leveraging Experimental Data in Machine Learning and Screening to Get From Computational Model to Real World Materials Fast

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Abstract

Machine learning in transition metal chemistry has lagged behind other areas of chemistry due to the combination of diversity of chemical bonding and limitations in high quality data sets, experimental or computational. I will describe our efforts to overcome these limitations to accelerate the discovery of novel transition metal containing materials using machine learning. I will discuss how we have leveraged experimental data sets through both text mining and semantic embedding to uncover relationships between structure and function, disseminating high quality datasets of transition metal complexes with known function [1]. I will describe how we've used these data sets to build machine learning models that predict the structure of transition metal complexes [2]. Then I will describe how we have leveraged large datasets of synthesized materials to uncover those with novel function in polymer networks. I will demonstrate the success of our design strategy through macroscopically visible changes in network scale properties of polymers once our transition metal complexes are incorporated.

Time permitting, I will also describe our efforts for data-driven discovery of metal organic frameworks (MOFs). MOFs have been widely studied for their ability to capture and store greenhouse gases. However, most chemical discovery efforts use computational study of hypothetical MOFs without consideration of their stability, limiting the practical application of novel materials. We have used natural language processing to extract experimental reports of numerous measures of stability of MOFs[3], including their thermal stability, stability upon activation (i.e., solvent removal), and in the presence of water or acid/base. I will show how we leverage these models to construct novel MOF candidates with vastly enriched stability over conventional hypothetical datasets. I will also describe how we pair these models with genetic algorithms to identify design principles for high mechanical stability and exceptional gas storage or for combined water and thermal stability.

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MACHINE LEARNING & ARTIFICIAL INTELLIGENCE

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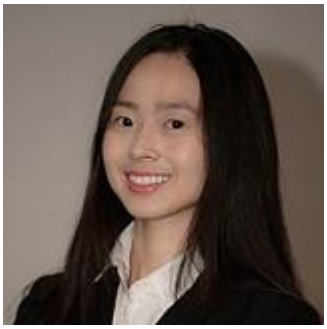

Dr. Grace X. Gu is an Assistant Professor of Mechanical Engineering at the University of California, Berkeley and currently holds the Don M. Cunningham Endowed Professorship. She received her BS in Mechanical Engineering from the University of Michigan, Ann Arbor and PhD in Mechanical Engineering from the Massachusetts Institute of Technology. The research interests of the Gu Group focus on creating new materials with superior properties for mechanical, biological, and aerospace applications using computational modeling and machine learning, developing intelligent additive manufacturing processes to realize complex material designs and in-situ monitoring and process optimization for additive manufacturing of sustainable materials such as biopolymeric, recycled and calcium carbonate-based materials, aiming to enhance their quality and reliability. Gu is the recipient of several awards, including the Presidential Early Career Award for Scientists and Engineers, ARO Early Career Program Award, DARPA Young Faculty Award etc. She has given dozens of invited lectures and seminars, including TEDxBerkeley. Gu has co-organized symposiums at various conferences and serves as an editor of Journal of Intelligent Materials Systems and Structures and Composites Science and Technology. She organizes an annual 3D printing workshop at Berkeley aimed at inspiring the next generation of students to pursue careers in science and engineering.

Learning from Nature, Mathematics, and Artificial Intelligence for Sustainable Materials Design and Manufacturing

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Abstract

The growing demand for sustainability in materials design and manufacturing is driving breakthroughs that reduce environmental impact while enhancing performance and efficiency. In this talk, I will present our research at the intersection of bioinspired design, mathematical tiling, and artificial intelligence (AI) to address key sustainability challenges. First, I will discuss our work on learning from natural systems such as sea sponges and chameleons to create synthetic metamaterials with tunable mechanical and electromagnetic properties. Next, I will explore composite structures based on aperiodic monotiles, which offer superior mechanical properties and durability compared to conventional periodic patterns. Finally, I will introduce an AI-driven monitoring system for additive manufacturing that detects and corrects anomalies in real-time, enhancing component quality and reducing waste. I will also discuss our recent work on in-situ monitoring and process optimization for additive manufacturing when considering environmental effects such as humidity. Together, these innovations can transform a wide range of applications, paving the way to create more resilient structures, design more sustainable materials, and develop greener manufacturing technologies along the way.

Transparent, Patternable and Stretchable Conducting Polymer Solid Electrode for Dielectric Elastomer Actuators

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Abstract

The growing interest in virtual and augmented reality has raised the importance of haptic devices to provide realistic sensations to users. Dielectric elastomer actuators (DEAs) are promising candidates for haptic applications due to their lightweight, stretchability, and conformability to human skin. To achieve large actuation strains, DEAs require compliant electrodes with low modulus and high electrical conductivity. While carbon grease has been commonly used as a compliant electrode, there has been limited research into the development of solid electrodes that can attain similar actuation performance as their non-solid counterparts.

In this study, we present a transparent, stretchable, and patternable solid electrode composed of poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) and poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethylene glycol) diacrylate (P123DA). The combination of PEDOT:PSS and P123DA enables tuning of electrical and mechanical properties by varying their ratio, which is critical for optimizing actuation performance. We investigated solid electrodes with different P123DA to PEDOT:PSS weight ratios of 1, 10, and 20 (denoted as R = 1, 10, 20), and found that increasing P123DA content enhanced mechanical compliance but reduced electrical conductivity. The optimal ratio (R = 10) achieved excellent performance, providing actuation comparable to carbon grease while maintaining high optical transparency (>95%).

The electrical conductivity of P123DA/PEDOT:PSS electrodes decreased from 198 S/cm for pristine PEDOT:PSS to 77.9, 1.43, and 0.08 S/cm for R = 1, 10, and 20, respectively. Morphological analysis by atomic force microscopy (AFM) revealed that fiber formation increased with higher P123DA content from R = 1 to 10, leading to the highest fiber density at R = 10. However, further increasing the ratio to R = 20 reduced fiber density due to insufficient PEDOT:PSS to form additional fibers. Derjaguin-Muller-Toporov (DMT) modulus measurements indicated that increasing the P123DA content lowered the modulus from 226 to 10.6 MPa, which is advantageous for achieving larger actuation strains.

Combining the electrical and mechanical results, actuation performance was found to increase from R = 1 to R = 10, primarily due to the reduced modulus. However, at R = 20, actuation performance decreased compared to R = 10 because the much lower electrical conductivity resulted in a slower electrostatic response. These results highlight the importance of balancing electrical conductivity and mechanical compliance to optimize DEA electrode performance.

In summary, this work developed transparent, stretchable, and patternable P123DA/PEDOT:PSS solid electrodes for DEAs. By systematically exploring different ratios, the study emphasizes the need to tailor electrode properties based on application demands. For static applications where larger actuation is prioritized, achieving low

modulus is critical, even at the expense of conductivity. Conversely, for dynamic applications requiring rapid responses, such as vibrotactile haptics and flying robots, high conductivity becomes a dominant factor. This study provides valuable insights into the electrode design strategies needed to maximize DEA actuation performance.

Development of Screen-Printed Boron-doped Diamond Nanoparticle for Electrochemical Sensor Application

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Abstract

Boron-doped diamond (BDD) electrodes have become a highly promising option for sensor applications due to their exceptional electrochemical properties, mechanical strength, and chemical inertness. BDD's distinctive features, such as a wide potential window and impressive stability in harsh chemical conditions [1]. In its nanoparticle powder form, known as boron-doped diamond nanoparticles (BDDNP), this material provides unique benefits, particularly in terms of easier modification and integration into composite materials, enhancing its versatility for various applications. Additionally, it can be produced as printed material, resulting in simple, portable, and cost-effective sensor devices. I am privileged to present this study on BDDNP, which marks the first research of its kind in Indonesia. Thus, not only contributing the research of BDDNP for electrochemical sensor, but also supporting the development of BDDNP research in Indonesia. Numerous applications of BDD and BDDNP electrodes have been published by our group, including sensors for antibiotics, bronchodilators, and heavy metal. Several antibiotics, such as ciprofloxacin, levofloxacin, ofloxacin, and azithromycin, have been successfully detected [2], [3]. These antibiotics are often used in livestock as growth promoters, which can lead to antibiotic resistance and residues in meat, milk, and eggs intended for human consumption. Furthermore, sensors for theophylline, a bronchodilator used to treat respiratory conditions like asthma and chronic obstructive pulmonary disease (COPD), have also been investigated [4]. Given its narrow therapeutic index, accurate monitoring of theophylline levels in patients is essential to prevent toxicity while ensuring therapeutic effectiveness. In Addition, we have demonstrated the detection of antimony in river water using BDDNP modified on screen-printed carbon electrode [5]. Both printed BDDNP electrodes and polycrystalline BDD demonstrate higher sensitivity compared to traditional electrode materials and commercial screen-printed carbon electrodes.

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Design and validation of laser-based vibrational circular dichroism spectroscopy using digitally referenced detection

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Abstract

By integrating polarization modulation with infrared spectroscopy, vibrational circular dichroism (VCD) measurements provide structurally sensitive information that allows us to examine molecular configurations and/or distribution of conformations. Many pharmaceutical and biological molecules possess an enantiomer pair, which interact and function differently in organisms. However, the associated signal is 10^{-4} to 10^{-5} times weaker than the sample absorption[1]. Relying on interferometry and a broadband thermal source, the measurement time of Fourier Transform infrared spectroscopy-based VCD ranges from 30 minutes to hours for sufficient SNR[2]. This slow speed precludes the rapid examination of samples and the development of imaging techniques. With three orders brighter infrared radiation than conventional thermal sources, quantum cascade laser (QCL) has promised sensitivity enhancement and high discrete frequency SNR enabled by the dispersive spectrometer nature, particularly advantageous for water-based solutions like proteins[3]. However, VCD detection demands orders of magnitude instrument sensitivity beyond what these spectrometers can provide, due to the noisy nature of broadly tunable QCLs[4,5]. Furthermore, QCL is intrinsically polarized and the interactions between optical elements can introduce depolarization undesired for VCD measurements[6].

Here, we demonstrate a QCL-based VCD spectrometer system using our developed digitally referenced detection scheme[7,8]. Incorporating dual detectors with high-speed digitization, noise sources including fluctuations in laser pulse emission, and imperfections in polarization modulation, are suppressed thus resulting in higher VCD sensitivity. Benefitting from the per-pulse acquisition scheme, we directly characterize the polarization of individual RCP and LCP pulses to optimize the design of the QCL-VCD configuration over the whole fingerprint spectra. The proposed method shows three times higher VCD spectral SNR compared to a single detector approach and enables faster VCD measurements of biomolecules. This optimization may also enable integration with an infrared microscope for chirality mapping of tissues and/or tracking of chiral biomolecules within.

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Ferroelectric Polarization for Enhanced Photoelectrochemical Water Splitting in $BiFeO_3/BiVO_4$ Photoanodes

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Abstract

Photoelectrochemical (PEC) application has attracted significant attention due to its potential as one of the promising clean energy systems, yet their practical use is limited by severe charge recombination and slow charge transfer kinetics. This study investigates the potential of ferroelectric polarization-controlled charge dynamics to exceed the performance of traditional static photoelectrodes.[1] We present significant photocurrent enhancements induced by ferroelectric polarization using a heterostructure of multiferroic bismuth ferrite (BFO) and photoactive bismuth vanadate (BVO) in a neutral pH electrolyte. Enhancements were observed for both poling directions: 136% for down-poled BFO/BVO and 70% for up-poled BFO/BVO at 1.23 V vs. RHE compared to the unpoled sample, achieving a Faradaic efficiency of over 95%. Extensive PEC and surface analyses, supported by density functional theory (DFT) calculations, attribute these improvements to the modulation of gradients in BFO band energies and changes in band-bending and offsets at the interfaces. The scalability of the sol-gel synthesis method and the use of environmentally benign materials and PEC conditions underscore the potential of these findings to pave the way for multifunctional materials as next-generation agile and dynamic catalysts and photoelectrode systems.

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Advancing the Stability and Performance of Vapor-Deposited Perovskite Solar Cells through Interface and Composition Engineering

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Abstract

Metal halide perovskites have shown tremendous promise as absorber layers for the next-generation of photovoltaic devices benefiting from their intriguing photophysical behaviours. Note that one of the most paramount challenges for the further industrialization of perovskite solar cells (PSCs) is their photoinduced degradation and thermal-stressing decomposition. The improvement of stability is closely tied to the fast improvement of the perovskite film quality based on composition engineering, precise control of the fabrication processes and a thorough understanding of the crystallization process during the film formation.

While fabrication of perovskite thin-films can be achieved through a variety of different techniques, thermal vapour deposition is particularly promising, allowing for high-throughput fabrication and large-scale production. Here, I will outline our recent results on key factors influencing vapor-deposited perovskite films, many of which have not been systematically explored. These studies encompass: the modulation of orientation of co-evaporated perovskite by employing the templating layer at the bottom interface [1], the influence of impurities in formamidinium iodide on perovskite film quality, device performance and long-term stability via both spin-coating and vapor-deposited methods [2], the crystallization and transformation of vapor-deposited aromatic ammonium salts and their passivation effect on co-evaporated 3D perovskite and those interfaced with different charge transport layers [3]. Collectively, these studies will shed important light on connecting the photophysical property and thermal-stability of vapor-deposited perovskite directly with orientation, chemical composition and crystallinity. These findings will pave the way for enhancing the stability and reproducibility of PSCs in large-scale fabrication.

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Synthesis and Characterization of Earth-Abundant Chalcogenide Perovskite $BaZrS_3$ for Photovoltaic Applications

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Abstract

Do we want an unlimited source of energy available around the Earth? Do we want to ensure that it does not cause pollution or adversely affect the climate in the long run? Do we want it to be affordable? Do we want it to be safe? The answer to all these questions is a resounding yes.

This work is focussed on developing non-toxic, earth-abundant materials for photovoltaic applications, leveraging the sun as the most abundant and cost-effective energy source. Specifically, we work on synthesizing and fabricating photovoltaic devices using chalcogenide perovskites. These materials, which crystallize in the ABX_3 structure (A = Ba, Sr, Ca; B = Zr, Hf; X = S), possess exceptional properties, including high light absorption, tunable bandgaps, a high dielectric constant, and remarkable stability against air, moisture, and heat[1]. These attributes make them highly promising for optoelectronic applications, particularly in tandem solar cells.

Historically, chalcogenide perovskites required high-temperature synthesis (over 900 °C), with most studies focusing on powders rather than thin films, making them unsuitable for device integration[2]. Additionally, their strong oxophilicity often led to oxide impurities and compositional inhomogeneities, while unoptimized methods produced inconsistent bandgaps (1.7–1.9 eV) instead of the ideal 1.8 eV.

Addressing these challenges, we systematically investigated factors influencing their high-temperature growth and identified three key requirements for synthesizing impurity-free $BaZrS_3$: precursor reactivity, the use of a liquid flux or transport agent, and an oxygen sink. By enhancing precursor reactivity, we developed solution-processing methods using various metal precursors, such as acetylacetonates, halides, sulfides, and organometallic compounds[3].

Additionally, we engineered a liquid flux to overcome mass-transfer barriers, enabling low-temperature synthesis, and employed an oxygen sink to eliminate oxide impurities. These innovations facilitated the synthesis of $BaMS_3$ (M = Zr, Hf) at temperatures below 600 °C, producing uniform $BaZrS_3$ films with an optimal bandgap of 1.85 eV, advancing the feasibility of these materials for practical photovoltaic applications. Furthermore, we demonstrated the superior performance of solution-processed $BaZrS_3$ by fabricating a photodetector with the fastest rise and decay times for transient photoconductivity reported in the chalcogenide perovskite literature.

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Building nanoscale laboratory using *in situ* electron microscopy: From nanomaterials dynamics to computational imaging

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Abstract

Functional nanomaterials such as catalysts operate through complex chemical and physical changes during reactions. *In situ* scanning/transmission electron microscopy (S/TEM) captures nanomaterial dynamics with an unprecedented spatial, spectroscopic, and temporal resolution combination [1,2]. However, current *in situ* S/TEM experiments have limits in revealing complete pictures of the catalyst dynamics since (1) they acquire partial information from limited image dimensions, (2) reaction conditions implemented for *in situ* S/TEM are often far from bulk-scale operating conditions, and (3) electron-beam induced damage on samples is unavoidable. In this work, we address these challenges to advance *in situ* S/TEM as a nanoscale laboratory that connects its atomic-scale findings to bulk-scale operations.

First, we introduce how to capture catalyst dynamics in multiple dimensions and apply findings to understand degradation mechanisms. Conventional *in situ* S/TEM only captures a 2D projection view where the catalyst/support morphology has a 3D nature. We implement simultaneous acquisition of (1) STEM (2D) and (2) secondary electron (3D) images for surface-topography information in controlled gas environments (**Figure 1a**). Using commercial-grade Pt catalysts as a model system, we explain the role of interplay between support, nanoparticle, and gas in degradation, which has not been revealed before with 2D projection images only.

Next, we explain how *in situ* S/TEM can be advanced into *operando* S/TEM by implementing realistic operating conditions. Catalyst operating conditions are a complex combination of external stimuli, and one of the most complicated examples is electrochemical cycling conditions at elevated temperatures in liquid phases. We develop liquid cell TEM with simultaneous control of temperature and electrochemistry. Combined with simulations of electrolyte concentration profiles (**Figure 1b**), we address the temperature-dependent nanoscale electrochemistry, which is applied to explain the electrocatalyst degradations.

Finally, we illustrate our unique approach to applying computational imaging for *in situ* S/TEM. Due to the continuous image acquisition, *in situ* S/TEM is inherently exposed to electron beam damage. 4D-STEM is a highly dose-efficient technique that acquires structural information as 2D diffraction pattern at every 2D image pixel while minimizing beam effect. We develop *in situ* 4D-STEM (5D-STEM) to record temporal evolution of the complete structure map. We introduce clustering algorithms for computationally efficient 5D data processing. We show that with our 5D-STEM, we can reveal the dynamic changes of orientation, strain, and thickness of the metal nanostructures, and it even enables imaging in a liquid phase by significantly improving the signal-to-noise ratio (**Figure 1c**).

We are excited by the opportunities presented by the approaches above to bridge the gap between the understandings from *in situ* S/TEM and engineering catalytic nanomaterials.

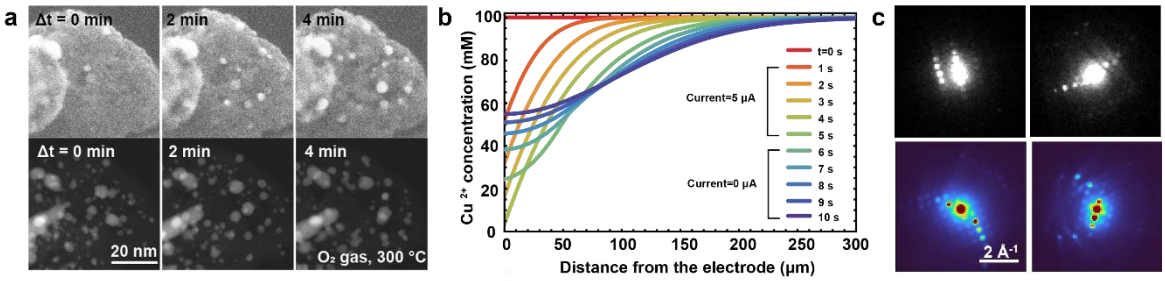

Figure 1. a) Simultaneously acquired 2D STEM (bottom row) and 3D SE images (top row) of supported Pt nanoparticle catalyst in an oxygen gas environment. b) Electrolyte concentrations profile simulation in liquid cell TEM with combined temperature and electrochemistry control using aqueous Cu^{2+} ion solution at 45 °C as a model system. c) 4D-STEM data of Au nanoparticles in the liquid phase, before (top row) and after (bottom row) applying 5D-STEM clustering algorithms.

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Unveiling Novel Phases in van der Waals Layered Magnets

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Abstract

Layered van der Waals compounds have attracted significant interests in recent decades, driven by the discovery of novel quantum states, from unconventional superconductors to non-trivial metallic behaviours. These non-trivial phenomena could lead to promising applications like spintronics, yet requires combined theoretical and experimental effort to establish an intrinsic understanding.

Among these, magnetic van der Waals materials provide a unique platform to explore strongly correlated electrons in low dimensions. Here, we focus on the transition metal phosphorous trichalcogenides ($TMPX_3$), in particular $FePS_3$ and $FePSe_3$, which have been recently reported to undergo insulator-to-metal and even to superconducting state transitions in the application of pressure. We comprehensively investigated the pressure-induced evolution of crystalline, magnetic structures and the transport properties using first-principles calculations and random structure search methodology under high pressure [1], and different experimental probes including synchrotron, neutron scattering and resistivity measurements [2]. Our work provides an unambiguous structural transition model for each compound respectively. Despite their similar stacking units, these two compounds exhibit substantially different physical properties and distinctive novel phases under pressure.

These works highlight the power of an integrated theoretical and experimental approach to explore the intrinsic properties of complex quantum materials. Such combined efforts are not limited just to one family of materials, and can extend to other systems (here, $BaFe_2Se_S$) to tackle problems beyond the scope of most scattering techniques [3].

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Hyper-gap transparent conductor

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Abstract

An elusive conductor with perfect optical transparency holds revolutionary potential for fields such as optoelectronics and nanophotonics. Such hypothetical metal would possess a spectral gap – a “hyper-gap” in its absorption spectrum, separating the intra-band and inter-band absorptions, in which the optical losses could vanish – currently, this property is achievable only within the bandgap of insulators. However, realizing such a hyper-gap metal demands an exotic electronic structure, where the conducting bands have a bandwidth narrower than their energy separations from the remaining electronic states. Here, we present such hyper-gap in a family of metals, through first-principal predictions coupled with both electrical and optical measurements. A transparent window, spanning from red to near-infrared wavelengths, is identified in bulk single crystals that remain transmissive over thirty microns thickness. The corresponding absorption coefficient is the lowest among known stoichiometric metals, rivaling thin films of transparent conductive oxides. This finding introduces a path, beyond traditional doping strategies in insulators, to combine electronic conduction and optical transparency.

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Advancing Epidermal Sensors for Personalized Healthcare

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Abstract

Advancements in flexible electronics have enabled the development of epidermal sensors that conform seamlessly to the skin, enabling noninvasive, real-time health monitoring [Ref. 1]. These wearable sensors hold great potential for remote patient monitoring and human-machine interfaces, forming the foundation for future digital health systems [Ref. 2]. However, key challenges remain in fabricating highly sensitive, durable, and biocompatible skin-like sensors capable of detecting both physical and chemical signals. Additionally, functional integration for enhanced breathability, sweat-ion detection, and long-term biosafety is critical for practical healthcare applications.

This talk will explore strategies for designing high-performance epidermal sensors, with a focus on functional nanomaterials, device architecture, and on-skin applications. I will discuss nanobridge-induced charge transfer and stress dissipation mechanisms using hierarchical 1D, 2D, and 3D nanomaterials, which enhance strain sensing performance and mechanical robustness (*Advanced Materials* 2017, 29, 1606411; *ACS Nano* 2018, 12, 56). Additionally, I will introduce ultra-stretchable elastomers for multi-dimensional mechanosensing and conformal skin adhesion, and remote sensing applications (*Science Advances* 2020, 6, eabb5367).

These sensors have demonstrated exceptional capabilities in detecting a broad range of signals, from subtle deformations—such as phonation, artery wrist pulse (AWP), jugular venous pressure (JVP), and respiratory patterns—to large-scale movements like walking, running, and jumping. Other applications include tactile pressure monitoring, proximity sensing, temperature tracking, and acoustic wave detection, making them promising for prosthetic feedback systems, wearable biomedical devices, and beyond.

Furthermore, our recent advancements in semiconducting MoS_2 monolayers (Science 2025, 387, 776) and conjugated polymer-based bioelectronic materials (*Nature Materials* 2022, 21, 1183; *ACS Nano* 2022, 16, 16677) have shown potential for highly selective, nanometer-thin chemical sensors, enabling high-precision sweat analysis and fluidic sensing. The integration of electrospinning techniques has further enhanced wear stability and biosafety, making these sensors suitable for continuous, long-term healthcare monitoring (*Nano Letters* 2024, 24, 12333). By combining these innovations with machine learning and big data analytics, this research lays the groundwork for next-generation wearable biosensors that offer enhanced precision, durability, and user comfort—advancing the future of digital health and personalized medicine.

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From 2D to 3D Electrochemical Microfabrication of Zinc Architectures: Synthesis, Microstructure, and Mechanical Properties Characterization

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Abstract

Biomedical implants require surface modifications that simultaneously promote cell attachment and provide antibacterial activity to enhance biointegration and reduce infection risk. Template-assisted electrodeposition (TAED) enables the transition from conventional 2D electrochemical coating processes to 3D microfabrication of complex metallic architectures, offering precise control over both geometry and microstructure which could help optimizing both cell-material interactions and antimicrobial efficacy due to [1] specific topography and enhanced surface area. Zinc (Zn) exhibits favorable properties for biomedical applications including biocompatibility, controlled biodegradation, and antibacterial properties, making it attractive for protective implants coatings as well as bulk material for temporary devices, though its low mechanical strength and room-temperature brittleness necessitate microstructural optimization strategies to enhance mechanical performance [2].

This work demonstrates systematic progression from 2D electrodeposited (ED) Zn coatings to 3D microcomponents through comprehensive microstructure characterization and ED process optimization. Micromechanical testing of focused ion beam (FIB)-milled micropillars, combined with electron backscattered diffraction (EBSD) and transmission electron microscopy (TEM) characterization established fundamental structure-property relationships in ED coatings. Systematic variation of current density and pulse characteristics during ED significantly affected grain size, shape, texture, and mechanical response, exhibiting Zn's characteristic inverse Hall-Petch behavior with compressive yield strengths varying from 800 MPa to 100 MPa upon grain refinement.

Meanwhile, TAED methodology was employed to fabricate Zn micropillar arrays using two-photon lithography templates and optimized ED conditions, demonstrating the ability to produce multiple microspecimens simultaneously. *In situ* micro compression testing across strain rates from 10^{-3} to 10^{-1} s^{-1} showed that TAED micropillars, despite exhibiting slightly different microstructure due to template-confined ED, followed similar mechanical trends as observed in FIB-milled micropillars in 2D coatings. We successfully extended this process to fabricate microlattice Zn structures, which coupled with finite element simulations of 3D structures' mechanical behavior, demonstrates the viability of this approach for designing biodegradable Zn metamaterials with potential applications in biomedical implant coatings.

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Reactive Oxygen Species-Adaptive Gel Coatings Promote Vascular Repair After Intervention

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Abstract

The application of drug - coated balloons in the treatment of coronary artery stenosis via interventional therapy is continuously evolving. However, it often leads to vascular injury, which triggers late - stage restenosis. A key pathological event in this process is the early disruption of the endothelial barrier function, which in turn initiates inflammation and hyperplasia. Currently, there is a lack of effective therapeutic strategies to promptly restore endothelial integrity. In this study, it was first determined that eliminating excessive reactive oxygen species (ROS) is a crucial pathway for strengthening intercellular tight junctions and restoring endothelial barrier function. Therefore, we proposed a sprayable ROS - responsive hydrogel coating OA@G-NO/B-EC for vascular balloons, aiming to reduce late - stage restenosis. The application of drug - coated balloons in the treatment of coronary artery stenosis via interventional therapy is continuously evolving. However, it often leads to vascular injury, which triggers late - stage restenosis. A key pathological event in this process is the early disruption of the endothelial barrier function, which in turn initiates inflammation and hyperplasia. Currently, there is a lack of effective therapeutic strategies to promptly restore endothelial integrity. In this study, it was first determined that eliminating excessive reactive oxygen species (ROS) is a crucial pathway for strengthening intercellular tight junctions and restoring endothelial barrier function. Therefore, we proposed a sprayable ROS-responsive hydrogel coating OA@G-NO/B-EC for vascular balloons, aiming to reduce late-stage restenosis.

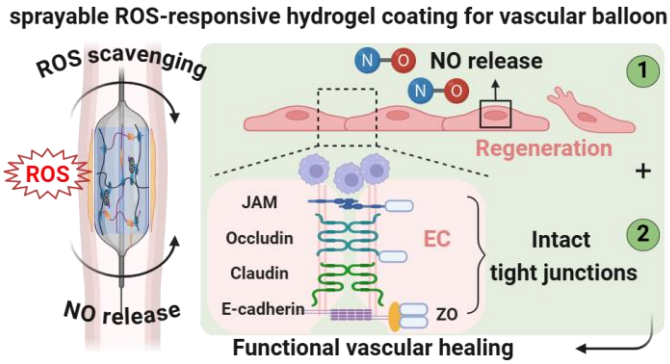

Figure 1. Sprayable ROS-responsive hydrogel coating for vascular balloons: restoring endothelial tight junctions and promoting endothelial regeneration for vascular healing

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Chalcogenide perovskites: a new class of functional materials?

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Abstract

Chalcogenide perovskite materials are highly robust, non-toxic and show strong light absorption but device development is hindered by the high-temperatures typically required for synthesis [1]. I will present our research, based on first-principles calculations and machine learned interatomic potentials, which explores the structural and thermodynamic properties of the most promising chalcogenide perovskite material for optoelectronic applications, $BaZrS_3$.

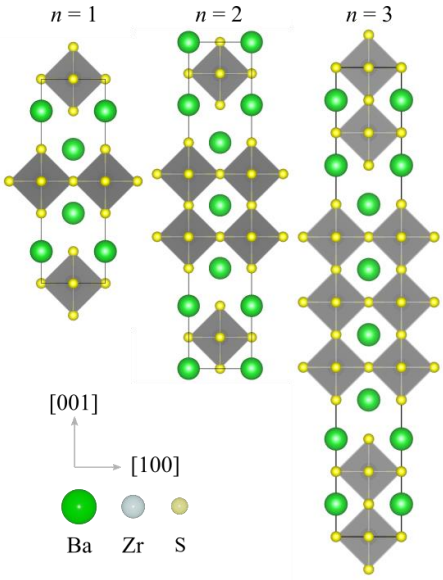

Figure 1: Crystal structures of the the n = 1,2,3 Ruddlesden-Popper phases in the Ba-Zr-S system. The 3D perovskite phase is recovered in the limit n→ ∞.

First I will consider perovskite stability against competing phases as a function of temperature and sulfur partial pressure [2,3], and compare our computational predictions against recent experimental measurements. This will give insight into the experimental conditions required for successful synthesis, and probe the thermodynamics underlying the common observation of low-dimensional perovskite analogues, the Ruddlesden-Popper (RP) series $Ba_{n+1}Zr_nS3_{n+1}$ (Figure 1). I will then share our latest work using the Neuroevolution Potential framework [4] and molecular dynamics to explore octahedral-tilt driven phase transitions in $BaZrS_3$ [5] and the RP-phases [6]. This will include a discussion on how first-principles predictions of X-Ray Diffraction Patterns and Raman spectra can be used to support experimental characterisation. I will conclude by outlining the key outstanding research questions which must be addressed so that chalcogenide perovskites can move from a research curiosity to a new class of functional materials.

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Bridging Atomistic Simulations and Real-World Catalyst Behaviours: A Multiscale Approach

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Abstract

Catalyst design is fundamental to advancing the storage and utilization of renewable energy. However, despite significant progress, catalyst systems remain extremely complex. They span a wide range of elemental compositions and structural forms, operate under highly dynamic reaction environments, and are often constrained by limited experimental and computational datasets. These challenges make it difficult to precisely locate active sites, predict catalyst evolution under operating conditions, and efficiently screen candidate materials across vast chemical spaces. As a result, many key scientific questions in catalyst discovery and optimization remain unanswered.

In this talk, I will present how incorporating reaction environment effects into catalyst design can help address these challenges (1). By integrating theoretical calculations with experimental insights, we can truly understand catalytic processes at the nanoscale. I will then discuss the development of a multiscale modelling framework, focusing on kinetic Monte Carlo (KMC) simulations designed to capture adsorbate-induced surface reconstructions under realistic reaction conditions. Unlike traditional static models, this approach dynamically tracks the atomic-scale evolution of catalyst surfaces, offering new perspectives on how structural transformations influence catalytic activity, selectivity, and stability over time (2–3). These simulations bridge the gap between atomistic theories and real-world catalyst behaviours, providing a powerful tool for understanding and engineering dynamic active sites. Finally, I will discuss the broader implications of these integrated strategies for the field of catalysis. By enabling predictive modelling of catalyst evolution under working conditions, multiscale simulations open new avenues for rational catalyst design across a variety of renewable energy and environmental applications. Looking ahead, I will outline future directions for expanding these methods and machine learning (ML) technologies to other catalytic systems, incorporating more complex reaction environments, and bridging simulations with experimental validation to drive catalyst innovation.

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Tuning metastability and deformation mechanisms in High entropy alloys using genetic algorithm machine learning predictions of Gibbs free energy

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Abstract

Gibbs free energy is a fundamental thermodynamic property that influences phase stability in materials. The variations in Gibbs free energy between phases play a crucial role in determining the metastability in the high entropy alloys (HEAs). Due to its vast compositional space, HEAs offer exceptional opportunities for tuning properties through compositional alterations [1]. Stacking fault energy is an essential parameter in determining the deformation behaviour of face-centred cubic metals and alloys, which can be derived from the Gibbs free energy[2]. Beyond stacking fault energy, the activation of deformation mechanisms like deformation twinning and transformation depends on the difference in Gibbs free energy between the phases[3].

The study develops a genetic algorithm machine learning model to predict the Gibbs free energy difference between phases in the HEAs, utilising the dataset generated from the thermodynamic calculations performed with ThermoCalc software[4]. The model identifies the key parameters influencing Gibbs free energy and establishes correlations between them. The crucial parameters affecting the Gibbs free energy are electronegativity, specific heat, atomic planar density and ionisation energy. The research offers a new approach for designing HEAs with tailored properties by accurately predicting metastability, leveraging their expansive deformation mechanism through strategic compositional tuning. The present study bridges the conventional thermodynamic calculations and the robust Machine learning approach.

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