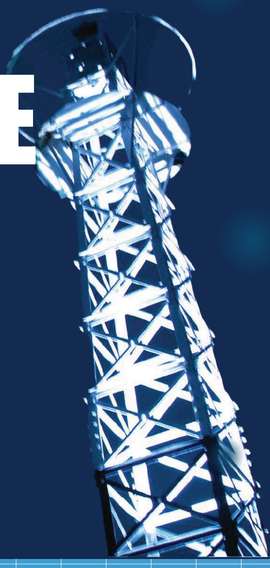
2nd Energy LEDARE Workshop



Venue : KNTEC, Frösundaviks allé 1, 169 70 Solna
Date : 11-13 September, 2023
Scientific Organizer : Nam Gyu Park(SKKU)

Participants

Korea

Nam-Gyu Park (SKKU)
Yun Jeong Hwang (SNU)
Tae-Woo Lee (SNU)
Ki Tae Nam (SNU)
Jong Hyeok Park (Yonsei Univ)
Hui-Seon Kim (Inha Univ)
Hyunjung Shin (SKKU)
Hyun Suk Jung (SKKU)
Jin Young Kim (UNIST)
Sang Il Seok (UNIST)

Sweden

Anders Hagfeldt (Uppsala Univ)
Tönu Pullerits (Lund Univ)
Ute Cappel (KTH)
Tomas Edvinsson (Uppsala Univ)
Thomas Wågberg (Umeå Univ)
Crispin Xavier (Linköping Univ)

Denmark, Finland, and Norway

Jens Wenzel Andreasen (Technical Univ. Denmark)
Paola Vivo (Tampere Univ., Finland)
Truls Norby (UiO, Norway)

Switzerland and EU

Michael Grätzel (EPFL, Switzerland)
Antonio Abate (HZB, Germany)

Ministry of Science and ICT

KNTEC

The 2nd Energy LEDARE Workshop 2023

September 11 - 13 (3 days)

Venue: KNTEC (www.kntec.org), Sweden

Organized by NRF, Korea

Timetable

Time	Sep. 11 (Mon)	Sep. 12 (Tue)	Sep.13 (Wed)
10:00-10:30		Anders Hagfeldt	Ki Tae Nam
10:30-11:00		Tae Woo Lee	Paola Vivo
11:00-11:30		Ute Cappel	Hyunjung Shin
11:30-13:00		Jens Wenzel Andreasen	Lunch
13:00-13:30	Registration /Opening	Lunch	
13:30-14:00	Michael Grätzel	Hui-Seon Kim	Jin Young Kim
14:00-14:30	Sang Il Seok	Thomas Wågberg	Tomas Edvinsson
14:30-15:00	Crispin Xavier	Free Discussion	Yun Jeong Hwang
15:00-15:30	Hyun Suk Jung		Coffee Break
15:30-16:00	Coffee Break		Truls Norby
16:00-16:30	Antonio Abate		Nam-Gyu Park
16:30-17:00	Jong Hyeok Park		Wrap-up
17:00-17:30	Tönu Pullerits		
17:30-18:00			
18:00-18:30	Dinner 19:00		Dinner 18:00
18:30-20:00		Dinner(18:00)	

Program

	Sep. 11 (Day 1)
13:00-13:20	Registration
13:20-13:30	Opening Remark (NRF and Nam-Gyu Park)

Session I (13:30-15:30) 🎙 *Presider:* ***Yun Jeong Hwang***

13:30-14:00 **Michael Grätzel**
Molecular Photovoltaics and the Rise of Perovskite Solar Cells

14:00-14:30 **Sang Il Seok**
Achieving Efficient Perovskite Solar Cells through Tailored Growth and Phase Control

14:30-15:00 **Crispin Xavier**
Biopolymers in organic batteries

15:00-15:30 **Hyun Suk Jung**
Close Loop Recycling Process for Ecofriendly Perovskite Solar Cells

15:30-16:00	Coffee Break

Session II (16:00-17:30) 🎙 *Presider:* ***Truls Norby***

16:00-16:30 **Antonio Abate**
Lead-Free Perovskite Solar Cells

16:30-17:00 **Jong Hyeok Park**
Overall Water Splitting by Lead Halide Perovskite Photoelectrodes

17:00-17:30 **Tõnu Pullerits**
Photonic processes in metal halide perovskite nanostructures, from 0D to 2D

18:00-20:00	Dinner
	Sep. 12 (Day 2)

Session III (10:00-11:30) 🎙 *Presider:* ***Thomas Wågberg***

10:00-10:30 **Anders Hagfeldt**
Stabilizing Grain Boundaries and Surfaces of the Perovskite Layer in Perovskite Solar Cells to Extend Device Durability

10:30-11:00 **Tae Woo Lee**
Perovskite nanocrystals enabling bright, efficient and stable light-emitting diodes

11:00-11:30 **Ute Cappel**
Energy alignment and charge dynamics in solar cells determined by time-resolved and operando photoelectron spectroscopy

11:30-12:00 **Jens Wenzel Andreasen**

	Understanding and controlling light-matter interactions in organic solar cells
12:00-13:30	Lunch

Session IV (13:30-15:00) *Presider:* ***KI Tae Nam***

13:30-14:00	**Hui-Seon Kim**
	Interface engineering for perovskite solar cells
14:00-14:30	**Tomas Wågberg**
	Novel strategies for efficient water electrolysis
18:30-20:00	Dinner

Sep. 13 (Day 3)

Session V (10:00-11:30) *Presider:* ***Tomas Edvinsson***

10:00-10:30	**KI Tae Nam**
	432 Symmetric Chiral Gold Nanoparticle
10:30-11:00	**Paola Vivo**
	Air-stable perovskite-inspired absorbers for sustainable indoor light-harvesting
11:00-11:30	**Hyunjung Shin**
	Structure – Property Relation in Formamidinium Lead Triiodide ($FAPbI_3$)
11:30-13:30	Lunch

Session VI (13:30-15:00) *Presider:* ***Ute Cappel***

13:30-14:00	**Jin Young Kim**
	Improving Performance and Stability of $FAPbI_3$-based Perovskite Solar Cells via Methylammonium Chloride and Formate Anion Engineering
14:00-14:30	**Thomas Edvinsson**
	Nature of the excited states in Lead halide perovskites and Quantum Mechanical Guided Machine Learning
14:30-15:00	**Yun Jeong Hwang**
	Electrolyte effect on electrochemical CO_2 reduction reaction
15:00-15:30	Coffee Break

Session VII (15:30-16:30) *Presider:*

15:30-16:00	**Truls Norby**
	Improving Performance and Stability of $FAPbI_3$-based Perovskite Solar Cells via Methylammonium Chloride and Formate Anion Engineering
16:00-16:30	**Nam-Gyu Park**
	Facet engineering for stable and efficient perovskite solar cells
16:30-17:00	Wrap-up and Closing Remark (NRF and Nam-Gyu Park)
18:00-20:00	Dinner

Invited Speakers

► **Korea Delegates**

1. Nam-Gyu Park (SKKU) npark@skku.edu
2. Yun Jeong Hwang (SNU) yjhwang1@snu.ac.kr
3. Tae-Woo Lee (SNU) twlees@snu.ac.kr
4. Ki Tae Nam (SNU) nkitae@snu.ac.kr
5. Jong Hyeok Park (Yonsei Univ.) lutts@yonsei.ac.kr
6. Hui-Seon Kim (Inha Univ.) hui-seon.kim@inha.ac.kr
7. Hyunjung Shin (SKKU) hshin@skku.edu
8. Hyun Suk Jung (SKKU) hsjung1@skku.edu
9. Jin Young Kim (UNIST) jykim@unist.ac.kr
10. Sang Il Seok (UNIST) seoksi@unist.ac.kr

► **Sweden Delegates**

11. Anders Hagfeldt (Uppsala Univ.) anders.hagfeldt@uu.se
12. Tönu Pullerits (Lund Univ.) tonu.pullerits@chemphys.lu.se
13. Ute Cappel (Royal Institute of Technology (KTH)) cappel@kth.se
14. Tomas Edvinsson (Uppsala Univ.) Tomas.Edvinsson@angstrom.uu.se
15. Thomas Wågberg (Umeå Univ.) Thomas.wagberg@umu.se
16. Crispin Xavier (Linköping Univ) xavi.er.crispin@liu.se

► **Denmark, Finland, and Norway Delegates**

17. Jens Wenzel Andreasen (Technical Univ. Denmark) jewa@dtu.dk
18. Paola Vivo (Tampere Univ., Finland) paola.vivo@tuni.fi
19. Truls Norby (UiO, Norway) truls.norby@kjemi.uio.no

► **Switzerland and EU Delegate**

20. Michael Grätzel (EPFL, Switzerland) michael.graetzel@epfl.ch
21. Antonio Abate (HZB, Germany) antonio.abate@helmholtz-berlin.de

Biography and Abstract

► Michael Grätzel (Ecole Polytechnique Fédérale de Lausanne, Switzerland)

Professor of Physical Chemistry at the Ecole polytechnique fédérale de Lausanne (EPFL), **Michael Graetzel**, PhD, directs there the Laboratory of Photonics and Interfaces. He pioneered research on energy and electron transfer reactions in mesoscopic systems and their use to generate electricity and fuels from sunlight. He is credited with pioneering the field molecular photovoltaics which in turn served as a launch pad for perovskite solar cells producing a revolution in the photovoltaics. His over 1700 publications have received some 464'000 citations with an h-factor of 295 (Google Scholar 2024) demonstrating the strong impact of his scientific work. A recent bibliometric ranking by Stanford University places Michael in the first position on top of a list of 100'000 world-wide leading scientists across all fields. Michael has been awarded a large number of prestigious international awards, the latest ones being the 2022 Rank Prize in Optoelectronics (UK) and the BBVA Foundation Frontiers of Knowledge Award in Basic Science. He is a member of several learned societies including the Swiss Academy of Technical Science the German Academy of Science (Leopoldina) and the Royal Spanish Academy of Engineering and was elected foreign member of the Chinese Academy of Science and of the Royal Society (UK). He has received honorary doctors (Dr. honoris causa) degrees from 13 Universities including the Universities of Lund and Uppsala in Sweden.

Molecular Photovoltaics and the Rise of Perovskite Solar Cells

Photovoltaic cells using molecular dyes, semiconductor quantum dots or perovskite pigments as light harvesters have emerged as credible contenders to conventional devices. Dye sensitized solar cells (DSCs) use a three-dimensional nanostructured junction for photovoltaic electricity production and reach currently a power conversion efficiency (PCE) of over 15 % in full sunlight. They possess unique practical advantages in particular highly effective electricity production from ambient light, ease of manufacturing, flexibility and transparency, bifacial light harvesting, and aesthetic appeal, which have fostered industrial production and commercial applications. They served as a launch pad for perovskite solar cells (PSCs) which are presently being intensively investigated as one of the most promising future PV technologies, the PCE of solution processed laboratory cells having currently reached 26..1 %. Present research focusses on their scale up to as well as ascertaining their long-term operational stability. My lecture will cover our most recent findings in these revolutionary photovoltaic domains.

► Sang Il Seok (Ulsan National Institute of Science and Technology, Korea)

Sang Il Seok is a Distinguished Professor in the Department of Energy and Chemical Engineering at the Ulsan National Institute of Science and Technology (UNIST) in Korea. He holds a B.S. in Chemistry from Kyung Pook National University, Korea, and a Ph.D. in Inorganic Materials Engineering from Seoul National University, Korea. After completing his Ph.D., he conducted postdoctoral research at Cornell University in the USA, focusing on defects and transport in the Fe-Ti-O Spinel structure. He also gained valuable experience as a visiting scholar at the University of Surrey in the UK in 2003 and École Polytechnique Fédérale de Lausanne (EPFL) in Switzerland in 2006. Prior to joining UNIST in 2015, Sang Il Seok served as the principal investigator at the Korea Research Institute of Chemical Technology (KRICT) and held a dual appointment as a professor at the Department of Energy Science at Sungkyunkwan University. He is a highly cited researcher, selected by Clarivate Analytics as one of the leading researchers since 2018. He has published over 200 peer-reviewed papers, including several articles in Nature and in Science as a main corresponding author. Such notable publications showcase the depth and significance of his research contributions to perovskite solar cells as one of the pioneers in the field. Throughout his career, he has received several awards for his outstanding contributions. The Korean government honored him with the prestigious "Korean Scientist Award" in 2017. In 20019, he was awarded the Kyung-Ahm Prize. Notably, in 2022, his groundbreaking work in perovskite solar cells led to him being honored with the esteemed Rank Prize. His research primarily revolves around functional inorganic-organic hybrid materials and their application to the devices, particularly perovskite solar cells. His expertise and dedication to advancing the field have solidified his standing as a respected energy and chemical engineering figure.

Achieving Efficient Perovskite Solar Cells through Tailored Growth and Phase Control

Halide perovskite photovoltaic solar cells (PSCs) have garnered significant global attention in the past decade due to their distinctive characteristics, such as being lightweight, flexible, and utilizing a solution coating process. Within a relatively short timeframe, PSCs have achieved a power conversion efficiency (PCE) of 26%, comparable to silicon solar cells. This remarkable enhancement in PCE is attributable to optimizing the device architecture, depositing uniform thin films, and adjusting the perovskite material composition to attain an appropriate bandgap. The exceptional material properties of perovskite materials have also played a crucial role. The strategic use of mediators to hinder rapid crystallization between organic cations and PbI_2, accomplished through solvent engineering or intramolecular exchange processes, as well as stabilizing the α-phase of optically active formamidinium lead iodide ($FAPbI_3$) perovskite at room temperature, have emerged as critical factors in depositing uniform thin films with reduced defects. The attainment of high-efficiency PSCs necessitates precise control over the crystallinity and surface morphology of the perovskite layers. This presentation will delve into the methods employed to achieve tailored growth and the formation of the α-phase in the crystalline $FAPbI_3$ layer on the substrate.

► Crispin Xavier (Linköping University, Sweden)

Xavier Crispin obtained his PhD in 2000 with Prof. J.L. Brédas (University of Mons, Belgium), postdoc at Linköping University with Prof. W.R. Salaneck. In 2004, Xavier joined the Laboratory of Organic Electronics headed by Prof. M. Berggren. For his work on organic thermoelectrics, he received the ERC-starting grant (2011), the Tage Erlander Prize (2012) and the Göran Gustafsson prize (2016). Since 2014, he is appointed as a Professor in Organic Energy Materials. In 2019, he became vice-director of the national program Advanced Functional Materials. He is cofounder and scientific advisor of Ligna Energy AB (2017) and Cellfion AB (2021). Today, he explores materials for organic batteries, solid state or redox flow batteries.

Biopolymers in organic batteries

The most common elements in the periodic table are carbon, oxygen, and hydrogen, all of which are abundant in the biosphere and define organic materials. This, in combination with the wealth of variation in molecular structures that organic synthetic chemistry can propose, provides the conditions for tailoring new organic materials for batteries. They may not be able to meet the requirements for batteries in vehicles because they typically have lower energy density per volume due to the lower density of organic matter compared to metals and inorganics. But bulky batteries are much less of an issue for large stationary energy storage needed in the electrical grid, in buildings or as a large power bank to charge the electrical cars. For that type of batteries, it is most important to have robust, safe, and sustainable battery technology with as low as possible cost/kwh/cycle.

We summarize our recent works following various new concepts for organic batteries: (i) First, a new class of electrolyte working in the regime of “water-in-polymer salt electrolyte”, which combines non-flammability, high ionic conductivity, wide electrochemical stability windows and enables aqueous organic batteries to get low self-discharge behavior.[1-4] (ii) Second, we review our effort to reach low-cost lignin electrodes by either combining with conducting polymers or carbon based nanoconductors.[5-7]

1. D. Kumar et al., Self-Discharge in Batteries Based on Lignin and Water-in-Polymer Salt Electrolyte. Advanced Energy and Sustainability Research 3, 2200073 (2022).
2. D. Kumar et al., Zinc salt in “Water-in-Polymer Salt Electrolyte” for Zinc-Lignin Batteries: Electroactivity of the Lignin Cathode. Advanced Sustainable Systems, 2200433 (2022).
3. Z. Khan et al., Water-in-Polymer Salt Electrolyte for Slow Self-Discharge in Organic Batteries. Advanced Energy and Sustainability Research 3, 2100165 (2022).
4. Z. Khan et al., Towards printable water-in-polymer salt electrolytes for high power organic batteries. Journal of Power Sources 524, 231103 (2022).
5. U. Ail et al., Optimization of Non-Pyrolyzed Lignin Electrodes for Sustainable Batteries. Advanced Sustainable Systems, 2200396 (2022).
6. U. Ail et al., Effect of Sulfonation Level on Lignin/Carbon Composite Electrodes for Large-Scale Organic Batteries. ACS Sustainable Chemistry & Engineering 8, 17933-17944 (2020).
7. C. Che et al., Twinning Lignosulfonate with a Conducting Polymer via Counter-Ion Exchange for Large-Scale Electrical Storage. Advanced Sustainable Systems 3, 1900039 (2019).

► Hyun Suk Jung (Sungkyunkwan University, Korea)

Hyun Suk Jung is a SKKU fellow professor in school of advanced materials science & engineering at Sungkyunkwan university (SKKU). He received his BS, MS, and PhD degrees in materials science & engineering from Seoul National University (SNU), in 1997, 1999, and 2004, respectively. He joined Los Alamos National Laboratory (LANL) as a director's postdoctoral fellow in 2005. He has published over 200 peer-reviewed papers including Nature Sustainability, Nature Communications, Energy and Environmental Science, Advanced Materials and Advanced Energy Materials, and holds more than 70 patents regarding synthesis of inorganic nanomaterials and solar energy conversion devices such as photovoltaic and photoelectrochemical devices. So far, his H-index is 61. He has received many awards including Top 50 outstanding research achievements from Ministry of Science and Education (2012), Minister award from Ministry of Future Creation and Science (2013), Young ceramist award from Korean Ceramic Society (2017), Excellence in Research (2020), and Minister award from Ministry of Science and ICT. He presently researches perovskite solar cells and flexible solar cells.

Close Loop Recycling Process for Ecofriendly Perovskite Solar Cells

All solid-state solar cells based on organometal trihalide perovskite absorbers have already achieved distinguished power conversion efficiency (PCE) to over 25% and further improvements are expected up to 27%. Now, the research on perovskite solar cells has been moving toward commercialization. To facilitate commercialization of these great solar cells, some technical issues such as long-term stability, large scale fabrication process, and Pb-related hazardous materials need to be solved. Also, flexible perovskite solar cell using plastic substrate can be used in niche applications such as portable electrical chargers, electronic textiles, and large-scale industrial roofing.

This talk is dealing with our recent efforts to facilitate commercialization of perovskite solar cells. For examples, we introduce a recycling technology of perovskite solar cells, which covers the regeneration process of Pb contained perovskite layer as well as recycling process of Au electrodes and transparent conducting oxide glass. Also, the recycling process of toxic solvents that have been used in fabrication or recycling process of perovskite solar cell is proposed for demonstrating close loop recycling process. The ecofriendly solvent-based green process for realizing highly efficient perovskite solar cell is also demonstrated.

► Antonio Abate (Helmholtz-Centrum Berlin, Germany)

Antonio Abate is the director of the "Novel Materials and Interfaces for photovoltaic solar cells" department at the Helmholtz-Centrum Berlin in Germany. He is researching solar energy conversion with halide perovskites.
Before his current position, Antonio led solar cell research at the University of Fribourg in Switzerland as a team leader. He was a Marie Skłodowska-Curie Fellow at École Polytechnique Fédérale de Lausanne within the group of Prof. Grätzel. He worked for four years as a postdoctoral researcher at the University of Oxford under the supervision of Prof. Snaith and at the University of Cambridge under the supervision of Prof. Steiner. Antonio graduated summa cum laude from the University of Naples Federico II in 2006. He got his PhD summa cum laude at Politecnico di Milano in 2011 under the supervision of Prof. Resnati and Prof. Metrangolo.

Lead-Free Perovskite Solar Cells

Halide perovskites quickly overrun research activities in new materials for cost-effective, high-efficiency photovoltaic technologies. Since the first demonstration from Kojima and co-workers in 2007,[1] several perovskite-based solar cells have been reported and certified with rapidly improving power conversion efficiency, now approaching the theoretical limit. Recent reports demonstrated that perovskites outperform the most efficient photovoltaic materials to date. At the same time, they still allow solution processing as a potential advantage in delivering a cost-effective solar technology.
The most stable and efficient perovskites contain lead, among the most toxic elements on earth.[2] Lead-free alternatives have been reported with impressive progress in power conversion efficiency for tin-based (lead-free) perovskites. However, the stability of tin-based perovskite solar cells still needs to be explored. In the present talk, we will focus on stability with a particular interest in tin-based (lead-free) perovskite solar cells.

1. Akihiro Kojima et al 2007 Meet. Abstr. MA2007-02 352
2. Trends in Ecology & Evolution, Volume 37, Issue 4, April 2022, Pages 281-283

► Jong Hyeok Park (Yonsei University, Korea)

Jong Hyeok Park is professor at Department of Chemical and Biomolecular Engineering in Yonsei university, Republic of Korea. His research focuses on solar-to-hydrogen conversion devices, Li & Na ion batteries, perovskite solar cells.

He received his Ph.D. in chemical engineering from KAIST, Republic of Korea, in August 2004. Then, he joined University of Texas at Austin, USA, as a postdoctoral researcher in 2004 (under Prof. Allen J. Bard). He is an author and a co-author of 320 papers and 100 patents.

He has received various prestige awards such as PBFC Award (2012) from The Korean Electrochemical Society, SKKU Young Fellowship (2012) from SKKU, Horace G. Underwood Fellowship (2018) from Yonsei University, Award of Excellence (2017) from Korean Academy of Science and Technology, S-Oil Next Generation Researcher Award (2021).

Overall Water Splitting by Lead Halide Perovskite Photoelectrodes

Hydrogen is a promising future sustainable fuel candidate with boundless opportunities. Research into photoelectrochemical (PEC) water splitting based on a lead halide perovskite (LHP) has progressed significantly with the aim of more efficient solar hydrogen production. In this presentation, I unite a well-known photo absorbing LHP with cost-effective water splitting catalysts, and we introduce two types of monolithic LHP-based PEC devices that act as a photocathode and a photoanode for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), leading to efficient unbiased overall water splitting. Through the integration of these two monolithic LHP-based photoelectrodes, an unbiased solar-to-hydrogen (STH) conversion efficiency over 10% and ~ 400 hour stability are achieved.

► Tönu Pullerits (Lund University, Sweden)

Tönu Pullerits obtained his PhD from the Institute of Physics at Tartu University, Estonia, in 1991. He pursued his postdoc work in Free University of Amsterdam (1992–1993), Umeå University (1993–1994). He moved to Lund University 1994 where he is currently full professor and head of the Division of Chemical Physics. He is an elected member of the Royal Swedish Academy of Sciences since 2016. His research interests include energy transport in molecular systems, ultrafast charge carrier dynamics and photophysics in photovoltaic materials, and coherent multidimensional spectroscopy.

Photonic processes in metal halide perovskite nanostructures, from 0D to 2D

Examples of our recent studies on perovskite nanostructures will be presented. We investigate two-photon-excited photoluminescence of $CsPbBr_3$ perovskite quantum dots on a silicon photonic crystal slab. By systematic excitation of optical resonances using a pulsed near-infrared laser beam, we observe an enhancement of two-photon-pumped photoluminescence by more than 1 order of magnitude when compared to using a bulk silicon film. Experimental and numerical analyses allow relating these findings to near-field enhancement effects on the nanostructured silicon surface. In another study, we investigate hot carrier (HC) cooling in two-dimensional (2D) perovskite single crystals by applying two complementary ultrafast spectroscopy techniques – transient absorption (TA) and time-resolved two-photon photoemission (TR-2PPE) spectroscopies. TR-2PPE directly maps the hot electron distribution and its dynamics in the conduction band to the detected photoelectron distribution. While TR-2PPE selectively probes the upper layer of the material, TA provides information on the whole bulk. Two cooling regimes are resolved in both techniques. The fast timescale of 100–200 fs is related to the electron scattering by longitudinal optical (LO) phonons and the slow timescale of 3–4 ps corresponds to the LO phonon relaxation. The HC cooling dynamic of TA measurement has faster initial stage and higher starting temperature for the slower stage than in TR-2PPE measurements. Conclusions about spatial sensitivity of the cooling dynamics across the 2D perovskite single crystals constitute valuable information that can guide the future development of HC solar cells and thermoelectric applications based on 2D perovskites.

► Anders Hagfeldt (Uppsala University, Sweden)

Anders Hagfeldt is Vice-Chancellor (President) of Uppsala University. A physical chemist, he obtained his PhD from Uppsala University in 1993 and is a specialist in the field of solar energy conversion. His research has established him as an international leader in the fields of dye-sensitised solar cells, perovskite solar cells and solar fuels.

Hagfeldt became Professor of Chemical Physics at Uppsala University in 2004 and Professor of Physical Chemistry in 2007. He has served as head of department and dean of chemistry at Uppsala University. From 2014 to 2020, Hagfeldt was Professor of Physical Chemistry at the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland. He has held visiting professorships at numerous universities, including Nanyang Technological University, Singapore; Sungkwunkwan University, Korea; Université Paris Diderot; Institut Català de Nanociència i Nanotecnologia (ICN2), Barcelona, Spain; Alagappa University, India; King Abdulaziz University, Saudi Arabia; and Dalian University of Technology, China. He is a fellow of four academies: the Royal Swedish Academy of Sciences, Royal Swedish Academy of Engineering Sciences, Royal Society of Sciences at Uppsala, and European Academy of Sciences. He holds an honorary doctorate from Université Paris Diderot, France. He is presently a SIEST Distinguished Faculty (Sungkyunkwan University/SKKU Institute of Energy Science and Technology, SIEST, Korea).

He has published more than 650 scientific papers that have received over 130,000 citations with an h-index of 166 (Google Scholar). Times Higher Education ranked Hagfeldt as number 46 in the top 100 material scientists during 2000–2010, and he was among the top 1% cited chemists in the Times Higher Education ranking for each year 2014–2022.

He is co-founder and board member of the company Dyenamo AB, Stockholm, Sweden.

Stabilizing Grain Boundaries and Surfaces of the Perovskite Layer in Perovskite Solar Cells to Extend Device Durability

Stabilizing grain boundaries and surfaces of the perovskite layer is critical to extend device durability. Here we introduced an unexplored class of molecule to post-treat formamidinium lead iodide (FAPbI3) perovskite films, which shows outstanding stability upon light soaking and remarkably remains in black-phase after 2 years ageing under ambient condition without encapsulation. The treated PSCs deliver a breakthrough record in operational stability of highly-efficient PSCs with less than 1% performance loss after more than 4500 h at maximum power point tracking, yielding an extraordinarily high theoretical T80 of over 9 years under continuous 1-sun illumination. They also present less than 5% PCE drops under various ageing conditions (including thermal cycling and damp heat test).

▶ Tae-Woo Lee (Seoul National University, Korea)

Tae-Woo Lee is a professor in the Department of Materials Science and Engineering at Seoul National University, Korea. He received his Ph.D. in Chemical Engineering from Korea Advanced Institute of Science and Technology (KAIST), Korea, in 2002. He joined Bell Laboratories, Lucent Technologies, USA, as a postdoctoral researcher in 2002 and then worked at Samsung Advanced Institute of Technology as a member of the research staff (2003–2008). He was an assistant and associate professor in the Department of Materials Science and Engineering at Pohang University of Science and Technology (POSTECH), Korea, until August 2016. He is author and co-author of 270 papers in high-impact journals including Science, Nature, Nature/Science sister journals, Joule, PNAS, Energy and Environmental Science, and Advanced Materials. His research focuses on organic/perovskite/carbon materials, their applications to flexible/printed electronics, displays, photovoltaics, and bioinspired neuromorphic devices.

Perovskite nanocrystals enabling bright, efficient and stable light-emitting diodes

Metal halide perovskites (MHPs) have emerged as a promising light emitter for next-generation display applications due to their high color purity (FWHM ~ 20 nm) and low processing cost. Despite various strategies being reported, the electroluminescence efficiency and stability of MHPs still lag that of existing light-emitting diodes (LEDs). In this presentation, we will discuss the advantages and strategies for commercializing MHPs. First, to achieve high electroluminescence efficiency, we have developed a comprehensive material strategy to suppress defect formation in colloidal perovskite nanocrystals (PNCs). Doping formamidinium lead bromide ($FAPbBr_3$) PNCs with guanidinium (GA^+) leads to smaller PNCs with enhanced carrier confinement. Additionally, a bromine-based small molecule, 1,3,5-tris(bromomethyl)-2,4,6-triethylbenzene (TBTB), was applied as a halide vacancy healing agent to stabilize the PNC surface.[1] Moreover, for large-area applications, we have developed a modified-bar coating method to fabricate large-area devices with comparable efficiency to those made by the spin-coating method.[2] Lastly, we report on the development of efficient, bright, and stable perovskite LEDs by introducing an in-situ core/shell PNC structure. By splitting large 3D crystals into nanocrystals and surrounding them with small organic ligands, we achieved significant improvement in both efficiency and lifetime while maintaining excellent charge transport and confinement.[3]

1. Y.-H. Kim et al., Nat. Photonics, 15, 148–155 (2021)
2. Y.-H. Kim et al., Nat. Nanotechnol., 17, 590–597 (2022)
3. J. S. Kim et al., Nature, 611, 688–694 (2022)

► Ute Cappel (KTH – Royal Institute of Technology, Sweden)

Ute Cappel is an Associate Professor at the Department of Chemistry at KTH – Royal Institute of Technology. She received her PhD degree in Chemistry at Uppsala University in 2011 with a thesis on the characterization of organic dyes for dye-sensitized solar cells. She then was a Marie-Curie fellow at Imperial College London from 2012-2014 focusing on ultrafast spectroscopy of hybrid solar cells. She then worked as a researcher at the Department of Physics and Astronomy at Uppsala University, where she combined time-resolved and photoelectron spectroscopy to study materials for solar cells. Since 2017, she has been a group leader at KTH, where her research focusses on understanding materials properties and processes in hybrid solar cells. For this she uses photoelectron spectroscopy at synchrotron light sources to study the chemical and electronic structure of surfaces and interfaces. She also develops time-resolved and operando photoelectron to measure electron dynamics and energy alignment in solar cell devices during the light-to-electricity conversion process. She received Göran Gustafssons prizes for her research in 2018 (small prize) and 2020 (large prize).

Energy alignment and charge dynamics in solar cells determined by time-resolved and operando photoelectron spectroscopy

Solar cells have a great potential in replacing fossil fuels in electricity generation, if requirements of low production costs can be met. In the last years, much research has focused on developing new solar cells made from organic or hybrid materials, which can be fabricated by cheap methods. This includes solar cells with a hybrid organic inorganic perovskite as the active layer in the solar cell, which have now reached power conversion efficiencies of more than 25%. In a typical solar cell, the perovskite layer is sandwiched between two selective contacts, one for holes and one for electrons.

The future success of these developments crucially depends on understanding the details charge separation, charge transport and charge recombination at the interfaces between the different layers in a solar cell as well as what parameters limit solar cell stability. X-ray based techniques such as photoelectron spectroscopy (PES) are powerful tools for obtaining electronic structure information of materials at an atomic level. By varying the photon energy from soft to hard X-rays, photoelectron spectroscopy can be used for non-destructive depth profiling of the solar cell interfaces giving information about the energy alignment and chemical structure and composition at the interface.

In this presentation, I will describe how we have used photoelectron spectroscopy for time-resolved and operando studies of complete solar cells. I will present results, where we were able to measure PES of a complete perovskite solar cells while applying an external bias and during visible illumination. This allowed us to determine the electronic structure and energy alignment of the active layer / back contact interface of the solar cell under operating conditions. Furthermore, I will discuss how time-resolved pump-probe measurements can be used to determine electron transfer dynamics in solar cells. The described methods provide new ways of gaining insights into the working mechanism of solar cells based different combinations of materials.

► Jens Wenzel Andreasen (Technical University of Denmark, Denmark)

Jens Wenzel Andreasen was born in Copenhagen, Denmark in 1969. He graduated as M.Sc. in geology from University of Copenhagen in 2000 and received his PhD degree in chemistry from the Technical University of Denmark in 2005.
He is currently Professor at the Technical University of Denmark, Department of Energy Conversion and Storage and has previously worked as Senior Researcher at the Risø National Laboratory for Sustainable Energy in Roskilde, Denmark. He has authored or co-authored 128 peer-reviewed papers in international journals and one book-chapter in Conjugated Polymers and Oligomers : Structural and Soft Matter Aspects. Knaapila, M. (ed.). World Scientific, p. 159-174 (Materials and Energy, Vol. 9), 2017. His research interests include the atomic to mesoscale structure of materials for sustainable energy as well as their dynamical coupling to electronic structure.
Prof. Andreasen is a member of the International Union of Crystallography and the American Crystallographic Association. He has until recently held a Consolidator Grant from the European Research Council (ERC) has coordinated an Innovative Training Network and currently coordinates a Doctoral Network under the Marie Curie-Sklodowska Actions.

Understanding and controlling light-matter interactions in organic solar cells

We demonstrate a method to manipulate the morphology of thin film semiconducting polymers. The manipulation is achieved by optical excitation of the polymer during roll-to-roll slot-die coating, providing a technique that is viable for large-scale production. Along with establishing the technique, the entire knowledge chain from fundamental insight in polymer physics and structure to application is presented. By correlating X-ray and neutron scattering techniques with density functional theory and molecular dynamics simulations of solvent evaporation, we successfully determine the packing of the polymers in the ground state and excited state. The findings are coupled with measurements of dynamical physical properties and solar cell device performance to pinpoint the structure-property relationship.

► Hui-Seon Kim (Inha University, Korea)

Hui-Seon Kim is an Associate Professor in the Department of Chemistry at Inha University. She received B.Eng. and Ph.D. at Sungkyunkwan University, Korea in 2011 and 2016 under the supervision of Prof. Nam-Gyu Park. She worked as a post-doc at the laboratory of Prof. Anders Hagfeldt at École Polytechnique Fédérale de Lausanne in Switzerland from 2016 to 2019. She joined Inha University in 2019 and established Nanomaterials and Energy Device Laboratory. She has been mainly working on the perovskite solar cells (PSCs) and has published articles with over 19100 citations since the first paper about the solid-state PSC in 2012.

Interface engineering for perovskite solar cells

Perovskite solar cells (PSCs) have been promptly raised to a strong candidate, exhibiting a certified power conversion efficiency (PCE) of 26.1%. Intensive efforts have been still made to reach an extremely high PCE on one hand and to ensure the long-term stability of PSCs on the other hand, where the interface of PSCs plays a critical role. Interface engineering of perovskite layer was pursued by implementing the heteroepitaxial growth on the bottom and the surface recrystallization on the top. The heteroepitaxial growth of perovskite film enabled the residual lattice tensile strain to be tuned, affecting the interface recombination and the crystal phase stability as well. Furthermore, the recrystallization not only reduced the trap density but also promoted the favorable crystal orientation of the top surface, encouraging the efficient charge extraction at the interface. The effect of interface engineering was well reflected in both the photovoltaic parameters, particularly in open-circuit voltage and fill factor, and the long-term stability, which highlights the importance of the interface engineering for perovskite-employed electronic devices.

► Tomas Edvinsson (Uppsala University, Sweden)

Prof. **Tomas Edvinsson** (TE) is a leading expert on Raman spectroscopy with three spectrometers in his group at Uppsala University, Sweden, and he has a long experience within low-dimensional systems and computational quantum mechanics. The research focus is on experimental and theoretical investigations of low dimensional semiconductors for solar cell and photocatalytic applications (solar fuels and water cleaning). TE is established within energy related materials with studies ranging from quantum dots and catalysis to emerging solar cell materials with e.g. a recent book published within characterization techniques for perovskite solar cell materials, another one in the writing, and he was one of the 50 worldwide invited scientists for a Nobel symposium within solar cell materials (Nobel symposium, May 3-5, 2023). TE is an advisory board member of Chemical Data Collection (Elsevier), J Mater Chem A (RSC), and Materials Advances (RSC). Complementing the environment of the group at Uppsala University, TE has recently accepted a part-time position as professor of Energy Materials at Newcastle University, UK.

Nature of the excited states in Lead halide perovskites and Quantum Mechanical Guided Machine Learning

Lead halide perovskites have emerged as a promising class of materials with exciting optoelectronic properties, making them promising candidates for next-generation optoelectronics. The detailed electronic structure and photo excited charge density response in the excited state are here important to describe and optimize lead halide perovskites under operation.[1,2] In this contribution, we highlight the nature of the excited state in lead halide perovskites, with subsequent processes of importance for understanding the behaviour of the system. Experiments from photoinduced Stark-effect experiment as well as corroborating theoretical investigations using both ground state and time-dependent density-functional theory (TD-DFT) are presented.[2,3] We show that the excess energy after thermalization under blue-light illumination is large enough for overcoming the activation energy for iodide migration and can thus trigger ion movement and vacancy formation.[2,3] Here, in particular, a dipolar A-site cation would decrease the energy of defect formation, but instead impede defect migration[4] and also affect the excited state response and subsequently enhanced optoelectronic properties[5]. We will also briefly outline how quantum mechanical guided machine learning can be utilized to find optimal catalytic properties in complex high-entropy materials systems[6,7] and its relation to the perovskite field. The results form a basis for a fundamental understanding of the excited-state properties of lead halide perovskite material to reveal the underlying mechanism for photoinduced halide segregation, reported defect tolerance when using organic dipolar cations, provide a rationale for using mixed halide perovskites to decrease halide migration, and provide the origin of the reported stability issues of organic A-site cations under blue and UV-light illumination and the effect multiple element inclusion in complex materials.

1. Park B., SM Jain S.M., Zhang X., Hagfeldt A., Boschloo B., Edvinsson T. Resonance Raman and Excitation Energy Dependent Charge Transfer Mechanism in Halide-Substituted Hybrid Perovskite Solar Cells ACS Nano, 2015, 9, 2088–2101
2. Pazoki, M., Jacobsson, J. T., Kullgren, J., Johansson, E.M.J., Hagfeldt, A., Boschloo, G., Edvinsson, T. Photoinduced Stark Effects and Mechanism of Ion Displacement in Perovskite Solar Cell Materials, ACS Nano, 2017, 11, 2823–2834.
3. Pazoki, M, Edvinsson, T. Nature of the excited state in lead iodide perovskite materials: Time-dependent charge density response and the role of the monovalent cation.
4. Phys Rev B 2019, 100 (4), 045203
5. Pazoki, M., Wolf, M.J., Edvinsson, T, Kullgren, J. Vacancy dipole interactions and the correlation with monovalent cation dependent ion movement in lead halide perovskite solar cell materials,
6. Nano Energy 2017, 38, 537–543
7. Imani, R., Borca, C.H., Pazoki, M. Edvinsson, .T. Excited-state charge polarization and electronic structure of mixed-cation halide perovskites: the role of mixed inorganic–organic cations in CsFAPbI3, RSC Adv., 2022, 12, 25415
8. Araujo, R. B., , Pehlivan I. B., Edvinsson. T. High-entropy alloy catalysts: Fundamental aspects, promises towards electrochemical NH3 production, and lessons to learn from deep neural networks, Nano Energy, 2023, 105, 108027.
9. Araujo, R. B., Edvinsson. T. N2 adsorption on high-entropy alloy surfaces: unveiling the role of local environments, J. Mater. Chem. A, 2023, DOI: 10.1039/d2ta09348k

► KI Tae Nam (Seoul National University, Korea)

Professor **Ki Tae Nam** received his B.S. and M.S. in Materials Science and Engineering from Seoul National University, and his Ph.D. in Materials Science and Engineering from Massachusetts Institute of Technology, Cambridge, USA. In the previous year, he and his team had successfully developed the world's first electrochemical carbon dioxide conversion technology that mimics the biofuel synthesis system in nature for the synthesis of a "carbonate fuel," a new concept of e-fuel (electricity-based fuel). He received the 2018 Young Scientist Award, the 2020 Sinyang Engineering Research Award, and the 2022 POSCO Cheongam Award. Also, he was selected in 2020 by the Korean Academy of Science and Technology as one of the six "International Outstanding Young Scientists." In addition, he is an elected executive of the Young Korean Academy of Science and Technology (Y-KAST), a group of selected excellent scientists 45 years or younger. On 17th March 2022, Professor Nam was appointed as a committee member of the science, technology, and education division by the South Korean presidential transition committee.

432 Symmetric Chiral Gold Nanoparticle

Chiral structure controlled at nanoscale provides a new route to achieve intriguing optical properties such as polarization control and negative refractive index. However, asymmetric structure control with nanometer precision is difficult to accomplish due to limited resolution and complex processes of conventional methods. In this regards, utilizing chirality transfer occurring at organic-inorganic materials offers viable route to overcome these limitations. Previously we developed a unique synthesis strategy that characteristic of molecule is transferred to gold nanoparticle morphology. Based on the system, here, we demonstrated novel chiral gold nanostructures exploiting chirality transfer between peptide and high-Miller-index gold surfaces. Enantioselective adsorption of peptides results in unequal development of nanoparticle surface and this asymmetric evolution leads to highly twisted chiral element in single nanoparticle making unprecedented 432 helicoid morphology. The synthesized helicoid nanoparticle showed strong optical activity (dissymmetry factor of 0.2 at 622 nm) which was substantiated by distinct transmittance color change of helicoid solution under polarized light. Modulation of peptide recognition and crystal growth enabled diverse morphological evolution and the structural alterations provided tailored optical response, such as optical activity, handedness, and resonance wavelength. We believe that our peptide directed synthesis strategy offers a truly new paradigm in chiral metamaterial fabrication and will be beneficial in the rational design of chiral nanostructures for use in novel applications.

► Paola Vivo (Tampere University, Finland)

Paola Vivo is an Associate Professor at Tampere University (TAU). She has worked in the field of solution-processable organic and inorganic semiconductors for emerging photovoltaic technologies for over 15 years. After pursuing her Ph.D. in Chemistry (2010) at Tampere University of Technology, she received several major grants as Principal Investigator, including the Academy of Finland Fellowship for postdoctoral research in 2013–2017. She currently leads the Hybrid Solar Cells group (https://research.tuni.fi/hsc/) at the Faculty of Engineering and Natural Sciences at TAU. Her research interests include developing novel materials, as thin films and nanocrystals, for solar energy applications. Presently, the main emphasis of the research is on halide perovskites and perovskite-inspired materials for solar cells and indoor photovoltaics.

Air-stable perovskite-inspired absorbers for sustainable indoor light-harvesting

Perovskite-inspired materials (PIMs) based on Group VA cations, such as antimony (III) (Sb^{3+}) and bismuth (III) (Bi^{3+}), have recently gained popularity as eco-friendly and air-stable absorbers. Their wide bandgap of around 2 eV makes them potentially suitable for tandem solar cells, indoor photovoltaics (IPVs), or photocatalysis. However, despite outstanding indoor power conversion efficiencies up to 60% have been theoretically predicted for PIM-based indoor photovoltaics (IPVs), this research is still in its early infancy.

In this talk, I will summarize some of our key findings on two-dimensional PIMs for IPV applications. In particular, I will focus on Sb- and/or Bi- based halides with a bandgap in the 1.9-2.0 eV range. The considerable presence of both intrinsic and surface defects in wide-bandgap PIMs is the key responsible of the modest indoor power conversion efficiency (PCE(i)) reported so far up to ~5% at 1000 lux white LED illumination. We propose effective compositional engineering strategies that enable a significant improvement in the PCE(i) up to nearly 10%. Our characterizations at both material and device level suggest that the PCE(i) enhancement is linked to the successful defect mitigation within the PIM domains and/or at their surface.

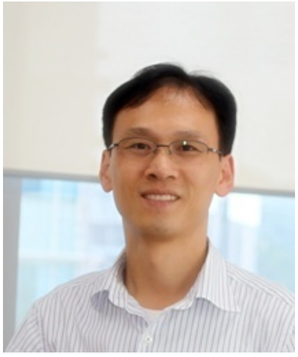
► Hyunjung Shin (Sungkyunkwan University, Korea)

Hyunjung Shin is a professor of department of Energy Science at Sungkyunkwan University, Republic of Korea. He received his M.S. and Ph.D. in Materials Science and Engineering from Case Western Reserve University, Cleveland, OH, USA in 1994 and 1996, respectively. He joined Max-Planck Institute fur Metallforschung, Stuttgart, Germany as an Alexander von Humboldt research fellow in 1997 and worked at Samsung Advanced Institute of Technology as a member of the research staff (1997 – 2002). He was an assistant, associate, and full professor in School of Advanced Materials Engineering at Kookmin University, Seoul, Korea until Aug 2012. He moved to Sungkyunkwan University. Now he is a director of Nature Inspired Materials Processing Research Centre and a Deputy Director of SKKU Institute of Energy Science and Technology (SIEST) in SKKU. His research focuses on organic-inorganic hybrid perovskite, inorganic nanostructured materials, 2-D sulphides, atomic layer deposition, and their applications to solar energy conversion devices, photoelectrochemical cells, electrochemical CO_2 reduction, memory switching devices and bio-inspired bone tissue materials. He is author and co-author of more than 220 peer-reviewed scientific papers including Nature Energy, Nature Nanotechnol., Science Advances, Advanced Energy Materials and Advanced Materials, as well as an inventor and co-inventor of around 30 patents.

Structure – Property Relation in Formamidinium Lead Triiodide ($FAPbI_3$)

Formamidinium lead triiodide ($FAPbI_3$) is gaining much interest with an optimal band gap of ~ 1.5 eV. Although α-$FAPbI_3$ is the most thermodynamically stable photoactive phase, it can kinetically stabilize δ-$FAPbI_3$ in ambient. Many attempts were studied to stabilize the black α-phase, for example, pseudo-halide anion engineering, ionic liquid engineering, and incorporation of additives. Incorporating with methylammonium chloride (MACl) as an additive not only induces the stabilized α-$FAPbI_3$, but also affects the crystallization kinetics of α-$FAPbI_3$. Along with the role of methylammonium chloride (MACl) as a 'stabilizer' in the formation of α-$FAPbI_3$,we pointed out the additional role as a 'controller' in the crystallization kinetics. Herein, we examined the crystallization process of MACl, as higher concentration of MACl induces slower crystallization kinetics. Which results in larger grain size and [001] preferred orientation in α-$FAPbI_3$ films as the MACl concentration increased from 10 to 20, 30, and 40%. Microscopic observations, such as electron back-scattered diffraction (EBSD), confocal photoluminescence (PL), time-resolved photoluminescence (TRPL) mapping, and conductive atomic force microscopy (C-AFM), were conducted to examine the optoelectronic properties of [001] preferentially oriented grains. Reduction in the non-radiative recombination, a longer lifetime of charge carriers and less photocurrent deviation between each grain induce higher short-circuit current density (J_{sc}) and fill factor (FF) in α-$FAPbI_3$ based perovskite solar cells (PSCs) with MACl40%. Resulting the PSCs with MACl40% to attain the highest power conversion efficiency (PCE) of 23.5%. Furthermore, we confirmed these observations by enhancing the grain size and [001] preferred orientation of the MACl10% sample through a two-step heat treatment. As the lower heat treatment induced suppression of nucleation and enhancement of the crystal growth in a-$FAPbI_3$ films with MACl10%. The two-step processing resulted in an improvement in the PCE from 18.4% to 21.8%. It indicates the impact of adding MACl to control the crystallization kinetics resulting in a preferred orientation and a large grain size. It highlights the importance of crystallization kinetics resulting in desirable microstructures for device engineering.

► **Jin Young Kim (Ulsan National Institute of Science & Technology, Korea)**



Jin Young Kim is a professor of School of Energy and Chemical Engineering and Carbon Neutrality at Ulsan National University of Science and Technology. He received Ph.D. degree from Pusan National University in 2005. From 2005 to 2007, he was a postdoctoral research fellow in the Center for Polymers and Organic Solids at UC Santa Barbara. His current research topics include organic solar cells, perovskite solar cells, perovskite light emitting diodes, and water splitting devices.

Improving Performance and Stability of $FAPbI_3$-based Perovskite Solar Cells via Methylammonium Chloride and Formate Anion Engineering

This study investigates the influence of Methylammonium Chloride (MACl) additive in formamidinium lead iodide ($FAPbI_3$)-based perovskite solar cells and introduces a novel approach using the pseudo-halide formate ($HCOO^-$) to enhance performance and stability. Through density functional theory, we discover that MACl facilitates the formation of an intermediate phase in α-$FAPbI_3$ without annealing, where the formation energy depends on the MACl amount. By controlling MACl incorporation, we significantly improve perovskite film quality, resulting in larger grain size, enhanced phase crystallinity, and improved photoluminescence lifetime. This leads to a certified efficiency of 23.48%. Furthermore, we explore the use of formate as an anion engineering concept to reduce anion vacancy defects in perovskite films. Formate effectively enhances film crystallinity, reducing defects at grain boundaries and the surface. The resulting perovskite solar cells achieve a record power conversion efficiency of 25.6% (certified 25.2%) and demonstrate long-term operational stability (450 hours) and high electroluminescence with external quantum efficiencies exceeding 10%. This work highlights the potential of MACl additives and formate anion engineering for high-performance and stable perovskite solar cells, offering a promising strategy to eliminate common lattice defects in metal halide perovskites and enabling efficient solution-processable optoelectronic devices.

► Thomas Wågberg (Umeå University, Sweden)

Professor **Thomas Wågberg** conducted his Ph.D. studies at Umeå University with Professor Bertil Sundqvist at Umea University, and Professor Per Jacobsson (Chalmers) as supervisors. During his PhD studies he also conducted research at UC Berkeley, USA in the group led by Professor Alex Zettl, as well as at Université Orsay, Paris, France in the group led by Professor Roger Moret. After his PhD degree in 2002, he became a Wenner-Gren Fellow and conducted postdoctoral research at Université Montpellier, in the group of Professor Patrick Bernier. Now, he is head of the Physics department at Umeå University, and leads the “Nano for Energy” group in nanostructured materials with an emphasis on energy conversion technologies at Umeå University.

Novel strategies for efficient water electrolysis

A growing global population in parallel with an increased prosperity seen from a global perspective have raised the need for energy and raw material resources exponentially. These increased needs have led to a number of negative consequences such as pollution, raw material shortages, increasing carbon dioxide levels in the atmosphere, and not least a threatening global warming. Renewable energy will be essential to break the dependence of fossil fuels, but due to the intermittency of renewables a storable non-fossil alternative is needed. Hydrogen represents one of very few sustainable options to store renewable energy on large scale and for seasonal variations. Here, we present novel strategies on water electrolysis driven by photovoltaics, with a focus on the development of state-of the art electrocatalysts based on earth-abundant transition metals, doped with sulphur and phosphor. We show that by tuning parameters such as adsorption energy, morphology and conductance of the electrocatalysts we can achieve solar-to hydrogen efficiency reaching 20 %. We discuss on strategies, mechanisms and challenges in the field of PV-driven electrolysis.

► Yun Jeong Hwang (Seoul National University, Korea)

Yun Jeong Hwang is an associate professor in department of Chemistry, Seoul National University since 2021. She received a Bachelor's degree and a Master's degree from Chemistry Department of Korea Advanced Institute of Science and Technology (KAIST). She continued her graduate study at University of California, Berkeley studying on semiconductor nanowire synthesis for efficient photoelectrochemical water splitting. She worked in Clean Energy Research Center at Korea Institute of Science and Technology (KIST) until 2020.

Her main research approaches are contributing to addressing critical energy and environmental issues by realizing clean and sustainable chemical production. The major research topics are nanomaterial synthesis to have high catalytic activity, electrochemical synthesis for carbon/nitrogen/oxygen utilization, and in-situ/operando electrochemical characterization for understanding the reaction pathways and the catalyst surfaces which can give feedback for scientific research advances. Her research interests focus on the synthesis and characterization of nanomaterials for the use of electrocatalysts to understand the properties and the interaction between heterogeneous catalyst surfaces and small molecules such as CO_2, H_2O, N-containing small molecules, and biomass derivatives. Through direct CO_2 utilization and H_2O electrolysis, she is aiming to realize artificial photosynthesis, as a sustainable carbon cycle. In addition, she is interested in the development of new surface analysis chemistry to understand catalytic activities and reaction pathways on the electrode-electrolyte junction behavior.

Electrolyte effect on electrochemical CO_2 reduction reaction

Electrochemical CO_2 reduction (CO_2R) can be integrated with renewable energy sources and water can be utilized as a direct proton source which is promising to provide a sustainable net-zero carbon cycle. However, using water as the proton sources causes undesired competitive hydrogen evolution reaction (HER), and thus it is crucial to control selectivity for CO_2R. Various metal based electrocatalysts have been investigated to convert CO_2 to CO, formate, ethylene, ethanol, or other C2+ chemicals. Recent efforts to understand the electrocatalytic activity have found that the cations in the electrolyte play an important role to modulate the activity even for a given electrocatalyst. In addition, the influences of the cations vary depending on the types of the reactions and catalysts when the cations interact with the intermediate species, and CO_2R is a sensitive reaction to the presence of the cations. Therefore, the interface between the catalyst and electrolyte have to be carefully investigated. The relationship between the product distribution of CO_2R and its intermediate species can be monitored by operando spectroscopy studies that have been attracted the attention. We demonstrate that, *CO, one of the crucial intermediate, can be observed by Raman or Infra-red spectroscopy, and their vibrational wavenumbers depends on the electrolyte condition. Meanwhile, we also investigate selectivity for electrochemical CO_2 conversion to CO production between Ag nanoparticle and Ni-N-C single atom catalyst. The Ni-N-C was found to have low sensitivity to the type of the alkali metal cation and universally high selectivity of CO_2R to CO over HER compared to the Ag nanoparticle, which showed the importance of the catalyst-electrolyte interface on the CO_2R activity. This contributes to increase CO_2 conversion efficiency even under low concentration of available CO_2 gas. Modulation of the catalyst-electrolyte interface can provide new opportunities to promote challenging catalytic reactions.

► Truls Norby (University of Oslo, Norway)

Truls Norby (b. 1955), PhD from University of Oslo (UiO) 1986, became professor at Department of Chemistry UiO 1994 and since 1997 heads Group for Electrochemistry. He works with defects and transport in materials for solid-state fuel cells, electrolysers, batteries, membranes, and sensors, specialising in protons and protonic transport in oxides and on their surfaces. He also integrates materials chemistry and semiconductor physics in photoelectrochemistry, oxide thermoelectrics, and innovations in design and fabrication. Norby has published 300 journal papers, graduated more than 100 Master- and PhD-students, and is member of the Norwegian Academy of Science and Letters and three other national academies. He has founded three companies and won the UiO Innovation Prize 2012 and the Norwegian Guldberg-Waage medal for chemistry 2018.

Solar hydrogen from adsorbed water vapour in all-solid photoelectrochemical cells

The prospect of stand-alone devices for solar-driven water splitting faces many challenges to take efficiency and economy beyond the combination of separate photovoltaics (via grid if beneficial) and electrolysis. In a photoelectrochemical (PEC) cell with a solid-state proton conducting electrolyte[1] and utilising surface protonic conduction on the photoanode we may utilise adsorbed water as source of protons[2,3]. Unlike traditional PEC cells we may then utilise available grey water instead of pure water, which is a scarce commodity in many sun-rich regions. Driving the process with a tandem or dual photoelectrode allows the possibility of a wire-less self-sufficient monolithic design4. However, there are several requirements of properties, complementarity, and compatibility of the materials involved that we need to address in research ahead.

1. K.O. Iwu, A. Galeckas, A.Yu. Kuznetsov, T. Norby, ”Solid-state photoelectrochemical water splitting with gaseous reactants”, Electrochimica Acta, 97 (2013) 320-25.
2. Kaiqi Xu, A. Chatzitakis, T. Norby, ”Solid-state photoelectrochemical cell with TiO2 nanotubes for water splitting”, Photochemical & Photobiological Sciences, 16 (2017) 10-16.
3. Xiaolan Kang, L. Chaperman, A. Galeckas, S. Ammar, F. Mammeri, T. Norby, A. Chatzitakis, “Water Vapor Photoelectrolysis with CdS and CdSe Nanoparticles Loaded TiO2 Nanotubes in a Solid-State Photoelectrochemical Cell”, ACS Applied Materials & Interfaces, 13 [39] (2021) 46875-85.
4. Kaiqi Xu, A. Chatzitakis, E. Vøllestad, Qiushi Ruan, Junwang Tang, T. Norby, “Hydrogen from wet air and sunlight in a tandem photoelectrochemical cell”, Int. J. Hydrogen Energy, 44 [2] (2019) 587-93.

► Nam-Gyu Park (Sungkyunkwan University, Korea)

Nam-Gyu Park is Distinguished professor of School of Chemical Engineering and Director of SKKU Institute of Energy Science and Technology (SIEST), Sungkyunkwan University (SKKU). He received his B.S. degree in chemical education, M.S. and Ph.D. degrees in chemistry from Seoul National University in 1988, 1992 and 1995, respectively. He worked at ICMCB-CNRS, France, from 1996 to 1997 and at National Renewable Energy Laboratory, USA, from 1997 to 1999 as postdoctoral researchers. He was director of solar cell research center at Korea Institute of Science and Technology (KIST) from 2005 to 2009 and principal scientist at Electronics and Telecommunications Research Institute (ETRI) from 2000 to 2005 before joining SKKU as a full professor in 2009. He is a fellow of Korean Academy of Science and Technology (KAST) since 2017. He has been working on high efficiency mesoscopic nanostructured solar cells since 1997. He is pioneer of solid-state perovskite solar cell, which was first developed in 2012. He was selected as Citation Laureate (top 0.01% scientist); a New Class of Nobel Prize-Worthy Scientist in September 20, 2017 and included in highly cited researchers (HCR, top 1% scientists) in 2017, 2018, 2019, 2020, 2021, and 2022 by Clarivate Analytics. He received awards including Scientist Award of the Month (2008), KIST Award of the Year (2009), Dupont Science and Technology Award (2010), SKKU fellowship (three times in 2013, 2018 and 2021), PVSEC Hamakawa Award (2015), Dukmyung KAST Engineering Award (2016), ACS-KCS Excellence Award (2018), Ho-Am Prize (Samsung, 2018) and Rank Prize (UK, 2022). Prof. Park has currently more than 370 refereed publications and more than 70 patents. He received H-index of 108 (google scholar). He is Senior Editor of ACS Energy Letters and serves on the Editorial Advisory Board for Chem. Rev., ChemSusChem, and Solar RRL.

Facet engineering for stable and efficient perovskite solar cells

Since the seminal report on the 9.7% efficient and 500 h-stable solid-state perovskite solar cell (PSC) in 2012 based on methylammonium lead iodide, power conversion efficiency (PCE) was swiftly increased to 25.7% due to unique photophysical property of halide perovskite. According to Web of Science, number of publications on PSCs increases exponentially since 2012, leading to the accumulated publications of more than 30,900 as of December 2022. PSC is regarded as a game changer in photovoltaics because of low-cost and high efficiency surpassing the conventional high efficiency thin film technologies. High photovoltaic performance was realized by compositional engineering, device architecture and fabrication methodologies for a decade. Toward theoretical efficiency over 30% along with long-term stability, exquisite control of light management and photo-excited charges are highly required, along with thermodynamic phase stability. In this talk, facet engineering of perovskite films is reported. A specific crystal facet was found to have strong interaction with photon, leading to high photocurrent. Furthermore, a certain facet was found to be quite stable under moisture and PSC based on a perovskite film with abundant moisture-tolerant facet was remarkably stable in humid atmosphere even without encapsulation.