# HKICE Summit on Next-Generation Green Energy Materials and Applications

# 13 - 14 JUNE 2024

# **HKIAS Lecture Theatre**

Hong Kong Institute for Advanced Study LG/F, Academic Exchange Building, CityUHK



**Full Program** 

# **Featured Speakers**



**Michael GRAETZEL** École Polytechnique Fédérale de Lausanne



**Shi-Gang SUN**Xiamen University



Chennupati JAGADISH
Australian National University



Ben Zhong TANG
The Chinese University of
Hong Kong, Shenzhen



Alex K.Y. JEN
City University of Hong Kong



**Hua ZHANG**City University of Hong Kong



Chao-jun Ll McGill University



**Tianshou ZHAO**Southern University of Science and Technology

Day 1: 13 June 2024 (Thu)

Time	Speaker	Talk Title	
08:30 - 09:00	Welcome Reception		
09:00 - 09:30	Opening Ceremony		
	Welcome Address by <b>Prof. Freddy BOEY</b> ,		
	President and University Distinguished Professor, City University of Hong Kong		
	Opening Remarks by <b>Miss WONG Shuk Han, Diane, JP</b>		
	Under Secretary for Environment and Ecology, Environment and Ecology Bureau		
	Photo-Taking		
	Session Chair: Prof. Hua ZHANG		
09:30 - 10:15	Plenary Talk 1: Prof. Michael GRAETZEL	Molecular Photovoltaics and the Rise of	
	Ecole Polytechnique Fédérale de Lausanne	Perovskite Solar Cells	
10:15 - 10:35	Tea Break		
	Session Chair: Prof. Qiyuan HE		
10:35 - 11:20	Plenary Talk 2: Prof. Ben Zhong TANG	Green Chemistry: Making Functional Polymers	
	The Chinese University of Hong Kong, Shenzhen	on/in/from Water	
11:20 - 12:05	Plenary Talk 3: Prof. Alex K.Y. JEN	Printable Organic and Perovskite Solar Cells for	
	City University of Hong Kong	Clean Energy	
12:05 - 12:30	Keynote Talk 1: Prof. Zonglong ZHU	Interface-Enhanced Stability for Halide	
	City University of Hong Kong	Perovskite Photovoltaics: A Fundamental	
		Understanding	
12:30 - 14:00			
	Session Chair: Prof. Zhanxi FAN		
14:00 - 14:45	Plenary Talk 4: Prof. Tianshou ZHAO	Long-Duration Energy Storage: the Bridge to a	
	Southern University of Science and Technology	Net Zero Future	
14:45 - 15:10	Keynote Talk 2: Prof. Bin LIU	A Design Strategy Towards Oxygen	
45.40.45.25	City University of Hong Kong	Electrocatalysts	
15:10 - 15:35	Keynote Talk 3: <b>Prof. Qi LIU</b> City University of Hong Kong	Lithium-ion Battery Cathodes: From Cobalt-rich to Cobalt-free	
15:35 - 15:55	Tea Break		
13.33 - 13.33	Session Chair: Prof. Xue WANG		
15.55 16.40		Structure Design and Performance	
15:55 - 16:40	Plenary Talk 5: Prof. Shi-Gang SUN Xiamen University	Structure Design and Performance Enhancement of Proton-Exchange-Membrane	
	Alamen Oniversity	Fuel Cells Catalysts	
16:40 - 17:25	Plenary Talk 6: Prof. Hua ZHANG	Phase Engineering of Nanomaterials (PEN)	
10.10 17.23	City University of Hong Kong	Thuse Engineering of Nationalerials (LEN)	
17:25 - 17:50	Keynote Talk 4: Prof. Zuankai WANG	Nature-inspired surfaces for water-energy	
	The Hong Kong Polytechnic University	nexus	
18:30 - 21:00	Dinner - Seafood @ Sai Kung		

# Day 2: 14 June 2024 (Fri)

Time	Speaker	Title
	Session Chair: Prof. Ruquan YE	
09:00 - 09:45	Plenary Talk 7: Prof. Chennupati JAGADISH	Semiconductor Nanostructures for
	Australian National University	Optoelectronics and Energy Applications
09:45 - 10:10	Keynote Talk 5: <b>Prof. Yi-Chun LU</b>	Material Designs for High-Performance
	The Chinese University of Hong Kong	Aqueous Redox Flow Batteries
10:10 - 10:30	Tea Break	
	Session Chair: Prof. Guo HONG	
10:30 - 11:15	Plenary Talk 8: Prof. Chao-jun LI	Group III-Nitrides as Emerging Catalysts for
	McGill University	Energy and Chemical Conversions
11:15 - 11:40	Keynote Talk 6: Prof. Bolong HUANG	Advanced Atomic Catalysts Design for Energy
	The Hong Kong Polytechnic University	Systems
11:45 - 13:30	Lunch – Faculty Lounge, 9/F, BOC	

[Plenary 01] Prof. Michael GRAETZEL

#### Molecular Photovoltaics and the Rise of Perovskite Solar Cells

Michael GRAETZEL
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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 % and 30 % in full sunlight and ambient daylight respectively. They possess unique practical advantages in particular bifacial light harvesting, highly effective electricity production from ambient light, ease of manufacturing, flexibility and transparency, 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 the most promising future PV technology. 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, their use for the generation of fuels from sunlight and first commercial applications.

#### **Selected References**

- 1. M.Grätzel et.al *Nature* 1991, 353,737-740. https://doi.org/10.1038/353737a0, cited over 36'000 times.
- 2. M.Grätzel et.al.Nature 2013, 499, 316-319. https://doi.org/10.1038/nature12340
- 3. M.Grätzel Nature Mater 2014, 13, 838-842, https://doi.org/10.1038/nmat4065
- 4. M. Grätzel et.al Science 2017, 358, 768-771. DOI: 10.1126/science.aam5655
- 5. M.Grätzel et.al. Science 2022, 375, 302-306. DOI: 10.1126/science.abh1885
- 6. M.Grätzel et.al. Nature 2023, https://doi.org/10.1038/s41586-022-05460-z.
- 7. M Grätzel et.al. Science 2023, 379, 288.

#### **Biography**



Michael Graetzel is a Professor at EPFL where he develops photosystems for the generation of electricity and chemical fuels from sunlight. Michael graduated from the Technical University Berlin and was a postdoctoral fellow at the University of Notre Dame before joining the EPFL faculty as a professor of physical chemistry. There, he started his ground breaking investigations on colloidal semiconductors, which generated several new research fronts worldwide. Michael is well known for his discovery of mesoscopic dye sensitized solar cells, which

in turn prompted the rise of perovskite solar cells, triggering a second revolution in photovoltaics. Michael's pioneering work was recognized by a number of awards including the Rank Prize, BBVA Foundation Frontiers of Knowledge Award in Basic Science, Millennium Technology Prize, Global Energy Prize, Marcel Benoist Prize, Balzan Prize, Harvey Prize and the King Faisal International Science Prize and rthe Calveras award in photovoltaics. He is an elected member of the Royal Society (UK) and the Chinese and German Academy Science as well as the Swiss Academy of Technical Sciences and the Royal Spanish Academy of Engineering. He is a Honorary member of the Société vaudoise de science naturelle. Michael received 14 honorary doctor degrees from European and Asian Universities. His over 1800 publications had a major impact on the photovoltaic field. A recent bibliometric ranking by Stanford University places Michael first amongst 100'000 world-wide leading scientists across all areas of science. His publications have received so far some 485'000 citations with an H-factor of 302.

[Plenary 02] Prof. Chennupati JAGADISH

# **Semiconductor Nanostructures for Optoelectronics and Energy Applications**

Chennupati JAGADISH

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Semiconductors have played an important role in the development of information and communications technology, solar cells, solid state lighting. Nanowires are considered as building blocks for the next generation electronics and optoelectronics. In this talk, I will present the results on growth of nanowires, nanomembranes and microrings and their optical properties. Then I will discuss theoretical design and experimental results on optoelectronic devices. In particular I will discuss nanowire and micro-ring lasers and integration of nanowires and microrings. I will also present the results on polarization sensitive, broad bandwidth THz detectors operating at room temperature. Nanowire based energy devices such as solar cells and photoelectrochemical (PEC) water splitting will be discussed. Future prospects of the semiconductor nanostructures will be discussed.

# **Biography**



Professor Jagadish is the President of the Australian Academy of Science and a Distinguished Professor and Head of Semiconductor Optoelectronics and Nanotechnology Group in the Research School of Physics at the Australian National University. He is a Fellow of 13 Science and Engineering Academies of Australia, US, UK, India, China, Europe and Developing World-TWAS. He has received many awards including Australia's highest civilian honor, AC, Companion of the Order of Australia, for his contributions to physics and engineering, in particular nanotechnology. He has received 2023 Pravasi Bharatiya Samman Award, highest award given to overseas Indians from the President of India. He has in the past served as

President of IEEE Photonics Society, IEEE Nanotechnology Council and Australian Materials Research Society.

[Plenary 03] Prof. Alex K.Y. JEN

#### Printable Organic and Perovskite Solar Cells for Clean Energy

Alex JEN

Lee Shau Kee Chair Professor

Department of Materials Science & Engineering and Department of Chemistry Hong Kong Institute for Clean Energy, City University of Hong Kong, Hong Kong

Our recent study on charge generation and recombination in bulk-heterojunction and planar-mixed heterojunction blends comprising a crystalline polymer donor with Se-containing Y6-derived non-fullerene acceptors has shown both high photovoltaic internal quantum efficiencies and high external electroluminescence quantum efficiencies. Crystallographic and spectroscopic studies reveal that the pseudo-2D, fused-ring molecular acceptors are not only intrinsically highly luminescent but also meets the criteria in achieving intrinsically radiative recombination within the blend by promoting delocalized excitons with much longer luminescent lifetime and reduced exciton binding energies. These results provide the important demonstration of efficient OPV blends to achieve PCEs close to 20%. Regarding the development of perovskite solar cells (PSCs), several novel interface and additive engineering approaches have been developed to enable PSCs to show very high PCE (>26% certified) and stability in the inverted architecture devices. Moreover, new multifunctional redox mediators have also been developed to overcome the halide segregation issues that strongly hinder the development of highly efficient and stable large-bandgap PSCs. The resulting devices showed very low photovoltage loss and high PCE >20%. Their integration with OPV to form 2-T tandem devices has shown record-high PCE of 26.1% with good operational stability. Finally, the scalability and environmental stability of PSCs will be discussed to show their promise for commercialization.

#### References

- 1. "Redox Mediator-Stabilized Wide-Bandgap Perovskites for Monolithic Perovskite-Organic Tandem Solar Cells", S. Wu, Y. Yan, J. Yin, K. Jiang, F. Li, Z. Zeng, S-W. Tsang, A. K-Y. Jen, *Nature Energy*, **2024**, <a href="https://doi.org/10.1038/s41560-024-01451-8">https://doi.org/10.1038/s41560-024-01451-8</a>.
- 2. "Hydrogen Bond-Bridged Intermediate for Perovskite Solar Cells with Enhanced Efficiency and Stability", F. Li, X. Deng, Z. Shi, S. Wu, Z. Zeng, D. Wang, Y. Li, F. Qi, Z. Zhang, Z. Yang, S-H. Jang, F. R. Lin, S-W. Tsang, X. K. Chen, and A. K.-Y. Jen, *Nature Photonics*, **2023**, *17*, 478.
- 3. "Advances and Challenges in Understanding the Microscopic Structure—Property—Performance Relationship in Perovskite Solar Cells", Y. Zhou, L. Herz, A. K-Y. Jen, and M. Saliba, *Nature Energy*, **2022**, *7*, 794.
- 4. "Dilution Effect for Highly Efficient Multiple-Component Organic Solar Cells", L. Zuo, S. B. Jo, Y. K. Li, Y. Meng, R. J Stoddard, Y. Liu, F. Liu, F. Liu, D. S. Ginger, H-Z. Chen, A. K-Y. Jen, *Nature Nanotech*, **2022**, *17*, 53.
- 5. "Planar-Mixed Heterojunction Organic Photovoltaic Suppresses Recombination Loss", K. Jiang, J., Zhang, C. Zhong, F. Lin, F. Qi, Q. Li, Z. Peng, W. Kaminsky, S. H. Jang, J. Yu, X. Deng, H. Hu, D. Shen, F. Gao, H. Ade, M. Xiao, C. Zhang, and A. K-Y. Jen, *Nature Energy*, **2022**, *7*, 1076.
- 6. "2D Metal—Organic Framework for Stable Perovskite Solar Cells with Minimized Lead Leakage", Shengfan Wu, Zhen Li, Mu-Qing Li, Yingxue Diao, Francis Lin, Jie Zhang, Peter Tieu, Wenpei Gao, Feng Qi, Xiaoqing Pan, Zhengtao Xu, Zonglong Zhu, Alex K.-Y. Jen, *Nature Nanotech*, **2020**, *15*, 934.
- 7. "Prospects and Challenges for Perovskite-Organic Tandem Solar Cells", S. Wu, M. Liu, A. K.-Y. Jen, Joule, 2023, 7, 484.
- 8. "Renewed Prospects for Organic Photovoltaics", G. Zhang, F. R. Lin, F. Qi, T. Heumüller, A. Distler, H-J. Egelhaaf, N. Li, P. Chow, C. J. Brabec, A. K.-Y. Jen, H.-L. Yip, *Chem. Rev.*, **2022**, *122*, 14180.
- 9. "Designs from Single Junctions, Heterojunctions to Multijunctions for High-Performance Perovskite Solar Cells", X. Wu, B. Li, Z. Zhu, C-C. Chueh, A. K.-Y. Jen, *Chem. Soc. Rev.*, **2021**, *50*, 13090.

#### **Biography**



Alex Jen is the Lee Shau-Kee Chair Professor and Founding Director of the Hong Kong Institute for Clean Energy at the City University of Hong Kong. He also served as the Provost of CityU during 2016-2020. He received his B.S. from the National Tsing Hua University in Taiwan and Ph.D. from the University of Pennsylvania in USA. Before arriving at CityU, he had served as the Boeing-Johnson Chair Professor and Chair of the Department of Materials Science & Engineering at the University of Washington, Seattle. He was also appointed as the Chief Scientist for the Clean Energy Institute endowed by the Washington State Governor. He is a distinguished researcher who published more than 1000 SCI papers with >92,000 citations and an H-index of 155. He is also a co-inventor of 71 patents and invention

disclosures.

For his pioneering contributions in organic photonics and electronics, Professor Jen was elected as Academician by both the European Academy of Sciences and the Washington State Academy of Sciences. He was also elected as Fellow for several professional societies, including AAAS, MRS, ACS, PMSE, OSA, and SPIE. He was named by the Times Higher Education (THE) in 2018 as one of the "Top 10 University Researchers in Perovskite Solar Cell Research". In addition, he was recognized by Thomson Reuters as one of the "World's Most Influential Scientific Minds of 2015 and 2016 and by Clarivate as one of the "Highly Cited Researchers" in Materials Science from 2014-2023.

[Keynote 01] Prof. Zonglong ZHU

# Interface-Enhanced Stability for Halide Perovskite Photovoltaics: A Fundamental Understanding

Zonglong ZHU
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Organic-inorganic hybrid perovskite solar cells (PSCs) have shown great progress over the past decade, with power conversion efficiencies (PCEs) of single-junction devices approaching silicon photovoltaics (PVs). However, their long-term stability still lags behind silicon-based competitors, which has significantly decelerated their commercialization progress. Faced with this challenge, major efforts have been made to unravel instability mechanisms, develop long-term performance-tracking protocols, and explore various approaches for enhancing the stability of PSCs. Among these strategies, interface manipulation is the most critical as it could simultaneously passivate or anchor the perovskite surface defects and acts as a barrier to protect the bulk of perovskite from the external environment. Recently, the development of diversified interface modification molecules and interfacial regulation strategies has greatly contributed to the improvement of PSC stability. This presentation will elucidate the factors influencing the stability of PSCs, provide an indepth understanding of device degradation mechanisms, and present advanced approaches to reveal them. Additionally, we will discuss pressing topics on interface manipulation, including low-dimensional perovskite capping layers, interface modification and reaction, and charge transport layer design. Lastly, we will provide insights into the core aspects related to the future development of PSC stability.

# **Biography**



Dr. Zonglong Zhu is an associate professor at City University of Hong Kong. Since joining the university as an assistant professor in 2018, he has authored numerous papers as the corresponding author in renowned journals such as Science, Nat. Nanotech., Nat. Commun., Chem. Soc. Rev., Acc. Chem. Res., J. Am. Chem. Soc., Adv. Mater., Angew. Chem. Int. Ed., and others. Dr. Zhu has published over 110 SCI papers, with over 13,000 citations and an impressive H-factor of 50. Dr. Zhu's contributions to the field have earned him numerous accolades. He has been recognized as one of the top 2% of scientists with the most citations in the world in 2021, Emerging Investigator of Nanoscale in 2022, Emerging Investigator of J. Mater. Chem. A in 2021, and Highly Cited Researcher in Cross-Field in 2022. In addition,

he has received several awards, including the President's award and Yong research award from the College of Science at CityU in 2022.

[Plenary 04] Prof. Tianshou ZHAO

#### Long-Duration Energy Storage: the Bridge to a Net Zero Future

Tianshou ZHAO

Chair Professor of Mechanical & Energy Engineering Southern University of Science & Technology, China Email: zhaots@sustech.edu.cn

Flow cells are those in which a flowable storage medium (e.g.: hydrogen, methanol, ammonia, liquid electrolytes, etc.) allows decoupling power and energy. This talk will show that flow cells are scable, safe, and particularly flexiable in storage duration and site selections. Therefore, flow cells will become game-changing technologies to facilitate the widespread deployment of renewables. In particular, we will show that common scientific issues and practical challenges pertaining to flow cell technologies can be addressed by an interdisciplinary approach combining electrochemistry and engineering thermophyiscs.

#### **Biography**



Tianshou Zhao is Dean of Energy Institute for Carbon Netrality, Chair Professor of Mechanical & Energy Engineering, Southern University of Science & Technology (SUSTech). Befor joining SUSTech in 2021, he held the named professorship of Engineering and Environment at HKUST. Prof Zhao is an elected academician of the Chinese Academy of Sciences, Fellow of the American Society Mechanical Engineers, Fellow of the Royal Society of Chemistry, Fellow of the Chinese Society of Chemistry, and a Highly Cited Researcher by Clarivate/Thomson Reuters, and Editor-in-Chief of International Journal of Heat and Mass Transfer. His research aims to establish the scientific underpinnings for innovations and breakthroughs in energy storage devices. Using an interdisciplinary approach that combines

thermo-fluid sciences with electrochemistry, he is exploring the best combination of materials and system structures to enable revolutionary advances in the performance, cost, and lifetime of energy storage devices.

[Keynote 02] Prof. Bin LIU

# A Design Strategy Towards Oxygen Electrocatalysts

Bin LIU

Department of Materials Science and Engineering City University of Hong Kong E-mail: bliu48@cityu.edu.hk

In this talk, I am going to summarize our recent progresses towards design of efficient oxygen electrocatalysts for various electrochemical energy conversion and storage applications. The design strategies include: 1. How to experimentally determine binding strength of reactive intermediates. 2. How to tune binding strength of reactive intermediates by surface engineering. 3. How to break the scaling relationship.

# **Biography**



Bin Liu received his bachelor of engineering (1st Class Honours) and master of engineering degrees at the National University of Singapore, Singapore in 2002 and 2004, respectively, and completed his doctoral degree at the University of Minnesota, USA in 2011. After spending a year as postdoctoral fellow in the University of California Berkeley, USA, he joined School of Chemical and Biomedical Engineering at Nanyang Technological University as an Assistant Professor in June 2012 and was promoted to Associate Professor in March 2017. In February 2023, Professor Liu joined the Department of Materials Science and Engineering at City University of Hong Kong as a Global STEM Professor. His research focuses on photo(electro)catalysis and in-situ/operando characterization. Professor Liu was

awarded emerging investigator by Journal of Materials Chemistry A, Royal Society of Chemistry in 2016, class of influential researchers by Industrial & Engineering Chemistry Research, American Chemical Society in 2018, and listed in the "Highly Cited Researchers" in Cross-Field in 2019 and Chemistry in 2020-2023 by Clarivate Analytics.

[Keynote 03] Prof. Qi LIU

# Lithium-ion Battery Cathodes: From Cobalt-rich to Cobalt-free

Qi LIU

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Knowledge of atomic interactions with high energy photons or particles opened up a window to the microscopic structures of materials. In particular, X-rays and neutrons interact with electrons and nuclei of atoms in different ways, which enables their complementary scattering, spectroscopic, and imaging capabilities for structural characterizations. Over the past few decades, techniques based on X-ray and neutron interactions, capable of being time resolved and combined, have been well developed for encoding structures in various length, elemental and temporal levels, and, in turn, have ignited breakthroughs in the field of battery science and engineering. In this talk, we will firstly reviewed the advanced X-ray and neutron techniques for studying secondary rechargeable batteries such as lithium-ion batteries, sodium-ion batteries and et al. For each of the techniques, with a brief description of the theory on account of characterizing principles is given (i.e., scattering, excitation, and emission), followed by an introduction of operando methodologies including instruments, setups, and cell designs employed in synchrotron and neutron beamlines. Finally, a few practical examples are presented to demonstrate the applicability of these techniques in studying lithium/sodium ion batteries, with a particular emphasis on each of their structural sensitivities at various time, elemental, and length levels.

# **Biography**



Prof. Liu Qi is currently an associate professor in the Department of Physics, City University of Hong Kong. He obtained his Ph.D from Purdue University in 2014. Before joining CityU, he worked as a postdoctoral fellow at Argonne National Laboratory. His current research interests focus on the structure-property-studies of functional materials via multiple neutron- and synchrotron-based techniques. His broad research activities include the design and synthesis of novel energy storage materials, phase transition mechanism and neutron-/synchrotron physics. Currently, Dr. LIU authored over 130 peer reviewed journal papers and over 20 conference papers. He has a citation of >10,000 and H-index of 53.

[Plenary 05] Prof. Shi-Gang SUN

# Structure Design and Performance Enhancement of Proton-Exchange-Membrane Fuel Cells Catalysts

**Shi-Gang SUN** 

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The Proton Exchange Membrane Fuel Cells (PEMFCs) convert directly, and high-efficiently chemical energy stored in fuel molecules or hydrogen into electricity, and plays a key role in the carbon neutralization target and hydrogen energy society. At present, platinum-based materials are the unique and un-replaceable catalysts employed in operated PEMFCs. The rare resource and high price of platinum metals restricts the commercialization and wide applications of the PEMFCs in the one hand, and in the other, the extremely sluggish kinetics of oxygen reduction reaction (ORR) at cathode of PEMFCs (90% of total Pt amount used in a PEMFC is currently loaded in cathode) consists in the main challenging for fast development of PEMFCs. Therefore, in order to promote the application of PEEMFCs especially in the field of electric transportation, to increase the utilization efficiency of platinum-based catalysts and to explore non-precious metal (NPM) catalysts are the two most promising routes. This communication will present our recent progresses in studies of both Pt-based and NPM catalysts for PEMFC utilizations.

For increasing the utilization efficiency of platinum-based catalysts, we have developed electrochemical shape-controlled synthesis of high-index facet nanocrystal catalysts that expose high-density of catalytic active sites and Pt-alloy nanocatalysts, which exhibit high catalytic activity and stability for anode hydrogen oxidation reaction (HOR) in PEMFCs. For exploring non-precious metal (NPM) catalysts, we focused on the most most-promising Fe/N/C catalysts. Through optimizing the Fe/N/C composition and sulfur-doping, constructing active three-phase interface to enable efficient mass/electron transfer, developing the "surfaceization" strategy of pyrolysis to increase the density and utilization of active sites, we have continuously refreshed the records of out-put power density of non-precious metal catalyst PEMFCs.

# **Acknowledgements:**

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# **References:**

- 1. Z.Y. Zhou, S.G. Sun et al. *Energy Environ. Sci.* 2018, 11, 166-177
- 2. T. Wang, S.G. Sun, Z.Y. Zhou et al. J. Am. Chem. Soc. 2022, 144, 9292-9301
- 3. W.C. Xu, Z.Y. Zhou, S.G. Sun et al. JMCA, 2023, 11, 4078-4087
- 4. N Tian, ZY Zhou, SG Sun, et al., *Science*, 2007, 316, 732-735
- 5. L. Huang, S.G. Sun et al. *J. Electrochem*. 2016, 22, 123-128
- 6. C Xiao, N Tian, ZY Zhou, SG Sun et al. Joule, 2020, 4, 2562-259
- 7. Y.C. Wang, Z.Y. Zhou, S.G. Sun et al. Angew. Chem. Int. Ed. 2015, 54,9907–9910
- 8. X.D. Yang, Z.Y. Zhou, S.G. Sun et al., ACS Catal. 2017, 7, 139-145
- 9. J.M. Zhang, Y.X. Jiang, S.G. Sun et al. *Angew. Chem. Int. Ed.* 2020, 59, 21976–21979
- 10. J.M. Zhang, Y.X. Jiang, S.G. Sun et al. Appl. Catal. B: Environ., 2020, 263, 118345
- 11. Y.C. Wang, Z.Y. Zhou, S.G. Sun et al. Adv. Funct. Mater., 2021, 2009645
- 12. X.Y. Cheng, Y.X. Jiang, S.G. Sun et al. *Energy Environ. Sci.*, 2021, 14, 5958
- 13. P.Y. Zhang, Y.C. Wang, Z.Y. Zhou, S.G. Sun et al. J. Phys. Chem. Lett. 2021, 12, 7797–7803
- 14. Y.C. Wang, Z.Y. Zhou, S.G. Sun et al. 2022, 8, eadd8873
- 15. S.H. Yin, Y.X. Jiang, S.G. Sun et al. Energy Environ. Sci. 2022, 15, 3033
- 16. Y.Y. Li, Z.Y. Zhou, S.G. Sun et al. *Electrochem. Commun.* 2022, 141, 107357
- 17. T. Wang, Z.Y. Zhou, S.G. Sun et al. J. Am. Chem. Soc. 2022, 144, 9292-9301
- 18. Y.C. Wang, N.F. Zheng, S.G. Sun et al. J. Am. Chem. Soc. 2023, 145, 15528-15537
- 19. L.T. Cui, Y.C. Wang, S.G. Sun et al. Sus. Energy & Fuels, 2024, 8, 178-191

#### **Biography**



Shi-Gang Sun obtained his Bachelor of Science from Xiamen University, China, in 1982, Doctorat d'Etat (Docteur ès Sciences Physiques) from Université Pierre et Marie Curie (Paris VI), France, in 1986. After one-year post-doctoral research in the Laboratoire d'Electrochimie Interfaciale du CNRS, France, he returned to China by the end of 1987, and served as associate professor and later full professor in 1991 at the Department of Chemistry of Xiamen University till now.

Prof. Sun is Academician of Chinese Academy of Sciences (CAS), fellow of International Society of Electrochemistry (ISE), Royal Society of Chemistry (RSC), Chinese Chemical Society (CCS), China Society of Chemical Engineering (CSCE), and China Society of micron and Nanotechnology (CSMN).

The main research interests of Prof. Sun include Electrocatalysis, Electrochemical Surface Science, Spectroelectrochemistry, Nanomaterials and Chemical power sources (Batteries, Fuel Cells). He has published more than 850 SCI papers with peer citation over 45,000, H-index 107 (Google Scholar Data), awarded 40 innovation patents, authored 5 books.

Prof. Sun has awarded the "Brian Conway Prize" from International Society of Electrochemistry (ISE), "Distinguished Contribution Award" from the Chinese Society of Electrochemistry, "Le prix Franco-Chinois 2014-2015" jointly from Société Chimique de France (SCF) and Chinese Chemical Society (CCS), and the State Natural Science Award (2nd Degree) of China, "Achievement award" from International Automotive Lithium Battery Associetion, and "Achievement award in spectroscopy" from Chinese Chemical Society and Chines Optics Society.

Prof. Sun is now editorial board member of Journal of Electroanalytical Chemistry, Functional Materials Letters, ACS Energy Letters, Electrochemical Energy Review, National Science Review, Applied Chemistry, Journal of Solid State Electrochemistry and Journal of Material Chemistry A, serving as associate editor to Electrochimica Acta, Spectral Analysis and Spectroscopy, Chinese Journal of Chemical Education, Acta Chimica Sinica, and editor-in-chief of the Journal of Electrochemistry.

[Plenary 06] Prof. Hua ZHANG

# **Phase Engineering of Nanomaterials (PEN)**

Hua ZHANG

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In this talk, I will summarize the recent research on phase engineering of nanomaterials (PEN) in my group, particularly focusing on the rational design and synthesis of novel nanomaterials with unconventional phases for various promising applications. For example, by using wet-chemical methods, for the first time, we have successfully prepared novel Au nanostructures (e.g., the hexagonal-close packed (hcp) 2H-Au nanosheets, 4H-Au nanoribbons, and crystal-phase heterostructured 4H/fcc and fcc/2H/fcc heterophase Au nanorods), epitaxially grown metal nanostructures on the aforementioned unconventional Au nanostructures and 2H-Pd nanoparticles, and amorphous/crystalline heterophase Pd, PdCu, Rh and Rh alloy nanosheets. By using gas-solid reactions, metastable 1T'-phase group VI transition metal dichalcogenides (TMDs), e.g., WS2, WSe2, MoS2, MoSe2, WS2xSe2(1-x) and MoS2xSe2(1-x), have been prepared. Impressively, the 1T'-MoS<sub>2</sub>-supported single-atomically dispersed Pt (s-Pt) atoms with Pt loading up to 10 wt% exhibit superior performance in hydrogen evolution reaction. Importantly, 1T'-TMD monolayers can be stabilized on 4H-Au nanowires, which can be used for ultrasensitive SERS detection Moreover, the salt-assisted 2H-to-1T' phase transformation of TMDs have been achieved, and the phase transformation of TMDs during our developed electrochemical Li-intercalation process has been observed. Impressively, the lithiation-induced amorphization of Pd₃P₂S<sub>8</sub> has been achieved. Currently, my group focuses on the investigation of phase-dependent physicochemical properties and applications in catalysis, (opto-)electronic devices, clean energy, chemical and biosensors, surface enhanced Raman scattering, photothermal therapy, etc., which we believe is quite unique and very important not only in fundamental studies, but also in future practical applications. Importantly, the concepts of phase engineering of nanomaterials (PEN), crystal-phase heterostructures, and heterophase nanomaterials are proposed.

**Reference:** (1) *Nature*, 2023, *621*, 300. (2) *Nat. Mater.*, 2024, *23*, in press. (3) *Nat. Mater.*, 2021, *20*, 1113. (4) *Nat. Rev. Chem.*, 2020, *4*, 243. (5) *J. Am. Chem. Soc.*, 2020, *142*, 18971. (6) *Nat. Chem.*, 2018, *10*, 638. (7) *Nat. Chem.*, 2018, *10*, 456. (8) *Nat. Catal.*, 2018, *1*, 460. (9) *Adv. Mater.*, 2018, *30*, 1803234. (10) *Chem. Sci.*, 2017, *8*, 795. (11) *ACS Nano*, 2015, *9*, 9451. (12) *Nat. Commun.*, 2015, *6*, 7684. (13) *Nat. Commun.*, 2013, *4*, 1444. (14) *ACS Nano*, 2012, *6*, 74. (15) *Nat. Commun.*, 2011, *2*, 292. (16) *Angew. Chem. Int. Ed.*, 2011, *50*, 11093.

# **Biography**



Dr. Hua Zhang obtained his B.S. and M.S. degrees at Nanjing University in China in 1992 and 1995, respectively, and completed his Ph.D. with Prof. Zhongfan Liu at Peking University in China in July 1998. He joined Prof. Frans C. De Schryver's group at Katholieke Universiteit Leuven (KULeuven) in Belgium as a Research Associate in January 1999. Then he moved to Prof. Chad A. Mirkin's group at Northwestern University as a Postdoctoral Fellow in July 2001. He started to work at Nanolnk Inc. (USA) as a Research Scientist/Chemist in August 2003. After that, he worked as a Senior Research Scientist at Institute of Bioengineering and Nanotechnology in Singapore from November 2005 to July 2006. Then he joined the School of Materials Science and Engineering in Nanyang Technological University (NTU) as an

Assistant Professor. He was promoted to a tenured Associate Professor on March 1, 2011, and Full Professor on Sept. 1, 2013. In 2019, he joined the Department of Chemistry in City University of Hong Kong as a Chair Professor, and currently he is the Herman Hu Chair Professor of Nanomaterials.

He has published 8 invited book chapters, 90 patent applications (including granted 1 China patent, 1 European patent, 3 Singapore patents, and 10 US patents), and over 500 papers. Some of his papers have been published in Nature (1), Science (1), Nat. Mater. (4), Nat. Chem. (5), Nat. Catal. (2), Nat. Rev. Mater. (2), Nat. Rev. Chem. (1), Nat. Commun. (13), Sci. Adv. (2), Nat. Protocols (1), Chem. Rev. (5), Chem. Soc. Rev. (16), Acc. Chem. Res. (4), Acc. Mater. Res. (1), J. Am. Chem. Soc. (29), Angew. Chem. Int. Ed. (29), Adv. Mater. (74), Energy Environ. Sci (12), Mater. Today (1), Adv. Energy Mater. (9), Chem (3), Natl. Sci. Rev. (4), ACS Nano (33), Nano Lett. (17), Adv. Funct. Mater. (5), Nano Energy (6), Energy Storage Mater. (1), ACS Catal. (1), Small (70), Small Methods (3), Nano-Micro Lett. (1), Mater. Horizons (2), Biomater. (1), Biosens. Bioelectron. (2), J. Mater. Chem. A (4), Matter (2), NPG Asia Mater. (1), J. Hazard. Mater. (1), Nanoscale Horizons (2), Appl. Mater. Today (1), J. Mater. Chem. (9), etc. As at May 2024, the total cited times are over 129,800 with H-index of 178 (Web of Science), and over 146,600 with H-index of 188 (Google Scholar). He has been invited to give more than 300 Plenary, Keynote or Invited Talks in international conferences, universities and institutes. He has organized several tens of international conferences and served as the Conference (Co-)Chair or Symposium Chair.

He is the co-Editor-in-Chief of *SmartMat* (2020-) and co-Chairman of the Editorial Board of *ChemNanoMat* (2015-), and sits on the Advisory Board of *Chemical Society Reviews* (2012-2019), *Aggregate* (2020-present), *Chemical Journal of Chinese Universities* (2019-), *Energy Materials and Devices* (2023-), *Materials Chemistry Frontiers* (2016-), *Matter* (2019-), *Nanoscale* (2012-), *Nanoscale Horizons* (2015-) and *NPG Asia Materials* (2018-), the Editorial Advisory Board of *ACS Nano* (2014-), *Advanced Functional Materials* (2018-), *Advanced Materials* (2019-), *Small* (2012-), *ACS Appl. Mater. Interfaces* (2014-2019), *Chem. Mater.* (2014-2019) and *Nanofabrication* (2012-2020), the Editorial Board of *2D Materials* (2022-), *ACS Omega* (2016-), *Acta Physico-Chimica Sinica* (2020-), *Applied Materials Today* (2015-), *Carbon* (2013-), *CHEM* (2016-), *Chemical Reviews* (2024-), *Chemistry-Methods* (2020-), *Chinese Science Bulletin* (2014-), *Electron* (2023-), *Energy Storage Materials* (2015-), *EnergyChem* (2018-), *eScience* (2020-), *Graphene Technology* (2016-), *Materials Today Energy* (2016-), *NANO* (2007-2020), *Nano Convergence* (2020-), *Transactions of Tianjin University* (2019), and *Science China Materials* (2014-), the International Advisory Board of *ChemPlusChem* (2012-2015), and the Scientific Advisory Board of *Small Methods* (2017-).

In 2020, he was elected as a *Foreign Fellow* of the European Academy of Sciences (*EurASc*). In 2015, he was elected as an *Academician* of the Asia Pacific Academy of Materials (*APAM*). In 2014, he was elected as a *Fellow* of the Royal Society of Chemistry (*FRSC*). He was listed in the "*Highly Cited Researchers*" in *Materials Science* (Clarivate Analytics/Thomson Reuters, 2014-2023 (10 consecutive years)), in *Chemistry* (Clarivate Analytics/Thomson Reuters, 2015-2023 (9 consecutive years)), and in *Environment and Ecology* (Clarivate Analytics, 2022). In 2015, he was listed as one of 19 "*Hottest Researchers of Today*" in the world in the *World's Most Influential Scientific Minds 2015* (Thomson Reuters, 2015). In 2014, he was listed as one of 17 "*Hottest Researchers of Today*" and No. 1 in *Materials and More* in the world in the *World's Most Influential Scientific Minds 2014* (Thomson Reuters, 2014). Moreover, he also got the IUMRS-Frontier Materials Scientists Award (2023, IUMRS-ICFM), *EcoMat Mid-Career Research Award* (2023, Wiley-VCH), *Outstanding Research Award* (2022, City University of Hong Kong), *President's Award* (2021, City University of Hong Kong), *Young Investigator Award* (Young Giants of Nanoscience 2016, Hong Kong), *Vice-Chancellor's International Scholar Award* (University of Wollongong, Australia, 2016), *ACS Nano Lectureship Award* (2015), *World Cultural Council (WCC) Special Recognition Award* (2013), the *ONASSIS Foundation Lectureship* (Greece, 2013), *Asian Rising Stars* (15<sup>th</sup> Asian Chemical Congress, 2013), *SMALL Young Innovator Award* (Wiley-VCH, 2012) and *Nanyang Award for Research Excellence* (2011).

Dr. Zhang's research is highly interdisciplinary. His current research interests focus on phase engineering of nanomaterials (PEN) and controlled epitaxial growth of heterostructures, including the synthesis of ultrathin two-dimensional nanomaterials (e.g., metal nanosheets, graphene, metal dichalcogenides, metal-organic frameworks, covalent organic frameworks, etc.), novel metallic and semiconducting nanomaterials, novel amorphous nanomaterials, and their hybrid composites for various applications, such as catalysis, clean energy, (opto-)electronic devices, chemical and biosensors, and water remediation.

[Keynote 04] Prof. Zuankai WANG

# Nature-inspired surfaces for water-energy nexus

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Water and energy are not separate entity, but closely coupled together. Current water energy nexus suffers from low energy efficiency and high environment impact. Fundamentally, water-energy nexus is governed by surfaces. However, surface innovation to address water and energy nexus is not easy, because individual water and energy processes often involve trade-off on surface properties. In this talk, I will discuss our recent efforts in developing a new and generic nature-inspired surface design theory that can fully unleash the inherent advantages of water (flowing, high latent heat and large surface tension) for efficient water-energy nexus, with typical applications in water collection, energy harvesting, thermal management.

#### **Biography**



Zuankai Wang is the Associate Vice President (Research and Innovation), Kuok Group Professor in Nature-Inspired Engineering, Chair Professor in the Department of Mechanical Engineering, and Director of Research Center for Nature-Inspired Science and Engineering at The Hong Kong Polytechnic University (PolyU). He received his BSc from Jilin University, his MSc from the Shanghai Institute of Microsystem and Information Technology, and his PhD from the Rensselaer Polytechnic Institute. Before joining PolyU, Prof. Wang was a Chair Professor at the Department of Mechanical Engineering and was the Associate Dean in the College of Engineering at the City University of Hong Kong. He is the Executive Editor-in-Chief of Droplet (Wiley).

Prof. Wang is a Fellow of the Hong Kong Academy of Engineering Sciences, the Royal Society of Chemistry, and the International Society of Bionic Engineering. He has won numerous awards, including the Nukiyama Memorial Award (2024), Falling Walls Science Breakthroughs of Year 2023 (Engineering and Technology), Croucher Senior Research Fellowship, Research Grant Council Senior Research Fellowship, BOCHK Science and Technology Innovation Prize, Green Tech Award, Xplorer Prize, and the 35th World Cultural Council Special Recognition Award. He was named as "Highly Cited Researcher" by Clarivate Analytics (2022, 2023).

[Plenary 07] Prof. Ben Zhong TANG

# Green Chemistry: Making Functional Polymers on/in/from Water

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Water, as an omnipresent substance, plays a vital role in many aspects of our lives, ranging from sustaining living organisms to driving technological advancements. The exploration of organic reactions in water and utilization of water as a reactant for synthesizing functional materials has attracted much attention due to their advantages, including unique reaction kinetics, environmental friendliness, and reduction of harmful wastes. In this talk, the recent research progresses in the development green polymerization processes involving water and triple-bond monomers (e.g., diynes, isocyanides, etc.) will be introduced. Furthermore, new click polymerization methods in aqueous media will be discussed. The "on water" effect facilitates polymerization in aqueous media much more effectively than in conventional organic solvents. Additionally, biogenic luminogens possessing aggregation-induced emission (AIE) attibutes (BioAlEgens) are developed in aqueous systems. The synthesized polymers, small molecules, and BioAlEgens show unique characteristics and functions such as AIE, clusteroluminescence, bioimaging, and stimuli response. With the aim of exploring polymerizations on/in water, we hope this talk will provide insight into polymerizations of water and triple-bond monomers, as well as preparation of functional materials under mild reaction conditions through the utilization of water.

#### References

- [1] Tang, B. Z.\*; Poon, W. H.; Leung, S. M.; Leung, W. H.; Peng, H. Macromolecules 1997, 30, 2209.
- [2] Deng, H.; Han, T.; Zhao, E.; Kwok, R. T. K.; Lam, J. W. Y.; Tang, B. Z. Polym. Chem. 2016, 7, 5646.
- [3] Zhang, J.; Wang, W.; Liu, Y.; Sun, J. Z.; Qin, A.; Tang, B. Z. Macromolecules 2017, 50, 8554.
- [4] Hu, R.; Chen, X.; Zhou, T.; Si, H.; He, B.; Kwok, R. T. K.; Qin, A.; Tang, B. Z. Sci. China Chem. 2019, 62, 1198.
- [5] Cai, X.-M.; Lin, Y.; Zhang, J.; Li, Y.; Tang, Z.; Zhang, X.; Jia, Y.; Wang, W.; Huang, S.; Alam, P.; Zhao, Z.; Tang, B. Z.\* *Natl. Sci. Rev.* **2023**, 10.1093/nsr/nwad233.
- [6] Liu, X.; Zhang, C.; Hu, L.; Wang, J.; Li, K.; Feng, H.-T.; Lam, J. W. Y.; He, B.; Tang, B. Z.\* CCS Chem. 2023, 5, 385.
- [7] Song, B.; Zhang, J.; Zhou, J.; Qin, A.; Lam, J. W. Y.; Tang, B. Z. Nat. Commun. 2023, 14, 3115.

#### **Biography**



Prof. Tang received BS and PhD degrees from South China University of Technology and Kyoto University in 1982 and 1988, respectively. He conducted postdoctoral research at the University of Toronto in 1989–1994. He joined the Hong Kong University of Science & Technology in 1994 and was promoted to Chair Professor in 2008. He was elected to the Chinese Academy of Sciences in 2009, the Asia Pacific Academy of Materials in 2017 and the World Academy of Sciences for the Advancement of Science in Developing Countries in 2020. In 2021, he joined the Chinese University of Hong Kong, Shenzhen, as Dean of the School of Science and Engineering, with a concurrent appointment of X.Q. Deng Presidential Chair Professor.

Prof. Tang has published >2,000 scientific papers, which have been cited >191,000 times. His h-index is 193. He has delivered >500 invited talks at international conferences and has been granted >100 patents. He is currently serving as Editor-in-Chief of Aggregate published by Wiley, and is sitting in the editorial boards of >20 international scientific journals.

Mainly engaged in materials science, macromolecular chemistry and biomedical theranostics. He coined the concept of aggregation-induced emission (AIE), and his labs are spearheading the AIE research in the world.

Prof. Tang has been listed as a Highly Cited Researcher in both areas of Chemistry and Materials Science since 2014. He received a series of awards, scholarships and honors, such as Croucher Senior Research Fellowship Award in 2007, MACRO Lecture Award (American Chemical Society) in 2012, Honorary Citizen of Guangzhou City in 2015, National Natural Science Award (1st Class) in 2017, Scientific and Technological Progress Award (Ho Leung Ho Lee Foundation) in 2017, Nano Today Award in 2021, and Biomaterials Global Impact Award in 2023.

[Keynote 05] Prof. Yi-Chun LU

#### **Material Designs for High-Performance Aqueous Redox Flow Batteries**

Yi-Chun LU

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Energy storage system is a critical enabling factor for deploying unstable and intermittent renewable power sources, such as solar and wind power sources. Non-aqueous lithium ion batteries dominate the battery markets owing to its high energy density. However, they are flammable, which could bring catastrophic damages in large-scale applications. Aqueous redox flow battery (RFB) is one of the most competitive technologies for scalable, safe and long-duration energy storage owing to its design flexibility in power and energy. All-vanadium RFB is the most well-established chemistry, but its widespread deployments are hindered by the low abundance and high cost of vanadium. Aqueous polysulfide electrolyte has been extensively studied as a low-cost and high-capacity electrolyte for RFBs owing to its high earth abundance and low material cost. However, they are limited by crossover and sluggish kinetics. In this presentation, we will discuss strategies to improve polysulfide redox flow batteries and it's future perspectives.

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#### **Biography**



Prof. Yi-Chun Lu received her Ph.D. degree from MIT in 2012. She is a Professor in the Department of Mechanical and Automation Engineering at The Chinese University of Hong Kong (CUHK). She serves as the Associate Editor of Journal of Materials Chemistry A and Materials Advances from Royal Society of Chemistry. She is Fellow of Royal Society of Chemistry, Founding Member of Young Academy of Science of Hong Kong and was the recipient of RGC Research Fellow 2022, Xplorer Prize 2021, IBA Early Career Award 2021, Excellent Young Scientists, National Natural Science Foundation of China (2019), Young

Researchers Award (2016), and Hong Kong SAR Research Grants Council Early Career Award (2014). Dr. Lu's research interest centers on developing fundamental understandings and material design principles for clean energy storage and conversion. Specifically, her research group is studying: Electrode and electrolyte design for high-energy metal-air and metal sulfur batteries; Redox-active components and solution chemistry for redox-flow batteries; Electrode and electrolyte design for high-voltage aqueous batteries; Mechanistic understanding of interfacial phenomena governing electrochemical energy conversion and storage processes.

[Plenary 08] Prof. Chao-jun LI

#### **Group III-Nitrides as Emerging Catalysts for Energy and Chemical Conversions**

Chao-Jun LI

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Group III-nitrides, touted as the next-generation semiconductors beyond Si, have brought dramatic changes to our everyday life over the past three decades with revolutionary applications in LED lighting and power electronics. The use of III-nitride semiconductors as catalysts for chemical reactions has also attracted extensive interests recently. The activation of covalent bonds in organic compounds, exemplified by C-H, O=C=O, N = N, O-H, etc., represents wide chemistry applications. From pharmaceuticals to clean energy, the manufacturing of almost every daily product can be impacted by the development of such bond activation. This talk will discuss some recent developments in the PI's laboratory on this topic.

#### **Biography**



Prof. C.-J. Li received his Ph.D. at McGill University 1992 and was a NSERC Postdoctoral Fellow at Stanford University (US). He was an Assistant (1994), Associate (1998) and Full Professor (2000) at Tulane University (US). Since 2003, he has been a Canada Research Chair (Tier I) in Green Chemistry and E. B. Eddy Chair Professor at McGill University. He also serves as the Co-Director for Quebec's FQRNT Center for Green Chemistry and Catalysis since 2009. He was a pioneer in using water as a green solvent and a leader in developing Green Chemistry for chemical synthesis. He received US NSF's CAREER Award (1997), US Presidential Green Chemistry Challenge Award (2001), 2010 Canadian Green Chemistry and Engineering Award, 2015 R. U. Lemieux Award and 2018 Alfred Bader Award of the Canadian Chemical Society, the 2020 Catalysis Award and the 2022 CIC Medal of CIC, the 2021

Alexander von Humboldt Research Award, and the 2018 Killam Research Fellow of the Canadian Council of Arts among others. Dr. Li was elected as a Fellow of the Royal Society of Canada (2012), the Royal Society of Chemistry (UK) (2007), the American Association for the Advancement of Science (AAAS) (2012), the Chemical Institute of Canada (2013), the American Chemical Society (ACS) (2015), the Chinese Chemical Society (2020), the American Chemical Society (ACS) (2013), as well as a Fellow of The World Academy of Sciences (TWAS) (2016) and the European Academy of Sciences (2020).

[Keynote 06] Prof. Bolong HUANG

# **Advanced Atomic Catalysts Design for Energy Systems**

**Bolong HUANG** 

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Currently, atomic catalysts (ACs) as the frontier research topics have attracted tremendous attention due to their ultrahigh electroactivity and broad applications in different energy systems. However, a large number of possible combinations between metals and support materials, the complexity of catalytic materials, as well as the complicated reaction mechanisms are still the main difficulties for designing novel ACs. To supply theoretical guidance for designing novel electrocatalysts, we have carried out comprehensive theoretical studies of ACs supported on graphdiyne (GDY) through density functional theory (DFT) calculations and machine learning (ML) techniques. First, we have proposed the "Redox Barrier Model" to quantify the capability of electron exchange and transfer. For the hydrogen evolution (HER) process, we have extended the conventional indicator of proton binding energy to more diverse criteria, where the screened electrocatalysts for HER are also verified ML. To design dual atomic catalysts (DACs), the formation stability and electronic modulations for all the combinations between transition metals (TMs) and lanthanide (Ln) metals are compared. Due to the electronic self-balance effects by f-d orbital coupling, the combinations of the Ln metals and TMs achieve optimized stability and electroactivity of GDY-DACs. For the applications of GDY-ACs in the CO2 reduction reaction (CO2RR), a comprehensive reaction pathway mapping of C<sub>1</sub> and C<sub>2</sub> products is achieved for the first time, where the integrated largesmall cycle mechanism and double-dependence correlations are identified. Moreover, the first principles machine learning (FPML) approach is proposed to predict the reaction trends for different products and C-C couplings for novel C₃ products. Therefore, these theoretical explorations have supplied important insights and effective approaches for the design of novel ACs, opening a new avenue to enable broad applications of ACs towards different energy systems.

# References

- [1] M. Sun, B. Huang\*, Adv. Energy Mater. 2024, 14: 2400152.
- [2] M. Sun, B. Huang\*, Adv. Energy Mater. 2023, 13: 2301948.
- [3] M. Sun, H. H. Wong, T. Wu, Q. Lu, L. Lu, C. H. Chan, B. Chen, A. W. Dougherty, B. Huang\*, *Adv. Energy Mater.* **2023**, **13**: 2203858.
- [4] M. Sun, H. H. Wong, T. Wu, A. W. Dougherty, B. Huang\*, Adv. Energy Mater. 2022, 12: 2103781.
- [5] M. Sun, H. H. Wong, T. Wu, A. W. Dougherty, B. Huang\*, Adv. Energy Mater. 2021, 11: 2101404.
- [6] M. Sun, T. Wu, A. W. Dougherty, M. Lam, B. Huang\*, Y. Li, C. -H. Yan, Adv. Energy Mater. 2021, 11: 2003796.
- [7] M. Sun, A. W. Dougherty, B. Huang\*, Y. Li, C. -H. Yan, Adv. Energy Mater. 2020, 10: 1903949.

#### **Biography**



Dr. Bolong Huang has received his PhD in 2012 from the University of Cambridge, and his BSc in condensed matter physics from the Department of Physics, Peking University in 2007. Following systematic training periods of Post-doc at Peking University, and in Hong Kong, he started his independent research at the Hong Kong Polytechnic University in 2015. He is now the Associate Professor at the Department of Applied Biology and Chemical Technology and Director of the Research Centre for Carbon-Strategic Catalysis. His main research fields are electronic structures of nanomaterials, energy materials, solid functional materials, and rare earth materials, as well as their applications in multi-scale energy conversion and supply systems. Dr. Huang has published 309 research papers in peer-reviewed international

journals with 260 papers as the corresponding author/first author/co-first author including *Nature, Science, Chem. Soc. Rev., Energy Environ. Sci., Sci. Adv. J. Am. Chem. Soc., Angew. Chem. Int. Ed., Nat. Commun., Adv. Mater., Adv. Energy Mater., Chem (Cell)*, etc., and has received citations over 22000 times with an h-index of 80. He has been recognized as 2022-2023 Highly Cited Researcher by Clarivate Analytics and 2022-2023 World's Top 2% Most-Cited Scientists by Stanford University.