FUTURE ENERGY MATERIALS
MARCH 22-23, 2021

VIRTUAL CONFERENCE ON

FUTURE ENERGY MATERIALS

March 22-23, 2021

YUKTAN TECHNOLOGIES

DAY-01

Keynote Talks

Halide Perovskites Beyond PV: A New Path to Energy Materials Sustainability?

David Cahen

Weizmann Institute of Science & Bar-Ilan University, Israel

Abstract

The vast majority of research on Halide Perovskite (HaP)- materials, focusses on the devices made with them, specifically solar PV cells, LEDs and radiation detectors cells; this holds also for academic research. While the fact that all high-performing devices are based on Pb (lead), is a serious drawback, in terms of several, aspects of the aims of global sustainability. However, from scrutinizing root causes for the remarkable opto-electronic properties of these materials, I will show how their facile soft chemical synthesis ("chimie douce"), and that such synthesis can yield materials with (ultra)low densities of active defect, are connected to what makes the materials a window on material sustainability. Both features derive from the ability of the materials to heal damage, inflicted on them, heal point, and even line defects. In inanimate systems such feat involves thermodynamics.* The phenomenon, which at times is distinguished from self-repair in that it does not require an external component, is known for some H-bonded polymers. At the core of this behaviour lies the strong dynamic disorder, within exquisite average periodic order.

We can generalize from the experimental findings to the somewhat counter-intuitive idea: as the main direct cause for such healing, for the remarkably low densities of (static) defects in HaPs and their ability to function even as efficient high-energy radiation detectors, we identify the very small free energy of, and activation energy for formation (and decomposition) of the materials from their binaries, and that, critically, those energies are well above the ones for static defect formation. Thus, the bulk material is left with only the thermodynamically (entropy) dictated densities of static defects (but high density of dynamic defects that do not affect the electronic and optical properties).

This property turns the materials into a testing ground for finding criteria for self-healing, and thus for improving material sustainability. This is, apart from the importance for materials as a resource per se, also a necessary condition for sustainable use of renewable energy sources.**

* cf. Rakita, Lubomirsky, DC; When defects become 'dynamic': Halide Perovskites: a new window on Materials?

Mater. Hor. 6, 1297 (2019);

Kumar, Hodes, DC; Defects in Halide Perovskites: The Lattice as a *Boojum*; *MRS Bull.*, 45, 478 (2020).

** DC, Lubomirsky; Self-Repairing Energy Materials: *Sine Qua Non* for a Sustainable Future *Acc. Chem Res.*, 50, 573 (2017);

Lubomirsky, DC; Energy Limitations on Materials Availability *MRS Bulletin,* 37, 412 (2012)

Biography

Prof. David Cahen is a full professor (emer.) in the WIS Dept. of Materials & Interfaces and in the Bar Ilan Univ, BIU, Chem. Dept. and a member of BINA, Bar Ilan Centre for Nanotechniology and Advanced Materials. Prof. Cahen studied chemistry & physics at Hebrew Univ. of Jerusalem (HUJ), materials science & physical chemistry at Northwestern Univ., and, as PD, biophysics of photosynthesis at the HUJ and the WIS. After joining the WIS

faculty he specialized in optoelectronic materials chemistry & physics. His research centers on fundamentals of materials for solar cells, and of electron transport across proteins, including implications for bio-optoelectronics. He is an AVS and MRS fellow.

Functional 2D Materials and Devices for High-Power Energy Storage

Xinliang Feng

Technische Universität Dresden, Germany

Biography

Prof. Feng is the head of the Chair of Molecular Functional Materials at Technische Universität Dresden. His current scientific interests include graphene-based 2D nanomaterials and low-dimensional nanostructured functional as well as hybrid materials for energy storage and conversion; mesoporous covalent-bonding organic frameworks and nanostructured functional carbon materials for energy storage and conversion; new energy devices and technologies. Prof. Feng has published more than 598 research articles which have attracted more than 54,570 citations with H-index of 116 (Web of Science) (Google Scholar Citations: >66,554 citations, H-index ≥124).

From Atom to System - How to Enable the Tera-scale Energy Transition

Ying Shirley Meng

University of California San Diego, USA

Abstract

High energy long life rechargeable battery is considered as key enabling technology for deep de-carbonization. Energy storage in the electrochemical form is attractive because of its high efficiency and fast response time. Besides the technological importance, electrochemical devices also provide a unique platform for fundamental and applied materials research since ion movement is often accompanied by inherent complex phenomena related to phase changes, electronic structure changes and defect generation. In this seminar, I will discuss a few new perspectives for energy storage materials including new fast ion conductors, new intercalation compounds and their interfacial engineering. With recent advances in characterization tools and computational methods, we are able to explore ionic mobility, charge transfer and phase transformations in electrode materials in-operando, and map out the structure-properties relations in functional materials for next generation energy storage and conversion. Moreover, I will discuss a few future priority research directions for electrochemical energy storage.

Biography

Prof. Ying Shirley Meng currently holds the Zable Endowed Chair Professor in Energy Technologies and is Professor of NanoEngineering and Materials Science at the University of California San Diego (UCSD). She received her Ph.D. in Advance Materials for Micro & Nano Systems from the Singapore-MIT Alliance in 2005, after which she worked as a postdoc research fellow and became a research scientist at MIT. Prof. Ying Shirley Meng is the founding Director of Sustainable Power and Energy Center. Prof. Shirley received the National Science Foundation (NSF) CAREER award in 2011, UCSD Chancellor's Interdisciplinary Collaboratories Award in 2013, Science Award in Electrochemistry by BASF and Volkswagen in 2014, C.W. Tobias Young Investigator Award of the Electrochemical Society (2016), IUMRS-Singapore Young Scientist Research Award (2017),International Coalition for Energy Storage and Innovation (ICESI) Inaugural Young Career Award (2018), American Chemical Society ACS Applied Materials & Interfaces Young Investigator Award (2018) and Finalist for the Blavatnik

National Award (2018). Her research group focuses on functional nano and micro-scale materials for energy storage and conversion. She is the author and co-author of more than 200 peer-reviewed journal articles, 2 book chapter and 6 patents. She serves on the executive committee for battery division at the Electrochemical Society and she is the Editor-in-Chief for MRS Energy & Sustainability.

Developing Next Generation Energy Storage Technologies

Jun Liu

University of Washington and Pacific Northwest National Laboratory, USA

Abstract

Energy storage is very important for modern computation and communication, electrification of transportation, renewable energy and secure electric infrastructures. Currently Li-ion batteries are the most prominent candidates for energy storage, while other traditional technologies such as pumped hydro and compressed air offer much cheaper solutions if available. Large scale deployment requires significant cost reductions in both capital and long-term operation cost. Many different approaches are pursued for next generation energy storage materials and technologies, but most studies have been conducted on the materials and component levels. Among the different materials, Li metal is a key electrode material for developing high energy batteries with a much higher specific energy and a lower cost. This talk will summarize our current understanding of the scientific and technological challenges, discuss recent progress and propose potential directions based on a high-energy cell design, fabrication and testing.

Biography

Prof. Jun Liu is the Washington Research Foundation Innovation Chair in Clean Energy, Campbell Chair Professor of Materials Science & Engineering, Professor of Chemical Engineering, and a Battelle Fellow at the Pacific Northwest National Laboratory (PNNL). He also serves as the Director for Innovation Center for the Battery500 Consortium, a multi-institute program supported by the U.S. Department of Energy (DOE) with the goal of developing next generation batteries. In the past, he has served as senior researchers at the Pacific Northwest National Laboratories, Bell Laboratories and Sandia National Laboratories. Prof. Jun is the recipient of the Battery Division Technology Award from The Electrochemical Society (ECS), two R&D100 Awards and the DOE EERE Exceptional Achievement Award. He is an elected member of Washington Academy of Science, a Materials Research Society Fellow, and an American Association for the Advancement of Science Fellow. He has been ranked in the top one percent of highly cited researchers since 2014 (Clarivate Analytics). He was named a Distinguished Inventor of Battelle in 2007, and was selected as PNNL's Inventor of the Year in 2012 and again in 2017.

Next Generation Rechargeable Zinc-Air Batteries

Zhongwei Chen

University of Waterloo, Canada

Biography

Prof. Zhongwei Chen is a Tier 1 Canada Research Chair, Professor in Advanced Materials for Clean Energy at the University of Waterloo, Fellow of the Royal Society of Canada, Fellow of the Canadian Academy of Engineering, Director of Waterloo Center for Electrochemical Energy, Associate Editor of ACS Applied Materials & Interfaces, and Vice President of International Academy of Electrochemical Energy Science (IAOEES). His research interests

are in the development of advanced energy materials and electrodes for fuel cells, metal-air batteries, and lithium-ion batteries. He has published 3 book, 9 book chapters and more than 300 peer reviewed journal articles. He is also listed as inventor over 30 US/international patents, with several licensed to companies internationally. He was the recipient of the 2016 E.W.R Steacie Memorial Fellowship, the member of the Royal Society of Canada's College of New Scholars, Artists and Scientists in 2016, the fellow of the Canadian Academy of Engineering in 2017, the Rutherford memorial medal from The Royal Society of Canada in 2017, which followed shortly upon several other prestigious honors, including the Ontario Early Researcher Award, an NSERC Discovery Supplement Award, the Distinguished Performance and Research Award.

What to Expect From Silicon Photovoltaics Over the 2020-2030 Decade

Martin Green

University of New South Wales, Australia

Abstract

Over the last decade, the cost of photovoltaic solar energy conversion has dropped very dramatically with solar photovoltaics *"now the cheapest source of electricity in most countries"* and *"now offering some of the lowest cost electricity ever seen"*, according to the International Energy Agency. However, improvements are in the pipeline that are leading to an era of "insanely cheap" solar power, within the coming decade.

The developments leading to these cost reductions will be described as well as the pending improvements that will allow solar to continue on its trajectory to even lower future costs over the 2020-2030 decade.

Biography

Prof. Martin Green is Scientia Professor at the University of New South Wales, Sydney and Director of the Australian Centre for Advanced Photovoltaics, involving several other Australian Universities and research groups. His group's contributions to photovoltaics are well known and include holding the record for silicon solar cell efficiency for 30 of the last 34 years, described as one of the "Top Ten" Milestones in the history of solar photovoltaics. Prof. Green's Major international awards include the 1999 Australia Prize, the 2002 Right Livelihood Award, also known as the Alternative Nobel Prize, the 2007 SolarWorld Einstein Award, the 2016 Ian Wark Medal from the Australian Academy of Science and the prestigious Global Energy Prize in 2017.

Invited Talks

Solution-Processed Perovskite Photovoltaics: From In situ Characterization to Robotic Experimentation

Aram Amassian

North Carolina State University, USA

Abstract

Semiconductor inks promise a new manufacturing paradigm for thin film (opto)electronic devices. Hybrid metal halide perovskites in particular are making tremendous inroads in (opto)electronic and photovoltaic applications. The formation of solid-state materials from the ink phase is not well understood or controlled, especially in application-relevant processing conditions, which tend to be kinetically far-removed from equilibrium. Moreover, the chemical, structural and processing universe of these materials is vast, making it challenging to draw overarching design principals through traditional experimental approaches. In light of these challenges we have developed multi-modal in situ diagnostics techniques to help investigate and shed light on the mechanisms of ink-to-solid transformation of perovskite semiconductors and their impact on the operation and performance of photovoltaic devices. More recent efforts have focused on tackling the vast parameter space of these materials, which involves complex formulation science and engineering as well as thin film science and engineering. This presentation will present solution deposition behavior through the perspective of in situ characterization and discuss our most recent efforts toward use of robotics and automation of the experimental research workflow of formulation, deposition and characterization of ink-based semiconductors.

Biography

Prof. Aram Amassian obtained his PhD in Engineering Physics from Ecole Polytechnique (Montreal, Canada) in 2006, and completed a postdoctoral fellowship in Materials Science and Engineering at Cornell University. Amassian was appointed as Assistant Professor of Materials Science and Engineering in 2009 at the King Abdullah University of Science and Technology (KAUST), where he was one of only 75 founding faculty members at all ranks. Prof. Amassian has co-authored more than 170 publications in peer reviewed journals and has delivered over 100 invited and keynote lectures. He was awarded the Career Development SABIC Chair for his pioneering work on solution processed optoelectronic materials and is the recipient of the American Vacuum Society's Electronic Materials Postdoctoral, the NSERC (Canada) Postgraduate and Postdoctoral Fellowships. His work has been highly interdisciplinary and collaborative, at the intersection of chemistry, physics, materials science and engineering.

Myth and Truth of Oxygen Redox Activities in Battery Cathodes: A View from Soft X-Ray Spectroscopy

Wanli Yang

Lawrence Berkeley National Laboratory, USA

Abstract

The desire for rechargeable batteries that could operate under high-voltage and high-energy conditions, unfortunately, often triggers various undesirable chemical reactions and parasitic effects. Among these reactions, oxygen activities have become one of the most debated topics in transition-metal (TM) oxide-based cathode materials. However, detecting the different natures of the complex reactions in oxide cathode is non-trivial, especially for the unusual oxygen states. In this presentation, first we will briefly introduce our developments of high-efficiency mapping of resonant inelastic X-ray scattering (mRIXS) and its demonstration for revealing the intrinsic TM and oxygen redox states in oxide cathodes[1]. We will then discuss some recent findings from mRIXS in cathode systems involving

oxygen redox reactions, with the focus on clarifying several misconceptions on the oxygen activities in battery cathodes, especially its kinetics[2] and cycling stabilities[3]. We further discuss the possible reasons behind these misunderstandings by reflections on the source of the oxygen redox reactions in the Li-rich cathode materials[4]. We conclude that while controlling oxygen activities is critical for achieving high voltage operation of battery cathodes, the optimism of its practical use and its fundamental origin are yet to be confirmed and clarified.

Biography

Prof. Wanli Yang obtained his Ph.D. in Condensed Matter Physics from Institute of Physics, Chinese Academy of Sciences in 2000, and completed Postdoc in Condensed Matter Physics from Stanford University. He is currently a senior scientist in Advanced Light Source which is a U.S. Department of Energy scientific user facility at Lawrence Berkeley National Laboratory. His current focus on Materials include Materials for energy applications, including materials for energy storage, photovoltaic, and catalysts.

Leveraging Reversible Chemistry for Materials Sustainability in Energy Storage

Zheng Chen

University of California San Diego, USA

Abstract

The development of next-generation energy storage devices and systems for electric vehicles (EVs) relies on materials with significantly improved performance and lower cost. The increasing amount of lithium-ion battery (LIBs) consumption will result in the resource shortage and price increase of lithium and precious transition metals (Co, Ni etc.); the wastes generated from disposal of used batteries can cause severe environment pollution. In this context, design of energy-efficient recycling and regeneration process for spent batteries is attracting growing interest. From a reversible chemistry point of view, this talk will introduce a potential strategy to directly recycle and regenerate spent LIBs using a "non-destructive" approach, which will lead to new electrode materials that can show the same level of performance as the native materials. Such a strategy combines fundamental understanding and process optimization for remanufacturing of energy materials. Therefore, it can potentially offer a sustainable solution for future energy storage.

Biography

Prof. Zheng Chen is an Assistant Professor at UC San Diego. Prof. Chen has received the NASA's 2018 Early Career Faculty Award, the LG Chem Global Battery Innovation Contest (BIC) Award in 2018, and the 2018 ACF PRF New Investigator Award. Prof. Chen has been selected as a Scialog Fellow in Advanced Energy Storage by Research Corporation and as a participant of 2019 China-America Frontiers of Engineering Symposium (CAFOE). He has been recognized as a 2018 Emerging Investigators of Journal of Materials Chemistry C. (2018), Chem. Comm. (2020) and Nanoscale (2021).

100% Renewables and Pumped Hydro Energy Storage

Andrew Blakers

Australian National University, Australia

Abstract

Solar PV and wind constitute three quarters of net new generation capacity additions. Together, they can readily eliminate fossil fuels by 2040, allowing a 75% cut in global emissions at low or negative cost. Balancing high levels of solar and wind is straightforward through the use of enhanced high voltage transmission, pumped hydro storage and battery storage. The National Electricity Market in Australia has reached 30% renewable electricity and is tracking to 50% in 2025. South Australia has reached 70% and is tracking to 100% in 2024. The price of electricity is around US$35/MWh. Australia is demonstrating that high levels of renewables can be incorporated in a stable electricity systems at low cost.

Biography

Andrew Blakers is E2 Professor of Engineering at the Australian National University. He has held several personal Fellowships (Humboldt, ARC Queen Elizabeth II, ARC Senior Research and Radio Research Board). He is a Fellow of the Australian Academy of Technological Sciences and Engineering, the Australian Institute of Physics and the Australian Institute of Energy, and is a Life Member of the International Solar Energy Society and the Australian Conservation Foundation. He is a Public Policy Fellow at ANU in recognition of his extensive outreach activities. He has published more than 400 papers and patents, has won numerous national and international awards, and contributes to numerous review and granting panels. Leadership roles have included founder of the ANU photovoltaic group and research laboratories, Foundation Director of the Centre for Sustainable Energy Systems, Node Director of the ARENA Australian Centre for Advanced Photovoltaics, Director of the ARC Centre for Solar Energy Systems, and Node Director of the Australian CRC for Renewable Energy. He was a lead inventor of PERC silicon solar cell technology (cumulative module sales of $50 billion) and co-inventor of Sliver solar cell technology (subject of a $240 million commercialisation effort by Transform solar including $11 million royalties paid to ANU). He has extensive project management experience, and has procured about $120 million in externally-sourced research-related funding for ANU. In recent years he has contributed to analysis of 100% renewable energy futures, including a global search for pumped hydro energy storage sites.

Photovoltaics in the Atomically-Thin Limit: Promising or Pipe Dream?

Deep Jariwala

University of Pennsylvania, USA

Abstract

High efficiency inorganic photovoltaic materials (e.g., Si, GaAs and GaInP) can achieve maximum above-bandgap absorption as well as carrier-selective charge collection at the cell operating point. But thin film photovoltaic absorbers have lacked the ability to maximize absorption and efficient carrier collection, concurrently often due to due to surface and interface recombination effects. In contrast, Van der Waals semiconductors have naturally passivated surfaces with electronically active edges that allows retention of high electronic quality down-to the atomically thin limit. This presents interesting opportunities for remote power and applications that require high-specific power in place of cost or efficiency. This webinar will focus on a review of advances in photovoltaics based on 2D semiconductors to date for the first part.

In the second part, I will show some of our own results in this space which have been dedicated to systematically address the three major engineering challenges for efficient photovoltaics: 1. Light absorption 2. Carrier collection

3. Band alignments. I will present our experimental demonstration of near-unity light confinement in ultrathin (< 15 nm) Van der Waals semiconductors (MoS_2, WS_2 and WSe_2) leading to nearly perfect absorption.[1] I will further present the fabrication and performance of our, broadband absorbing, heterostructure photovoltaic devices using sub-15 nm TMDCs as the active layers, with record high quantum efficiencies.[2] I will then present ongoing work on addressing the key remaining challenges for application of 2D materials and their heterostructures in high efficiency photovoltaics[3] which entails engineering of interfaces and open-circuit voltage[4] as well as on going work on novel materials and light trapping[5,6] in them. I will conclude by giving a broad perspective of future work on 2D materials from fundamental science to applications.

Biography

Deep Jariwala is an Assistant Professor in Department of Electrical and Systems Engineering at the University of Pennsylvania (Penn). Deep completed his undergraduate degree in Metallurgical Engineering from the Indian Institute of Technology BHU, in 2010 and his Ph.D. in Materials Science and Engineering at Northwestern University in 2015. Deep was a Resnick Prize Postdoctoral Fellow at the Caltech from 2015-2017 before joining Penn in 2018 and starting his own group. His research interests broadly lie at the intersection of new materials, surface science and solid state devices for opto-electronics and energy harvesting applications as well as in the development of correlated and functional imaging techniques.

Electrochemical Capacitors: Electrode Materials and Performance

Andrew Burke

University of California-Davis, USA

Abstract

Electrochemical capacitor energy storage technologies are of increasing interest because of the demand for rapid and efficient high-power delivery in transportation and industrial applications. The shortcoming of electrochemical capacitors (ECs) has been their low energy density compared to lithium-ion batteries. Much of the research in recent years has focused on increasing the energy density of ECs. The two primary approaches to increasing the energy density are to increase the maximum voltage of the EC cell and to increase the specific capacitance (F g^{-1}) of its electrodes. This paper is focused on the research on new materials for electrodes. Most of the ECs currently on the market use activated carbon with nano-pore structure in the electrodes. Much of the research on advanced devices has involved carbon in combination with materials having inherently high specific capacitance (Fg^{-1}). These materials are either mixed with the carbon or coated as nano-layers on the carbon particles. The high specific capacitance materials include graphene and various metal oxides, conducting polymers, nitrides (MXenes) and metal–organic frameworks (MOFs). Electrodes with a wide range of specific of capacitance from 300-600 Fg^{-1} have been demonstrated in the lab. ECs assembled in the lab with combinations of carbon and the advanced electrodes have shown energy densities of 50-100 Wh/kg. Modeling of ECs using the advanced materials also showed energy densities in the same range.

Biography

Prof. Andrew Burke holds B.S. and M.S. degrees in Applied Mathematics from Carnegie Institute of Technology, a M.A. degree in Aerospace Engineering and a Ph.D. in Aerospace and Mechanical Sciences from Princeton University. Since 1974, his career work has involved many aspects of electric and hybrid vehicle design, analysis, and testing. Dr. Burke has authored over 150 reports and papers on electric and hybrid vehicles, batteries, and ultracapacitors. Dr. Burke joined the Research Faculty of the Institute of Transportation Studies at UC Davis in July 1994.

Oral Presentations

Halide Perovskite Solar Cells: Strategies for High Stability

Carlos Pereyra, Kenedy Tabah, Sonia Raga, Haibing Xie, Monica Lira-Cantu*

Catalan Institute of Nanoscience and Nanotechnology, Spain

Abstract

Single-junction halide perovskite solar cells (PSCs) have already achieved a certified power conversion efficiency (PCE) above 25 %, making them one of the most promising emerging photovoltaic technologies1. One of the main bottlenecks towards their commercialization is their long-term stability, which should exceed the 20-year mark. Many are the strategies applied to extend device lifetime, among them are the use of additives, the optimization of the fabrication process of perovskite thin films or the replacement of unstable organic transport layers such as Spiro-OMeTAD. Although most of these approaches can effectively improve device efficiency, they fail at providing stable PSCs as defined as those able to display less than 10 % degradation after 1000 h of continuous illumination under 1 sun[2]. In this talk, we will briefly review the different methods currently applied in PSCs to enhance not only their efficiency but also their long-term stability. We will discuss the modification of the different materials in the PSCs and the mechanism behind PSC degradation. We will present our most recent results on the different strategies applied in our laboratory to enhance the stability of PSC, for example the replacement of classical semiconductor oxides, used as transport layers, by ferroelectric materials; the use of organic additives to passivate defects or the application of hole transport layer-free carbon-based PSCs. We will discuss our results on the effect of these modifications in PSC stability. Refs: (1) NREL, "Best Research-Cell Efficiency Chart." https://www.nrel.gov/pv/cell-efficiency.html., (2) M. V. Khenkin, E. Katz…M. Lira-Cantu et al., Nat. Energy, vol. 5, no. 1, pp. 35–49, Jan. 2020.

Biography

Prof. Monica Lira-Cantu is Group Leader of the Nanostructured Materials for Photovoltaic Energy Group at the Catalan Institute of Nanoscience and Nanotechnology, ICN2 in Barcelona (Spain). She has more than 127 publications, among them 106 published papers, 8 patents, 12 book chapters and 1 edited book. She has published in top scientific journals such as Nature Energy (IF=47), Energ. & Env. Science (IF=33); Joule (IF=27); Adv. Energy Mater (IF= 25), among others. She has delivered more than 120 presentations in congresses as Keynote, Invited and Oral speaker.

Metal@Semiconductor Hetero-Nanocrystals: Heterointerface Control and Photocatalysis Applications

Jiatao Zhang[1, 2] * and Jia Liu, Hongzhi Wang, Xiaodong Wan, Yuemei Li

[1, 2]Beijing Institute of Technology, China

Abstract

The precise control of hetero-interface in colloidal Plasmonic metal@II-VI semiconductor hetero-nanocrystals (HNCs), is very important for the efficient energy or charge transfer through hetero-interface, better light harvest and then their efficient photocatalysis applications. Due to the large lattice mismatch between metal and semiconductor (lattice mismatch > 40%), growth of monocrystalline semiconductor based metal/semiconductor hybrid nanocrystals (core/shell and heterodimer) with modulated composition, morphology and interface strain are prerequisites for flexible control of plasmon-exciton coupling, efficient electron/hole separation and carriers transfer. By putting forward new reverse cation exchange induced non-epitaxial growth method, we realized

nanoscale monocrystalline growth of the semiconductor shell on Plasmonic metal core and the aliovalent doping in semiconductor shell synergistically. The efficient Plasmon enhanced electron/hole separation and hot electron injection have been realized (the hot electron injection efficiency reachs to 48%). Then revolutionary plasmon enhanced photocatalytic, PEC performance have been realized.

Biography

Jiatao Zhang earned his PhD in 2006 from chemistry department of Tsinghua University, China. Then he worked as postdoctoral research fellow in Prof. Dieter Fenske group of Karlsruhe institute of Technology from 2006 to 2007. From 2008 to 2011, he worked as research associate in Min Ouyang group of physics department, University of Maryland, College Park. From 2011 to now, he is working as Xu Teli Professor in Beijing Institute of Technology. In 2013, he was awarded Excellent Young Scientist foundation of NSFC. Fellowship of RSC (FRSC) since 2018. The IUPAC distinguished awards for novel materials and synthesis.

State of the Art and Research Directions for Thermal Energy Storage Materials at Sub-Zero Temperature Ranges

Alessandro Romagnoli[1]* and Yang Lizhong[2]

[1]School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore

[2]SJ-NTU Corporate Laboratory, Nanyang Technological University, Singapore

Abstract

Energy storage is playing an increasingly important role in combating climate change. Compared to the extensive research interests in creating new electrochemical storage materials, less attention is paid to develop thermal energy storage materials. However, thermal energy, including heating and cooling, is the most crucial end-use in the residential sector, accounting for around 50-80% of the total energy consumption. Among that, cooling and refrigeration already consume 25–30% of the global electricity production, and this consumption is expected to surge 33-fold by 2100. Meanwhile, despite the massive amount of energy dedicated to producing cold energy, various cold sources are not efficiently utilized or even generally wasted. The fast-growing demand and production of cold energy, along with the newly trending concept of "cold economy," triggered the urgent need to develop advanced cold thermal energy storage materials, systems, and applications. This study provides a systematic and comprehensive review of a wide range of existing and potential cold thermal energy storage materials at sub-zero temperatures (from around –270 ˚C to below 0 ˚C). Numerical and experimental work conducted for the containment and heat transfer of different material types is systematically summarized. Current and future applications of cold thermal energy storage materials, including recovering waste cold energy, enhancing refrigeration systems' performances, and improving renewable energy integration, are analyzed with their suitable material types and compatible storage technologies. Moreover, by identifying the research gaps where further efforts are needed, the review also outlines the potential development directions of the next generation cold thermal energy storage materials.

Biography

Alessandro is an Associate Professor in the School of Mechanical and Aerospace Engineering at the Nanyang Technological University of Singapore. Since 2020, Alessandro has been appointed as Co-Director of the NTU-Surbana Jurong Corporate Lab, a S$60M effort looking at Intelligent Urban Solutions, Active Solutions for Sustainability, and Future of Construction and Underground. Alessandro established the Thermal Energy Systems Lab @NTU which focusses on industrial energy efficiency, power generation - from large scale to distributed energy generation applied to micro-grids, and energy systems integration for different energy mix - including renewables and energy storage.

Thiosquaraines as Heavy-Atom-Free Photon Upconversion Sensitizers

Cody W. Schlenker* and Sarah R. Pristash

University of Washington, USA

Abstract

Photon upconversion through triplet–triplet annihilation is of interest for diverse applications, notably as a potential means of exceeding the Shockley–Queisser limits in solar cells. We demonstrate a heavy-atom-free triplet sensitizer based on a thionated squaraine. Using this all-organic sensitizer, we demonstrate upconversion through triplet sensitization of several organic annihilator molecules. Thionated squaraines provide an exciting new platform for developing heavy-atom-free upconversion systems.

Biography

Schlenker received his B.S. (Chemistry 2004) from Linfield College. He then earned his Ph.D. (Chemistry 2010) studying organic optoelectronics with Mark Thompson (USC). As an NSF SEES Fellow, Schlenker worked with David Ginger (UW), studying photophysics of semiconducting polymers. In 2014, Schlenker joined the UW Chemistry Faculty. His research focuses on energy conversion and storage in photocatalysts, photovoltaics, photon upconversion, and rechargeable batteries. He has been recognized with honors, including as an NSF CAREER Awardee, J. Am. Chem. Soc. Young Investigator, ACS Adv. Energy Mater. Young Investigator, Washington Research Foundation Innovation Assistant Professor, and Bernard and Claudine Nist Faculty Fellow.

DAY-02

Keynote Talks

Bridging the Gap Between Performance and Sustainability in the Next Generation Energy Storage and Conversion Technologies

Magda Titirici

Imperial College London, UK

Abstract

Materials sustainability is particularly important when building future energy storage and conversion technologies. Such energy technologies are crucial to ensure the transition towards a zero emissions society but are relying heavily on materials. We must address the fine balance between the development of emerging energy technologies and the materials we use to build them. Today, scarce metals are the most important components of energy storage and conversion systems. Cobalt and graphite are in the cathodes and anodes of Li-ion batteries. With the accelerated development of Li-ion battery technologies, there is a huge demand not only for Cobalt and graphite but also for Li itself, which is geographically confined to Bolivia Chile and Argentina. Hence, we need innovative energy storage technologies beyond Li. Iridium and Platinum are the catalysts of choice for H2 production from water and its utilization in fuel cells to generate clean electricity. The current available supply for these metals cannot sustain the expansion of such technologies at a global scale. We need alternative electrocatalysts and sources for H2 production and H2 use in fuel cells. Gallium, Tellurium, Indium are used in solar cells and photocatalytic systems for solar fuel production. These materials are scarce, and alternatives must be sought for the next generation of solar panels and photocatalytic systems.

In this talk I will present some of our innovations in the design of sustainable materials alternatives to be efficiently utilized in energy storage and conversion technologies. Examples will range from efficient and sustainable batteries beyond Li to alternative catalysts to Pt for fuel cell's cathodes as well as alternative biowaste sources to water for the production of affordable and clean H2. A new family of photoactive nanomaterials made from biomass, i.e carbon dots, will also be discussed for potential use in solar H2 production.

Biography

Prof. Magda Titirici is a chair in Sustainable Energy Materials at the Imperial College London. She received her PhD in Materials Chemistry from University of Dortmund in Germany. She then joined the Max-Planck Institute of Colloids and Interfaces as a Postdoctoral Fellow and later become a Group Leader, starting her independent research on sustainable carbon materials in 2006. Prof. Magda is the author of over 250 articles and is included in the Global Highly Cited Researchers (Clarivate Analytics) over the past four years. She has received the Rosenhein Medal from IoM3, an Honorary PhD from University of Stockholm in 2017, the Chinese Academy of Science President Fellowship, the Royal Society of Chemistry Corday-Morgen prize in 2018 and a Royal Academy of Engineering Chair in Emerging Technologies fellowship in 2019. Her current research interests include sustainable materials with focus on carbon and carbon hybrids produced via hydrothermal processes, waste recycling into advance products, avoidance of critical elements in renewable energy technologies and the development of truly sustainable clean energy storage and conversion paths including alternative chemistries beyond Li, flexible and structural supercapacitors made from lignin/cellulose, carbon-based O2 electrocatalysis, CO2 capture and conversion and exploring the optoelectronic properties of nanocarbons.

New Directions in Solid State Chemistry Enabling Clean Energy Conversion and Storage

John Irvine

University of St Andrews, UK

Abstract

Understanding and controlling the processes occurring at electrode/electrolyte interface are key factors in optimising fuel cells and electrolysers. Metal particles supported on oxide surfaces promote many of the reactions and processes that underpin the global chemical industry and are key to many emergent clean energy technologies. At present, particles are generally prepared by deposition or assembly methods which, although versatile, usually offer limited control over several key particle characteristics, including size, coverage, and especially metal-surface linkage. In a new approach, metal particles are grown directly from the oxide support though in situ redox exsolution. We demonstrate that by understanding and manipulating the surface chemistry of an oxide support with adequately designed bulk (non)stoichiometry, one can control the size, distribution and surface coverage of produced particles. We also reveal that exsolved particles are generally epitaxially socketed in the parent perovskite which appears to be the underlying origin of their remarkable stability, including unique resistance of Ni particles to agglomeration and to hydrocarbon coking, whilst retaining catalytic activity.

Biography

Prof. John Irvine FRSE, FRSC has made a unique and world-leading contribution to the science of energy materials, especially fuel cell and energy conversion technologies. This research has ranged from detailed fundamental to strategic and applied science and has had major impact across academia, industry and government. The quality and impact of Prof. Irvine's research has been recognised by a number of national and international awards, including the Lord Kelvin Medal from the Royal Society of Edinburgh in 2018, the Schönbeim gold medal from the European Fuel Cell Forum in 2016, the RSC Sustainable Energy Award in 2015, with earlier RSC recognition via Materials Chemistry, Bacon and Beilby awards/medals. He has almost 500 publications and has an WoS h-index of 64. He has strong international standing having held senior visiting appointments in the US, Australia and China and has strong links with a number of leading laboratories across the Chinese Academy of Science including being Thousand Talents professor at Fujian Institute of Research on the Structure of Matter.

Perovskite on Silicon: Towards 30 Percent Industrial, Stable and Cost-Effective Solar Cells ?

Christophe Ballif

EPFL and CSEM, Switzerland

Abstract

In this presentation, we review first shortly the status of the PV industry, emphasing the low manufacturing costs achieved by monocrystalline silicon, where ultra low price of 9-11$/m2 for wafers and 20-25/m2 for cells are achieved. This makes silicon a choice low cost absorber for tandem cells. We then show quickly empirically how the best tandem devices based on perovskite/silicon structure could reach practically 32-33%. We review then the progress made by such devices, with current record for small size devices (1 cm2, certified) at 29.5%. Then we illustrate with some of the results of the EPFL and CSEM teams in Neuchâtel, progresses on metallization, upscaling, and work on textured wafers. For instance 4 cm2 cells with screen-printed metallization can be made with over 27.5% efficiency. We discuss the challenges still facing perovskite technologies, with some insight into key degradation modes of devices. Providing those can be solved, we finally show in which market segments and at which typical pricing high efficiency tandem modules could penetrate the market, setting indirectly limits on the possible manufacturing costs of the perovskite top cells.

Biography

Prof. Christophe Ballif is director of the Phototovoltaics and Thin Film Electronics Laboratoryb) (PV-Lab at the institute of microengineering (IMT) in Neuchâtel (part of the EPFL since 2009). The focus of his lab is on the science and technology of high efficiency heterojunction crystalline cells, so-called passivating contacts for solar

cells, multi-junction solar cells include novel generation Perovskite on innovative optical high speed detector and on various macroelectronics application. Prof. Ballif graduated as a physicist from the EPFL in 1994, where he also obtained in 1998 his Phd degree working on novel PV materials. He accomplished his postdoctoral research at NREL (Golden, US) on compound semiconductor solar cells (CIGS and CdTe). He (co-) authored over 500 journal and technical papers, as well as several patents.

Invited Talks

One Dimensional Nanomaterials for Emerging Energy Storage

Liqiang Mai

Wuhan University of Technology, China

Abstract

One-dimensional nanomaterials can offer large surface area, facile strain relaxation upon cycling and efficient electron transport pathway to achieve high electrochemical performance. Hence, nanowires have attracted increasing interest in energy related fields. We designed the single nanowire electrochemical device for in situ probing the direct relationship between electrical transport, structure, and electrochemical properties of the single nanowire electrode to understand intrinsic reason of capacity fading. The results show that during the electrochemical reaction, conductivity of the nanowire electrode decreased, which limits the cycle life of the devices. We have developed a novel assembled nanoarchitecture was also presented, which consists of V2O3 nanoparticles embedded in amorphous carbon nanotubes that are then coassembled within a reduced graphene oxide network. The naturally integrated advantages of each subunit exhibit highly stable and ultrafast sodium-ion storage. In addition, we demonstrated a 3D nitrogen-doped graphene/titanium nitride nanowire (3DNG/TiN) composite as a freestanding electrode for Li–S batteries. The highly porous conductive graphene network provides efficient pathways for both electrons and ions and TiN nanowires attached on the graphene sheets have a strong chemical anchor effect on the polysulfides. As a result, the 3DNG/TiN cathode exhibits an initial capacity of 1510 mAh g–1 and the capacity remains at 1267 mAh g–1 after 100 cycles at 0.5 C. A commercial polypropylene (PP) separator decorated with TiO2 nanosheets with oxygen acancies (OVs-TiO2@PP) is fabricated to enhance the fast lithium-ion penetration and the high energy density of the whole cell. We also develop a bilayer-structured vanadium oxide (Mg0.3V2O51.1H2O) with synergistic effect of Mg2+ ions and lattice water as the cathode material for magnesium-ion batteries (MIBs). The pre-intercalated Mg2+ ions provide high electronic conductivity and excellent structural stability and the lattice water enables fast Mg2+ ions mobility because of its charge shielding effect. As a result, the Mg0.3V2O51.1H2O exhibits excellent rate performance and an unprecedented cycling life with capacity retention of 80.0% after 10,000 cycles. Moreover, a K+/vacancy disordered P3-type structure is designed and synthesized by simply modulating the K+ contents in Mn/Ni-based layered oxides. The K+/vacancy disordered K0.7Mn0.7Ni0.3O2 exhibits much better rate performance and higher discharge capacity. Our work presented here can inspire new thought in constructing novel one-dimensional structures and accelerate the development of energy storage applications.

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Biography

Prof. Liqiang Mai is a Chair Professor of Materials Science at Wuhan University of Technology and Laboratory Director of Wuhan University of Technology at Nano Key Lab. He is the Advisory Board of Nano Research and

International Advisory Board of Advanced Electronic Materials.

Copper-Substituted Na_xMO_2 (M=Fe, Mn) Cathodes for Sodium Ion Batteries

Xiaobo Ji

Central South University, China

Biography

Xiaobo Ji is Sheng hua Professor and associate dean in the Department of Chemistry and Chemical Engineering at Central South University. He is the Associate Editor for Electrochemistry Communications; Elsevier and has published more than 270 peer-reviewed papers. His current research is specializing in the research & development of battery and Supercapacitor materials and their systems.

Up- and Down Converting Light in Solar Energy Conversion Schemes

Dirk Guldi

Friedrich-Alexander-Universitaet Erlangen-Nuernberg, Germany

Abstract

The Shockley-Queisser limit places an upper bound on solar conversion efficiency for a single p-n junction solar cell at slightly more than 30%. To surpass this limit, multi-exciton generation is being explored in inorganic semiconductors, while singlet fission (SF) is being investigated in arrays of conjugated organic molecules. In an optimal SF process, the lowest singlet excited state of one molecule (S1) that is positioned next to a second molecule in its ground state (S0) is down-converted into two triplet excited states (T1) each residing on one of the two adjacent molecules. The two triplet states initially form a correlated pair state 1(T1T1), which then evolves into two separated triplet states (T1 + T1). As such, the energetic requirement for SF is $E(S1) \geq 2 \times E(T1)$.

We have set our focus in recent years on intramolecular SF in molecular materials and their studies in solution rather than on intermolecular SF investigations in crystalline films. Implicit in intramolecular SF is a resonant, direct excitation of the SF material. In pentacene dimers linked by a myriad of molecular spacers, SF takes place with quantum yields of up to 200%. In addition, all key intermediates in the SF process, including the formation and decay of a quintet state that precedes formation of the pentacene triplet excitons, have been identified. This approach is, however, limited to the part of the solar spectrum, where, for example, the pentacene dimers feature a significant absorption cross-section. To employ the remaining part of the solar spectrum necessitates non-resonant, indirect excitation of the SF materials via either up- or down-conversion. For example, the up-conversion approach is realized with singlet excited states in pentacene dimers, which are accessed by two-photon absorptions (TPA). TPA is then followed in the second step of the sequence by an intramolecular SF – similar to what is seen upon resonant, direct excitation. Quite different is the down-conversion approach, which is based on an intramolecular Förster resonance energy transfer (FRET) and thereby the (photo)activation of the SF material. FRET requires the use of a complementary absorbing chromophore and enables funneling its excited state energy unidirectionally to the SF performing pentacene dimer. Again, SF completes the reaction sequence.

Biography

The Guldi lab and its network belong to the cutting edge of worldwide research in solar-energy conversion with expertise not only in advanced photon- and charge-management, but also in the synthesis of tailored materials and molecular modelling.

Dirk Guldi is a professor of Chemistry and Pharmacy department and chair of Physical Chemistry I. His current

research activities include the application of a variety of spectroscopic and microscopic techniques to characterize chemical, physical and photophysical properties of new, molecular architectures. His experimental working techniques range from ultrafast spectroscopy (absorption and fluorescence) to vibrational spectroscopy (Raman and IR) and electrochemistry to microscopy (Raman, TEM and AFM). In practice, molecular light-controlled systems are extremely valuable for the implementation of solar energy conversion, photovoltaics, and catalytic processes.

Functionalization of Renewable Materials for Materials Sustainability

Jose Rajan

Universiti Malaysia Pahang, Malaysia

Abstract

Emergence of sustainability as the new normal and consequent concerns over material sustainability for various industrial sectors accelerated materials discovery process from renewable sources [1]. Energy storage become one of the dominant industries currently and most of the high performing energy storage devices such as lithium ion batteries use expensive mined materials as electrodes with enormous processing and value addition. Biomass derived carbon has been suggested as a possible material for energy storage, however, they mainly suffer from lower performance indicators [2 -3]. We have explored augmenting properties of biomass carbon with small amounts (~5 – 10 wt.%) of metals or metal oxides to enhance the charge storage parameters in lithium ion capacitors, battery – supercapacitor hybrids, and symmetric supercapacitive storage modes besides developing eco-friendly and green routes for their processing using physical means than chemical methods. Four strategies were adopted: (i) enhancing the charge storage sites by filling large voids in porous carbon by hierarchical 3D nanoflowers or composite nanostructures [4-6], (ii) developing a thin metal oxide film over porous carbon surface through a simultaneous activation and coating process [7], (iii) developing a thin metal film over porous carbon [8], and (iv) green reduction of graphene oxide to reduced graphene oxide by means of physical methods than chemical ways [9]. Several advanced carbon structures are thereby synthesized; in supercapacitive charge storage mode they gave charge storability of ~60% of lithium battery and ~10 times more power capability than lithium battery. Only 10% metal compositions could boost up the energy storage capabilities dramatically. Promising green processing routes are also developed which avoid large scale toxic chemicals for developing advanced materials.

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Biography

Rajan Jose is currently the Dean of Research (Technology), a member of Senate, and a Senior Professor at the Universiti Malaysia Pahang (UMP). He supervises the Nanostructured Renewable Energy Materials Laboratory in the UMP. He received his PhD degree in the year 2002 for his work on superconducting and microwave electronics. He was employed at the Indira Gandhi Centre for Atomic Research (India), AIST (Japan), Toyota Technological Institute (Japan), and the National University of Singapore (Singapore) before joining UMP. His current research interests include nanostructured materials and renewable energy devices.

Tailored Electrodes Based on Transition Metal Compounds for Hybrid Supercapacitors: A New Path to Enable Electrochemical Energy Storage

Fatima Montemor

University of Lisbon, Portugal

Abstract

Electrochemical Energy storage is crucial to enable a low carbon energy economy. In this field supercapacitors thanks to their high specific power and short response time are becoming crucial in a wide array of applications. However conventional carbon based devices lack energy density, a drawback that limits their use in certain applications. To overcome this problem, metal compounds, such as oxides, hydroxides and sulfides are presently considered very interesting materials to fabricate electrodes for redox supercapacitors and asymmetric capacitors. Other drivers enabling these materials also include the need to assemble devices using aqueous and more friendly electrolytes, use of non-scarce raw materials and the need for tailoring functional electrodes to meet the final application requirements.

Electrodes for asymmetric supercapacitors based on transition metal compounds can be fabricated by different routes that allow easy tailoring of the final physico – chemical properties, including chemical composition, morphology, crystal structure and electronic and ionic conductivity. These properties must be well designed and introduced in the electrode material, since they govern the electrochemical response of the electrode, and are the key to tailor the device metrics.

This work aims at highlighting the latest advances on the use of transition metal compounds for high power applications namely as asymmetric supercapacitor electrodes. This work also identifying new perspectives and strategies to explore further the material electrochemical response and to enhance its energy storage performance.

Biography

M.F. Montemor graduated in Chemical Engineering at INSTITUTO SUPERIOR TÉCNICO (IST), the school of engineering of the TECHNICAL UNIVERSITY OF LISBON in 1989 and obtained her Ph.D., also from the TECHNICAL UNIVERSITY OF LISBON, in 1995. Her research objectives are focused in the area of new surface functionalization strategies and development of novel coatings for improved performance of metallic parts used in various sectors. She is a Full Professor in the Department Of Chemical Engineering and researcher at CQE and Vice President for Research and International Affairs at Instituto Superior Técnico.

Oral Presentations

Two-dimensional Doping of Proton Conductors

P.Ngabonziza[1]*, R.Merkle[1] ,Y.Wang[1], P.A.van Aken[1], T.S.Bjørheim[2], J.Maier[1], J.Mannhart[1]

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[2]University of Oslo, Norway

Abstract

Ionic conducting heterostructures are of interest to explore interfacial effects in solid state ionics and to foster their potential deployment in clean energy technologies such as solid oxide fuel cells. How to achieve ion conduction in heterostructures is therefore a fascinating and relevant question.

In this presentation, we will report on the first realization and study of a two-dimensionally doped ion conductor. This work is based on epitaxial $BaZrO_3$–$BaYO_x$ heterostructures [1] in which entire ZrO_2-layers of the $BaZrO_3$ crystal are replaced by heterovalent layers (YO_x). The resulting charge carriers reside in the immediate vicinity of the substituted layer. These heterostructures show – if hydrated - significant proton conductivities increasing with the number of interfaces. They are comparable, yet somewhat lower than those of hydrated $Ba(Zr,Y)O_3$ ceramics. Pros and cons of 2d versus conventional 3d doping are discussed.

To explore the potential of inelastic electron tunneling spectroscopy to study ionic species at high temperatures, we then use the same $BaZrO_3$ based heterostructures as proton conductors and electron tunnel barriers in tunnel junction devices [2]. These junctions yield high resolution inelastic tunneling spectra of protons diffused along the interfaces in $BaZrO_3$–$BaYO_x$-based tunnel barriers up to at least 400 K, breaking the previously established fundamental resolution limit by a factor of nine By analyzing O H bond vibrations, the existence of protons in the tunnel barriers is confirmed.

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Inelastic Electron Tunneling Spectroscopy at High Temperatures.
Adv. Mater. 33 2007299 (2021).

Biography

Prosper Ngabonziza completed his PhD in 2016 in engineering physics from University of Twente in The Netherlands. He received the S2A3 Bronze Medal in 2013 awarded by the Southern Africa association for advancement of science to the best student who did a most meritorious master dissertation in a science department in South Africa. He works at the Max Planck Institute for Solid State Research in the department of solid-state quantum electronics of Prof. Jochen Mannhart.

Photovoltatronics: Intelligent PV-based Devices for Energy and Information Applications

Hesan Ziar, Patrizio Manganiello, Olindo Isabella* and Miro Zeman

Delft University of Technology, The Netherlands

Abstract

Electrification and digitalization are two significant trends in the energy sector. Large-scale introduction of variable renewable energy sources, energy storage and power-electronics components, all based on direct current (DC), is

fundamentally changing the electrical energy system of today that is based on alternating current (AC). This trend leads to a complex hybrid AC/DC power system with the extensive deployment of information and communication technologies (ICT) to keep the system stable and reliable. Photovoltaics (PV) is a technology that will play an essential role in local generation of clean electricity in expanding urban areas. To take full advantage of PV in the urban environment, PV technology must become intelligent. In this contribution, we identify, describe, and label a new research field that deals with intelligent PV and its application in components with multiple functionalities. We denote this field photovoltatronics, which brings together disciplines of energy and informatics. Since photons and electrons are carriers of both energy and information, photovoltatronics is the field that designs and delivers autonomous devices for electricity generation and information communication. It introduces a pathway from harvesting energy of photons (hn) to creating bits of information (01) through the energy of photo-generated electrons (eV). We show that B10 keV energy is at least needed for transceiving one bit of information in the energy-information chain of the photovoltatronics, while the ultimate efficiency of the chain can reach up to 33.4%.

Biography

Olindo Isabella is Associate Professor and head of the Photovoltaic Materials and Devices group at Delft University of Technology. He obtained his MSc degree in Electronic Engineering in 2007; was visiting researcher at AIST (Tsukuba, Japan) between 2011 and 2012; and received his PhD degree (cum laude) in advanced light management for thin-film silicon solar cells from Delft University of Technology in 2013. Since then, he has been in force at the Photovoltaic Materials and Devices group, expanding his research interests to photovoltaic technologies and applications. He has published more than 100 peer-reviewed journals articles (h-index 28).

Detailed Band Diagram Determination of Perovskite Solar Cells Using Photoelectron Spectroscopy on Step by Step Prepared Devices and Using Tapered Cross Sections of Full Devices

Thomas Mayer*[1], Tim Hellmann[1], Chittaranjan Das[2], Clément Maheu[1], Tobias Abzieher[3], Ulrich Paetzold[3], Wolfram Jaegermann[1]

[1]Darmstadt University of Technology, Germany

[2]Karlsruhe Institute of Technology, Germany

Abstract

The electronic structure of electronic devices to a large extent is governed by the interfaces of semiconductors with contact materials. In solar cells, thermodynamic equilibration of the electrochemical potential of electrons in the absorber and the contact phases leads to built in electric fields, which under solar excitation are the cause of the photo-potential. As photoelectron spectroscopy is a surface analytical method the band structure of buried interfaces can be determined by step by step deposition and analysis experiments using vacuum integrated systems. Different perovskite absorbers are demonstrated to be of n-type doping character comparing classical and inverted device stacks in the dark and operating at open circuit under light. In order to analyze the electronic structure of ex-situ solution processed devices, we developed tapered cross sections photoelectron spectroscopy (TCS-PES). Here we use a shallow angle wedge to project the nm scale of the normal cross section to the mm scale on the TCS that can be analyzed by line scan PES with local resolution in the 10µm range. In contrast to the current believe, we demonstrate that efficient MAPI3 and (FAPbI3)0.85(MAPbBr3)0.15 solar cells are of n-n-p and not n-i-p character.

Biography

Thomas Mayer is Leader of the Group Organic and Hybrid Electronic Materials at Surface Science Lab in the Materials Science Department TU-Darmstadt. He is an Expert in Photoelectron Spectroscopy on Semiconductor Interfaces using Integrated Systems for in-Vacuo Interface Preparation and Analysis.

Hybrid Electrode With High Optical & Electrical Property and Durability for Flexible Solar Cells

Soyeon Kim[1]* and Dong Chan Lim[1]

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Abstract

Mechanically durable transparent electrodes are needed in flexible devices to implement their long-term stable operating for applications in bendable, fordable and rollable fields. As it is well-known, Indium-tin-oxide (ITO), which is most typically used as a transparent electrode, is not suitable to be applied to flexible substrates. As such, several promising transparent electrodes have been previously reported to replace ITO. Among these, metal mesh has various advantages while being applicable to flexible substrate. However, the produced sample has a surface roughness despite being in the form of embedding, metal mesh has inherent voids problem, and problem that arise at the interface of contact with other organic layers. Therefore, we designed hybrid electrode constitute of conducting polymer with metal mesh to compensate that several problems. As the result, designed hybrid had good electrical and optical properties. And moreover, that electrode can maintain its mechanical durability even after a bending and rolling tests. Finally, due to the excellent properties of the hybrid electrode, we can get enhanced thin film solar cell which is contained organic and inorganic solar cell.

Biography

Soyeon Kim received her Ph.D. degree in chemical & biomolecules engineering from Yonsei University, Korea in 2017. After obtaining a Ph.D., she works senior researcher of department of energy & electronic material in surface materials division at the Korea Institute of Materials Science (KIMS), Korea. Her main research interests are in nanomaterials including synthesis and applications for energy & electronic devices.

Stability of the Oxidized Form of RuLL´(NCS)$_2$ Dyes in Acetonitrile in the Presence of Water and Pyridines – Why the Dye-Sensitized Solar Cell Electrolyte Should be Dry

Torben Lund*, Poul Erik Hansen, Jens Josephsen, Niels Jacob Krake, and John Mortensen

Roskilde University, Denmark

Abstract

The detrimental effect of electrolyte water contamination on the light-soaking lifetime of Dye-sensitized Solar Cells (DSCs) prepared with RuLL´(NCS)$_2$ dyes and N-additives like 4-*tert*-butylpyridine (TBP) is not well understood. A new explanation is presented based on investigation of the stability of the ruthenium(III) complexes Ru(bipy)$_2$(NCS)$_2^+$ (**1**$^+$) and RuLL´(NCS)$_2^+$ (L = 4,4´-dicarboxy-2,2´-bipyridine, L´= 4,4´-nonyl-2,2´-bipyridine) (Z907$^+$) in acetonitrile in the presence of water and pyridines covering a large variation in basicity. **1**$^+$ reacts with small amounts of water in the acetonitrile containing a pyridine base (X) according to the overall reaction:

$$6\ Ru(bipy)_2(NCS)_2^+ + 4\ H_2O + 8\ X \rightarrow 5\ Ru(bipy)_2(NCS)_2 + Ru(bipy)_2(NCS)(CN) + SO_4^{2-} + 8\ XH^+.$$

The reaction mechanism of **1**$^+$ (and Z907$^+$) is proposed to be initiated by an attack of OH^- giving Ru(bipy)$_2$(NCS)(NCS-OH). The stronger the base the faster the reaction. Extrapolating the life time of Z907$^+$ to a typical TBP concentration of 0.5 M in the DSC gives a degradation rate around 7 s^{-1}. Z907$^+$ bound to a layer of nano crystalline TiO_2 surface reacted fast too, when inserted in an acetonitrile solution containing 4-*tert*-butylpyridine. In a "wet" electrolyte, containing more than 500 mM of water the light-soaking lifetime of a DSC prepared with Z907 is predicted to be about 10 days at out-door light soaking conditions, whereas trace amounts of water (< 25 mM) in a "dry" electrolyte is used up by consumption of only 10% of the Z907 in a typical DSC. Therefore, the DSC is expected to have a long light-soaking lifetime with a "dry" electrolyte.

Biography

Prof. Torben Lund got his Ph.D in 1987 from Aarhus University. Since 1993 he is working as an Associate Professor at Roskilde University. His group has established a fundamental understanding of the degradation mechanism and kinetics of ruthenium dyes both under light soaking and thermal stress. As the first group in the DSC field we have used analytical methodologies based on HPLC coupled electro spray mass spectrometry (LC-MS) to characterize dye degradation mechanism and stability in DSCs.

Poster Presentations

3D Architected Pyrolytic Carbon Electrodes for Lithium Ion Batteries

Kai Narita

California Institute of Technology, USA

Abstract

The ability to design a particular geometry of porous electrodes at multiple length scales in a lithium-ion battery can significantly and positively influence battery performance because it enables control over distributions of current and potential and can enhance ion and electron transport. We developed 3D architected carbon electrodes, whose structural factors are independently controlled and whose dimensions span microns to centimeters, using digital light processing and pyrolysis. These free-standing lattice electrodes are comprised of monolithic glassy carbon beams, are lightweight, with a relative density of 0.1-0.35, and mechanically robust, with a maximum precollapse stress of 27 MPa. The specific strength is 101 kN m kg-1, comparable to that of 6061 aluminum alloy. The excellent mechanical resilience enables to preserve the three-dimensionally designed porous electrode structure under static pressure in a packaged cell and facilitates electrode recycling.

These architected carbon electrodes can reach a mass loading of 70 mg cm^{-2} and an areal capacity of 3.2 mAh cm^{-2} at a current density of 2.4 mA cm^{-2}. The capacity retained >80% over 100 cycles at 0 0.39 mA cm^{-2}. We demonstrate this approach allows for the independent design of structural factors, i.e. beam diameter, electrode thickness, and surface morphology, enabling control over Li-ion transport length, overpotential and battery performance, not available for slurry-based electrodes. This multi-scale approach to architecting electrodes may open substantial performance-enhancing capabilities for solid- and liquid-state batteries, flow batteries and fuel cells.

Biography

Kai Narita is a senior PhD student in Materials Science, California Institute of Technology. Kai joined Caltech after completing a bachelor's and master's degree at Tokyo Institute of Technology in Japan. Currently, Kai works with Prof. Julia Greer to develop 3D architected battery electrodes with controllable and flexible multi-scale form-factors using lithography-based 3D printing and pyrolysis. Kai is also interested in understanding the role of micron-scale battery dynamics (e.g. ion/electron transports) on nano-scale phenomena such as solid electrolyte interphase formation.

Phase Change Energy Storage Composite Material with Assembled Graphene Skeleton for Thermal Conductivity Enhancement

Li Kong*, Jia Yu, Haoqing Wang, Hongji Zhu , Qingshan Zhu, Jiawen Su

Harbin Engineering University, China

Abstract

This abstract presents a novel structure used as the heat transfer enhancement in phase change material. Based on the common graphene foam, graphene film was introduced through simple ice-templated method. Narrow strip of graphene film was wound into a roll, then immersed in an aqueous graphene oxide solution. With the help of liquid nitrogen, ice crystals grow lengthwise, driving the graphene oxide sheets to rearrange themselves into a honeycombed foam structure, while the graphene film roll is tightly wrapped inside. The Gfilm-Gfoam skeleton structure was obtained by vacuum freeze-drying and hydrazine hydrate reduction. Finally, the paraffin was filled by vacuum impregnation, and cooled to obtain a Gfilm-Gfoam/PW composite. The composite structure can increase the thermal conductivity of paraffin by 44 times to 11.594 W/mK, and the corresponding mass fraction is only 1.14 wt%. Faster heat conduction ability, coupled with the strong heat storage ability of phase change material, make the composite phase change material can improve the power generation of thermoelectric generator (TEG) in a

fluctuating thermal environment. Simulation results indicate that increasing thermal conductivity helps the PCM to better play a buffering effect, and significantly reduce the fluctuation of the power generation voltage.

Biography

Li Kong currently works as a PhD Candidate at Harbin Engineering University. The previous work focused on the preparation and simulation analysis of graphene-enhanced phase change materials, and then turned to the structural design analysis of thermoelectric generation devices and the study of thermoelectric power generation performance under fluctuating heat sources. The research results have been published in ACS applied energy materials and Journal of Electronic Materials. The efficient use of energy is Li's consistent research interest, including the recovery and conversion of heat energy.

Engineering Interface of TiC Electrodes for Li-air Batteries

Elmar Kataev*[1], Valerii Isaev[2], Anna Kozmenkova[2], Alexander Frolov[2], Denis Vyalikh[3], Daniil Itkis[2] and Lada Yashina[2]

[1]*Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Germany*

[2]*Lomonosov Moscow State University, Russia*

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Abstract

Li-air batteries (LABs) are considered one of the most promising energy storage devices due to their outstanding theoretical specific energy. Unfortunately, this type of battery faces severe challenges including low cycleability associated with reactivity of oxygen reduction reaction (ORR) products and intermediates, for instance, superoxide anion, towards positive electrodes which are commonly made of various carbons. Recently, transitional metal carbides were proposed as a stable alternative to carbon materials. Titanium carbide shows outstanding performance as positive electrode in LABs specifically providing no capacity loss for at least 100 discharge/charge cycles and no significant side products formation as compared to carbon-based materials. However, overall recharge performance of TiC-based electrode is strongly dependent on its surface chemistry. TiOx layer, unavoidably formed on TiC surface, as thin as 3 nm can completely block electron transfer reaction, while non-uniformity of the oxide layer leads to rapid TiC degradation. Thus, to obtain suitable cathode material it is necessary to tune surface chemistry of TiC.

Here we report a direct operando photoemission study of ORR pathway on pristine and oxidized surfaces of TiC. We designed the electrochemical cell with TiC nanoparticles deposited on glass-ceramics electrolyte to avoid side reactions of ORR products with liquid electrolyte. Combining operando photoemission data with in situ observation of superoxide anion attack on TiC in model chemical systems, we provide atomic-level understanding of TiC surface chemistry and present several ways for its stabilization in aprotic ORR.

Biography

Elmar Kataev received his Ph.D. in solid-state chemistry and electrochemistry from the Department of Materials Science at Lomonosov Moscow State University. After his Ph.D., he joined group of Prof. Steinrück at Friedrich–Alexander University Erlangen–Nürnberg. Currently, he is working at the Department of Interface Design at Helmholtz-Zentrum Berlin. His research topics cover batteries and electrocatalysis with special focus on synchrotron-based operando spectroscopy characterization.

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