

# Book of abstracts

## **Joint Chemical Science RSC-CSJ symposium 2024: Materials for energy storage and conversion**

31 October – 1 November 2024 | Burlington House, London, UK



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# Welcome

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from the Royal Society of Chemistry and *Chemical Science*

Dear Colleagues,

A warm welcome to the Joint *Chemical Science* RSC-CSJ symposium.

This meeting is the next iteration in the *Chemical Science* symposia series hosted by the Royal Society of Chemistry.

This year we are excited to join together with the Chemical Society of Japan (CSJ) to make this a joint event. The Chemical Society of Japan (CSJ) and Royal Society of Chemistry (RSC) have collaborated on many successful joint activities in the past. This symposium will be the eleventh time our two societies have come together to create a unique event for scientists to share ideas and experiences, this time in the field of energy materials.

Under the banner of our flagship journal, *Chemical Science*, we are shining a spotlight on cutting-edge chemistry research and giving it the sort of attention that drives scientific progress and makes a difference. Each year, we aim to keep the same format for the Symposium, with ample time available to support networking and discussion, while changing the theme to reflect the latest research developments, ensuring we bring together leading researchers from around the world. We also encourage strong participation from early career scientists and future leaders, who will be the future of this discipline. We are dedicating significant time in the programme to our poster session, and will hear from a selection of these scientists in our flash poster presentations. We strongly encourage all delegates to actively take part in these sessions.

The *Chemical Science* symposium also provides a way for our wider community to regularly stay in touch with the journal editors from RSC journals in this area, and fellow researchers across a broad range of topics in the chemical sciences.

This years' symposium is focussed on the topic of *materials for energy storage and conversion*.

We have a wide range of speakers in this symposium who are all internationally recognised experts in aspects of energy materials. Methods and topics that we will hear about will be varied including, amongst others: rechargeable battery materials, fuel cells, new perovskite materials for photovoltaics, molecular solar cells and solar fuel production.

We hope that the lectures and poster presentations will stimulate the exchange of ideas and experiences between all participants, setting a strong platform for discussion. We'd like to thank each of the speakers, poster presenters and participants for all their contributions.

A very warm welcome to what promises to be an exciting symposium. We hope that this event will act as a springboard for future activities and that it will help in fostering new research collaborations.



May Copsey,  
*Executive Editor, Chemical Science*



Andrew Cooper  
*Editor-in-Chief, Chemical Science*  
*University of Liverpool*



Helen Pain  
*Chief Executive Officer, Royal*  
*Society of Chemistry*

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## Welcome address

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from the Chemical Society of Japan

Dear Colleagues

It is a great pleasure for me as President of the Chemical Society of Japan (CSJ) to welcome you to the *Joint Chemical Science RSC-CSJ Symposium 2024: Materials for Energy Storage and Conversion*, hosted by the Royal Society of Chemistry (RSC) jointly with the RSC's flagship journal *Chemical Science*.

For CSJ the Royal Society of Chemistry is one of the closest international partner societies, and CSJ and RSC have been enjoying a continuing collaboration and scientific and human exchanges over decades, as symbolized by the Memorandum of Understanding (MOU) that just extended last year where Dr. Helen Pain, CEO of RSC, kindly visited the CSJ Headquarters in Tokyo for signing. The RSC-CSJ joint symposium is perhaps the most important activity in our bilateral collaboration, and this time its international significance has been enhanced by joining the annual symposium of *Chemical Science*.

The theme of the 2024 symposium "Materials for Energy Storage and Conversion" is, as I believe, quite timely: Obviously the world has been striving to achieve a sustainable society where attaining energy security is imminent, and the chemical sciences and technology are front-line key players and perhaps changemakers to meet the challenge. The theme is also important for CSJ, the mission of which literally states "to contribute through chemistry to the achievement of a sustainable human society". It is thus our pleasure to send four invited speakers from CSJ who are visibly active in the research and innovation in energy storage and conversion fields and will join the RSC counterparts and international speakers at the London event.

The last but not the least, I would like to thank Dr May Copsey, Executive Editor, *Chemical Science* along with all of RSC and *Chemical Science* colleagues for their superb preparation and organization of the symposium, collaboration and service.

We at CSJ do look forward to participating in the RSC-CSJ Joint Symposium both in person and online so as to deepen our discussion of, and possible contribution through chemistry to, the imminently challenging goal to the Earth.

With all the best wishes for the success of the symposium,



Professor Keiji Maruoka  
*President, The Chemical Society of Japan*

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## Speakers

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**Veronica Augustyn**

*North Carolina State University, USA*

Veronica Augustyn is the Jake and Jennifer Hooks Distinguished Scholar in Materials Science and Engineering and Associate Professor in the Department of Materials Science and Engineering at North Carolina State University. Her research focuses on the electrochemistry of materials for energy and environmental applications, including interfacial reactivity, ion-insertion coupled electron transfer mechanisms, and confinement phenomena. She is also the founder and faculty advisor of an award-winning international project, SciBridge, which develops renewable energy research and education collaborations between universities in Africa and the U.S.



**Francesca Brunetti**

*University of Rome Tor Vergata, Italy*

Prof. Francesca Brunetti, FRSC, received her PhD in Telecommunications and Microelectronics from the University of Rome Tor Vergata in 2005. In 2005, she was awarded of a Marie Curie Individual Fellowship spent in the Institute for Nanoelectronics of the Technical University of Munich, Germany. In 2006 she became researcher in the Department of Electronic Engineering of the University of Rome Tor Vergata, and since 2018, she is associated professor at the same Department.

Cofounder of the Centre for Hybrid and Organic Solar Energy at the University of Rome Tor Vergata (CHOSE, [www.chose.it](http://www.chose.it)) her current research is focused on the analysis, design and manufacture of electronic and optoelectronic devices through the use of organic and perovskites semiconductors realized on rigid and flexible substrates. In particular, she is working third-generation organic solar cells on flexible substrates, flexible perovskite solar cells and large area modules. Recently, she started an activity on the realization of supercapacitors on flexible and recyclable substrates, among which paper and their integration with photovoltaic devices (photocapacitors). Coordinator of several national and international projects, she is fellow of the Royal Society of Chemistry and Associated Editor of "Sustainable Energy and Fuels" a Royal Society of Chemistry Journal focused on renewables. She is the current director of CHOSE.

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**Sebastian Chirambatte Peter***Jawaharlal Nehru Centre for Advanced Scientific Research, India*

Prof. Sebastian C. Peter received his PhD in chemistry from the University of Münster, Germany (2006) and was post-doctoral fellow at Max Plank Institute for Chemical Physics of Solids, Dresden, Germany (2006-07) and Northwestern University, USA (2007-10). Dr. Peter joined as a faculty at New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore in 2010. His broad research interests include the development of solid-state inorganic materials for fuel cell, CO<sub>2</sub> reduction and hydrogen production. He is the founder and director of the start-up “Breathe Applied Sciences Pvt Ltd” to translate the fundamental works on CO<sub>2</sub> utilization. He is featured in the “75 under 50: Scientists Shaping Today’s India” by the DST and the convenor of the first ever CoE on CCU in India. He is commissioning first ever CO<sub>2</sub> to methanol plant in India. He received the National Technology Award, National Prize and National Start-up Award for his technology transition.

**Jillian L. Dempsey***National Laboratory, Yale University*

Jillian L. Dempsey is a professor at the University of North Carolina at Chapel Hill, and currently holds the Bowman and Gordon Gray Distinguished Term Professorship. She is the Deputy Director of the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE). Her research group explores charge transfer processes associated with solar fuel production, including proton-coupled electron transfer reactions and electron transfer across interfaces. Her research bridges molecular and materials chemistry and relies heavily on methods of physical inorganic chemistry, including transient absorption spectroscopy and electrochemistry. She also dedicates time to advancing electrochemistry education for all chemists.

**Marina Freitag***Newcastle University, UK*

Prof. Marina Freitag, a Royal Society University Research Fellow and Professor of Energy at Newcastle University, is a pioneering researcher in sustainable energy materials. Her innovative approach combines chemistry, engineering, and artificial intelligence to develop highly efficient and robust photovoltaic technologies. With her invention of the “zombie” solar cell and her ground-breaking work on self-powered IoT devices, Prof. Freitag is driving the transition towards a sustainable and intelligent energy future. Her contributions to the field have been recognized with prestigious awards, including the Göran Gustafsson Young Researcher Award and the Royal Society of Chemistry Harrison-Meldola Memorial Prize.

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**Elizabeth Gibson**  
*Newcastle University, UK*

Libby is a Professor of Energy Materials at Newcastle University. Research in her group focuses on developing materials and devices for sustainable power, fuel and feedstocks. This involves materials development, device assembly and characterization of the underpinning photophysics and electrochemistry. Her current roles include being the academic lead for the Northern Net Zero Accelerator PB-IAA, the EPSRC Northeast Transient Absorption Spectroscopy & Microscopy Facility, Institution Director of the EPSRC CDT Renewable Energy at Northeast Universities (ReNU), and she is the engagement lead for the UKRI Interdisciplinary Centre for Circular Chemical Economy.



**Alexis Grimaud**  
*Boston College, USA*

Dr. Alexis Grimaud received his PhD from the University of Bordeaux in 2011 and is currently an associate professor in the chemistry department at Boston College. Prior to that position, he served as CNRS Researcher from 2014 to 2022 at the Collège de France, Paris, France. Dr. His research efforts focus on understanding complex interfacial processes at the heart of electrochemical systems, including water electrolyzers and Li-ion batteries, for which he is developing and studying novel liquid electrolytes with tailored reactivity that he is using to allow intercalation into novel classes of materials. Dr. Grimaud's achievements were recognized by the French Young Researcher award as well as the Young Researcher award from the Energy Division of the French Chemical Society.



**Laurence J. Hardwick**  
*University of Liverpool, UK*

Professor Laurence Hardwick is the Director of the Stephenson Institute of Renewable Energy within the Department of Chemistry at the University of Liverpool, UK. Since 2011 he has led a group of 12-15 researchers that have focused on understanding real-time interface processes in batteries and electrochemical capacitors, a crucial step in improving energy materials to meet net-zero targets. His work has focused on developing cutting-edge technologies such as advanced operando Raman and infrared spectroscopic techniques that can probe the functionality of electrode interfaces at the nanoscale. He presently targets integration of automation into electrochemical methods for accelerating interface design and characterisation.



**Akari Hayashi**  
*Kyushu University, Japan*

Akari Hayashi received her PhD in Chemistry from University of California, Davis, the USA. After she received her PhD, she worked at the industry and national laboratory. She started her academic career as an associate professor at Nagoya Institute of Technology, and joined Kyushu University as an associate professor in 2011. She is now a professor of Kyushu University Platform of Inter-/Transdisciplinary Energy (Q-PIT). She also belongs to Department of hydrogen energy systems. Her research focuses on hydrogen energy through producing, storing, and using hydrogen. She has started fuel cell research since 2006. She is also working on combining renewable energy and hydrogen energy.

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**Prof Laura Herz**  
*University of Oxford, UK*

Laura Herz is a Professor of Physics at the University of Oxford and an EPSRC Open Fellow. She received her PhD in Physics from the University of Cambridge in 2002 and was a Research Fellow at St John's College Cambridge from 2001 - 2003. Her current research interests lie in the area of organic, inorganic and hybrid semiconductors, with a strong current focus on advanced materials for solar energy conversion. Her work has been recognized by several awards, including the Environment, Sustainability and Energy Division Mid-Career Award of the Royal Society of Chemistry, the Nevill Mott Medal and Prize from the Institute of Physics and the Friedrich-Wilhelm-Bessel Award from the Alexander von Humboldt Foundation. She has been listed by Clarivate Analytics as a Highly Cited Researcher since 2018. Laura is a Fellow of the Royal Society, the Royal Society of Chemistry, the Materials Research Society, and the Institute of Physics.



**Andreas Kafizas**  
*Imperial College London, UK*

Dr. Andreas Kafizas is a Senior Lecturer in the Department of Chemistry at Imperial College London (ICL). His research is focused on developing sustainable synthetic routes to photocatalytic coatings for a range of practical applications, including renewable fuels production (e.g. hydrogen fuel from water and carbon-based fuels from carbon dioxide), air remediation (e.g. nitrogen oxides removal) and water remediation (e.g. arsenic removal). To date, Andreas has published over 100 peer-reviewed papers and has written 6 book chapters (>7,100 citations, h-index = 52).

Andreas completed his MSci in Chemistry in 2007, and PhD in Chemistry in 2011 at University College London. His PhD was focussed on the development of photocatalytic materials synthesised by chemical vapour deposition, and he was awarded the Ramsay Medal for best graduating doctor. In 2012, he was awarded the Ramsay Fellowship, where studied the charge carrier behaviour of photocatalytic materials for solar fuels at ICL. In 2016, he was awarded a Junior Research Fellowship at ICL to develop heterojunction photoelectrodes for solar water splitting. In 2018, he was awarded a Lectureship at ICL, and now leads the Solar Coatings Group (<https://www.imperial.ac.uk/solar-coatings-lab/about-us/>), is the theme lead in Sustainable Power and Renewable Fuels at the Energy Futures Lab, and is a board member at the London Centre for Nanotechnology.



**Emilio J. Palomares Gil**  
*Institute of Chemical Research of Catalonia (ICIQ)-CERCA, Spain*

Emilio Palomares, born in Valencia in 1974, earned his Biology degree from UVEG in 1997, followed by a PhD at UPV/ITQ-CSIC in 2001. He received a Marie Slowdowska-Curie Fellowship at ICL, London, in 2001, delving into molecular devices for energy conversion. Joining ICMol-UVEG in 2004, he later moved to ICIQ-CERCA in 2006. Notable accolades include an ERC starting grant (2009), ERC PoC (2015), and ICREA Professorship (2009). Palomares received the Young Chemist Award (2006), INNOVA 2010 Award, and the E2S International Chair (2019). Elected ICIQ Director in 2020, he secured an ERC Advanced Grant in 2023. Palomares has co-authored 280+ peer-reviewed papers, focusing on materials for energy devices. His group specializes in interfacial charge transfer reactions, particularly in solar cells for electrochemical fuel cell applications.

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**Atsushi Wakamiya**  
*Kyoto University, Japan*

Atsushi Wakamiya is a full professor of Kyoto University. He received his Ph.D. from Kyoto University in 2003. He began his academic career at Nagoya University as Assistant Professor in 2003. In 2010, he moved to Kyoto University and was promoted to Professor in 2018. He received many awards: The Chemical Society of Japan Award for Creative Work (2020), Commendation for Science and Technology by MEXT Japan: Award for Science and Technology Research Category (2022), etc. He is a project leader of the Green Innovation Program (NEDO) and JST-Mirai Project. He is a co-founder and a director (as Chief Scientific Officer, CSO) of “EneCoat Technologies, Co. Ltd.”, a startup company for perovskite solar modules.



**Yuki Yamada**  
*Osaka University, Japan*

Yuki Yamada is currently a full professor at SANKEN, Osaka University in Japan. He majored electrochemistry and received his PhD from Kyoto University in 2010. In the same year, he moved to the University of Tokyo as an assistant professor and was promoted to a lecturer in 2018 and an associate professor in 2020. In 2021, he moved to SANKEN, Osaka University as a full professor. His current research interests focus on the development of liquid electrolyte (concentrated electrolytes, hydrate-melt electrolytes, new solvents, etc.) and its underlying design principles for various electrochemical applications such as batteries and conversion reactions.



**Miho Yamauchi**  
*Kyushu University, Japan*

Miho Yamauchi received her Ph. D degree from University of Tsukuba, Japan, and joined Kyushu University as an assistant professor and CRC (ICAT, now) Hokkaido University as an associate professor. She became a PI and a professor at WPI-I<sup>2</sup>CNER and moved to IMCE at Kyushu University and is currently a cross-appointed professor at Tohoku University. Her research interests include nanomaterials science with respect to hydrogen science, catalysis and efficient energy conversion. Recently, she is a group leader of GteX project for water electrolysis (JST) and a unit leader for CO<sub>2</sub> electrolysis for Moonshoot project (NEDO) and is focusing on the construction of CO<sub>2</sub> conversion systems using CO<sub>2</sub> captured directly from the air.

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## Oral presentations

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- O01      Proton-coupled electrochemistry of metal oxides: from insertion to interfacial phenomena**  
Veronica Augustyn  
*North Carolina State University, USA*
- O02      Flexible perovskite solar cells and modules: from fabrication to examples of possible applications**  
Francesca Brunetti  
*University of Rome Tor Vergata, Italy*
- O03      Carbon and water recycling for sustainable energy: a journey from fundamental chemistry to green technologies**  
Sebastian Chirambatte Peter  
*Jawaharlal Nehru Centre for Advanced Scientific Research, India*
- O04      Light-driven proton-coupled electron transfer reactions at passivated silicon photoelectrodes for solar fuel production**  
Jillian Dempsey  
*University of North Carolina, USA*
- O05      Molecular engineering for sustainable intelligence**  
Marina Freitag  
*Newcastle University, UK*
- O06      Project ViTAL: decarbonise power using integrated solar technology**  
Elizabeth Gibson  
*Newcastle University, UK*
- O07      Stabilizing unstable intercalation materials by mastery of solid/liquid equilibrium**  
Alexis Grimaud  
*Boston College, USA*
- O08      Understanding electrode reaction processes through operando vibrational spectroscopy of interfaces and interphases**  
Laurence Hardwick  
*University of Liverpool, UK*
- O09      Development of mesoporous carbon for fuel cell application**  
Akari Hayashi  
*Kyushu University, Japan*
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- O10**      **Metal halide perovskites for photovoltaic applications**  
Laura Herz  
*University of Oxford, UK*
- O11**      **Developing photoelectrochemical water splitting devices - from understanding charge carrier behaviour to testing prototypes in the field**  
Andreas Kafizas  
*Imperial College London, UK*
- O12**      **The chemistry of self-assembling molecules as selective conacts in molecular solar cells**  
Emilio J. Palomares Gil  
*Institute of Chemical Research of Catalonia (ICIQ)-CERCA, Spain*
- O13**      **Organic materials at interfaces for highly efficient perovskite photovoltaics**  
Atsushi Wakamiya  
*Kyoto University, Japan*
- O14**      **Rational design of liquid electrolytes for rechargeable batteries**  
Yuki Yamada  
*Osaka University, Japan*
- O15**      **Nanocatalyst systems for electrochemical upgrading of ubiquitous chemicals**  
Miho Yamauchi  
*Kyushu University, Japan*
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## Poster presentations

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- P01**      **Polyoxometalate enabled zinc-air battery at near neutral pH**  
Riccardo Argurio  
*ICN2, Spain*
- P02**      **Energy conversion in efficient thermoelectric monolayers using Monte Carlo simulation**  
Seyedehameneh Bahadori  
*Tarbiat Modares University, Iran*
- P03**      **NH<sub>4</sub>Cl-driven nanocrystal fragmentation enhances quantum efficiency of ionic carbon nitrides in photocatalytic H<sub>2</sub>O<sub>2</sub> generation**  
Jaya Bharti  
*Max Planck Institute of Colloids and Interfaces, Germany*
- P04**      **Investigation of anode-supported solid oxide fuel cells YSZ electrolyte prepared using screen-printing method**  
Tarik Chafik  
*Faculté des Sciences et Techniques de Tanger, Morocco*
- P05**      **Eco-friendly pectin/PEG binder for LiFePO<sub>4</sub> cathode enhances electrochemical performance**  
Yan-Ruei Chen  
*Academic Sinica, Chinese Taipei*
- P06**      **Enhanced fast charging capabilities in natural graphite/iron cross-linked pectin electrodes for lithium-ion batteries**  
Chin-Yi Chung  
*Institute of Physics, Academia Sinica, Chinese Taipei*
- P07**      **Layered double hydroxide-based materials for CO<sub>2</sub> conversion**  
Claire Coulthard  
*University of Oxford, UK*
- P08**      **A facile continuous approach for the high throughput synthesis of functionalised 2D derived nanocomposites**  
Conor Davids  
*London South Bank University, UK*
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- P09      Hybrid organic-inorganic plastic crystals for multiple energy applications: cold storage, barocaloric and dielectric properties**  
Javier García Ben  
*Universidade da Coruña, Spain*
- P10      Boosting heating and cooling technologies: metal-organic frameworks for transforming pressurized CO<sub>2</sub> into thermal energy**  
María Gelpi  
*Universidade da Coruña, Spain*
- P11      Exploring the thermal and ionic transport of Cu<sup>+</sup> conducting argyrodite Cu<sub>7</sub>PSe<sub>6</sub>**  
Anupama Ghata  
*University of Münster, Germany*
- P12      Long lasting lithium-ion batteries with lithium iron manganese phosphate cathode enabled by multi-electrolyte additive-mediated electrode-electrolyte interphase**  
Anupriya K Haridas  
*University of Warwick, UK*
- P13      Steel mesh-supported SNW-1/CsPbBr<sub>3</sub> nanocomposite: photocatalyst for sustainable ammonia production**  
Negin Khosroshahi  
*Iran University of Science and Technology, Iran*
- P14      Molecular structure descriptors for machine learning to develop highly efficient organic photovoltaics**  
Doo-Hyun Ko  
*Sungkyunkwan University, South Korea*
- P15      Development of novel antimony materials for next generation supercapacitors**  
Tianxin Liang  
*The University of Edinburgh, UK*
- P16      Synthesis and functional properties of bismuth doped reduce graphene oxide/gadolinium ferrite composites**  
Hina Liaquat  
*University of Liverpool, UK*
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- P17 Photocatalysts for solar driven simultaneous hydrogen generation and plastic degradation**  
Sarah Martell  
*Dalhousie University, Canada*
- P18 Photocatalytic hydrogen evolution by means of Ru NPs based dyads**  
Gerard Martí Balaguer  
*Universitat Autònoma de Barcelona, Spain*
- P19 Enhancing oxygen reduction electrocatalytic performance of MnO<sub>2</sub> / porous carbon composite by surface modification with a protic ionic liquid**  
Muhammed Shah Miran  
*Department of Chemistry, University of Dhaka, Dhaka 1000, Bangladesh*
- P20 Preparation, characterization and electrical studies of phosphonium polymeric ionic liquid as solid polymer electrolyte**  
Muhammad Syukri Mohamad Misenan  
*Yildiz Technical University, Turkey*
- P21 Hydrogen production and pollutant degradation with advanced dual photocatalytic-piezocatalytic TiO<sub>2</sub>-based nanocomposites**  
Kiem Giap Nguyen  
*London South Bank University, UK*
- P22 Using pump-probe spectroscopy to investigate metal oxides for solar water splitting**  
Louise Oldham  
*Imperial College London, UK*
- P23 Influence of Pt shell morphology on hot carrier extraction in plasmonic AuNRs**  
Diptiranjana Paital  
*Kings College London, UK*
- P24 Probing dielectric properties at frequencies relevant for light energy conversion: THz-permittivity of carbon nitrides and their enhancements from humidity**  
Filip Podjaski  
*Imperial College London, UK*
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- P25      Activating cobalt inverse spinel oxides via Fe substitution for enhanced water splitting reaction**  
Saraswati Roy  
*BITS-PILANI, Hyderabad Campus, India*
- P26      Single-ion conducting Zn-MOF-74 quasi-solid aqueous electrolyte for use in rechargeable zinc batteries**  
Jacob Rubel  
*KU Leuven, Belgium*
- P27      Designing lithium-ion batteries for recycling: the role of adhesives**  
Sean Scott  
*University of Leicester, UK*
- P28      Nanoparticle exsolution from complex oxides: tailoring catalyst properties through composition and process design**  
William Skinner  
*Imperial College London, UK*
- P29      Molecular interactions in ionic liquids, polymer membranes as fuel cells electrolytes and ion hopping in protic organic ionic plastic crystals**  
Anurag Prakash Sunda  
*J. C. Bose University of Science and Technology, YMCA, India*
- P30      Determining the structure and properties of solid electrolyte interphases in a battery-like environment with molecular resolution**  
Neave Taylor  
*University of Oxford, UK*
- P31      Dual modification of MnO<sub>2</sub> cathode improves performance and stability of Zinc-ion batteries (ZIBs)**  
Junru Wang  
*KU Leuven, Belgium*
- P32      Ultra-high surface area layered double hydroxide-based materials for oxygen evolution reaction catalysis**  
Matthew Williams  
*University of Oxford, UK*
- P33      Ferrosilicon electrodes for lithium ion batteries**  
Phillip Wu  
*Institute of Physics, Chinese Taipei*
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- P34**      **Bismuth-modified carbon nanotube electrodes for vanadium flow batteries**  
Jie Yang  
*Queen Mary University of London, UK*
- P35**      **Metal-organic nanosheets for synchronous harvest and storage of solar energy**  
Kezia Sasitharan  
*Newcastle University, UK*
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# Development of mesoporous carbon for fuel cell application

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Akari Hayashi

*Kyushu University Platform of Inter-/Transdisciplinary Energy Research*

Polymer electrolyte fuel cells (PEFCs) have been commercialized as fuel cell vehicles, but further improvement of current-voltage (IV) performance is required for applying to heavy-duty vehicles (HDVs). Regarding to TOYOTA MIRAI, 2nd generation MIRAI made a lot more improvement in comparison to 1st generation MIRAI, and mesoporous carbon (MC) supports are known to have largely contributed for such improvement.

Mesoporous carbon is a group of carbon materials which is composed of mesoporous structure, and mesopores are defined as pores of 2-50 nm. When Pt nanoparticles are encapsulated within relatively small mesopores, the mobility and then growth of Pt particles are reduced, leading to increase in durability of PEFCs. Additionally, relatively lower amount of ionomer covers Pt nanoparticles within mesopores, oxygen diffusion resistance is largely reduced although the proton conductivity is still kept through the ionomer staying outside of mesopores and water.

Our group have also been working on MC materials since 2006. Two types of MCs, MC bulk and MC fibers (MCF), with the different mesoporous structure have been developed since 2006 and 2017, respectively. More recently, new MC bulk has also been synthesized. With newly developed MC bulk, IV performance at the high current density region is very much improved, which is very important especially for the HDV application. Many factors, such as the Pt loading against the carbon support, Pt deposition method, ionomer/electrocatalyst ratio, and mesoporous structure, can contribute to this improvement. Therefore, in this paper, the effect of these parameters on IV performance is investigated.

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# Organic materials at interfaces for highly efficient perovskite photovoltaics

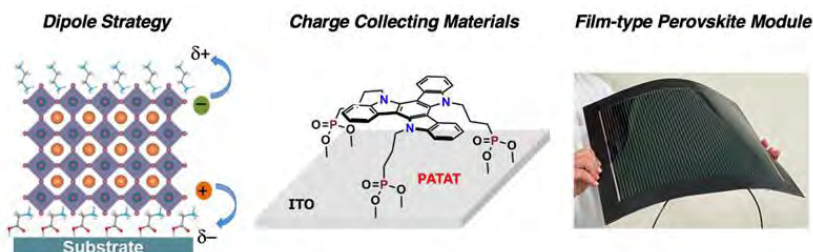
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Atsushi Wakamiya

*Institute for Chemical Research, Kyoto University, Japan,  
wakamiya@scl.kyoto-u.ac.jp*

Perovskite photovoltaics can be fabricated by coating process. The advantage is that these photovoltaics can be used in a variety of applications as a film type with lightweight and flexible shapes. So far, we have been working on the study of high-performance perovskite photovoltaics from the viewpoint of materials chemistry. Our research approaches for perovskite solar cells and modules are summarized as follows.<sup>[1-3]</sup>

1) Development of highly purified perovskite precursor materials:<sup>[4,5]</sup> We synthesis a series of complexes of lead halides or tin halides as purified precursor for perovskite materials. 2) Development of fabrication methods for perovskite layer by solution process: Based on "dipole strategy", we designed the surface passivation organic materials.<sup>[6-8]</sup> We develop the efficient fabrication methods of perovskite layer including top and bottom surface passivation based on the film formation mechanism. 3) Development of organic semiconductors as efficient charge-collection materials from perovskite layer: We design and synthesis novel pi-conjugated materials, PATAT, etc., in terms of control of the energy level of frontier orbitals, molecular orientation, and interface between perovskite layer.<sup>[9,10]</sup>



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# Rational design of liquid electrolytes for rechargeable batteries

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Electrolyte is an essential component in rechargeable lithium batteries, which functions as an ion-conductive and electron-insulating liquid medium between positive and negative electrodes. An ever-increasing demand for better batteries (with high voltage, high capacity, fast charging, and high safety) has set extraordinarily high standards for electrolyte materials, which has driven many researchers to work on the development of new liquid electrolytes.

One of the biggest challenges to liquid electrolytes is the reduction stability at negative electrodes. A conventional negative electrode in lithium-ion batteries is graphite ( $6C + Li^+ + e^- = LiC_6$ ), which shows a low electrode potential of -2.9 V vs standard hydrogen electrode (SHE). A promising negative electrode that may replace graphite in the future is lithium metal ( $Li^+ + e^- = Li$ ), whose electrode potential is even lower (-3.045 V vs SHE). At such low electrode potentials (i.e., strong reducing ability), almost all electrolyte components are reduced and decomposed as a preferable side reaction. In state-of-the-art liquid electrolytes (e.g.,  $LiPF_6$  or  $LiN(SO_2F)_2$  in ethylene carbonate), the decomposition products are deposited on the negative electrodes and function as a protective layer (so called “solid electrolyte interphase (SEI)”) that can alleviate the electrolyte decomposition. Nevertheless, the SEI layer cannot fully suppress the electrolyte decomposition, which leads to low charge-discharge efficiency and poor cycling performance especially at elevated temperatures.

In this talk, I will introduce two promising electrolyte design to address the negative electrode challenge. First, we demonstrate that the  $Li^+$  chemical potential ( $m_{Li^+}$ ) in electrolytes is an important factor to dominate the charge-discharge efficiency of such negative electrodes.<sup>1</sup> When we strategically increase the  $m_{Li^+}$  by specific electrolyte design (e.g., increasing salt concentrations<sup>2-6</sup> or employing weakly solvating solvents), it can significantly upshift the electrode potential of lithium metal and graphite, which can weaken the driving force for the reductive decomposition of electrolyte components. Second, we successfully design and synthesize a new solvent molecule for lithium-ion battery electrolytes based on our previous publication.<sup>7</sup> This solvent is not only nonflammable but also can create a rigid SEI on graphite negative electrolytes, which enable unprecedentedly stable charge-discharge cycling performance even at 70°C.

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# Nanocatalyst systems for electrochemical upgrading of ubiquitous chemicals

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Hydrogenation reactions using green hydrogen are indispensable for the energy storage and material synthesis without a great deal of CO<sub>2</sub> emission. Electrochemical CO<sub>2</sub> reduction (eCO<sub>2</sub>R) using H<sub>2</sub>O as a hydrogen source attracts much attention as a technology for carbon cycling on the earth and the selective eCO<sub>2</sub>R for the production of high-value chemicals is increasingly demanded.<sup>1-3</sup> Hydroxide-derived copper (OH/Cu) electrodes exhibit excellent performance for eCO<sub>2</sub>R. We have quantitatively evaluated surface OH for the first time and established a direct correlation between the OH amount and selectivity for the production of CH<sub>4</sub> and C<sub>2+</sub> on OH/Cu and demonstrated valuable selectivities using OH/Cu electrodes.<sup>4</sup> The eCO<sub>2</sub>R in acidic electrolytes would have various advantages due to the suppression of carbonate formation. Here, we designed an optimal architecture of a gas diffusion electrode (GDE) employing a copper-based ultrathin superhydrophobic macroporous layer (Cu-GDE), in which the CO<sub>2</sub> diffusion is highly enhanced and demonstrated Faradaic efficiency of 87% for C<sub>2+</sub> products.<sup>5</sup>

This presentation will also discuss highly efficient hydrogenation reactions using a structure controlled TiO<sub>2</sub> catalysts.<sup>5-8</sup>

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