Special Session: Advances in Fuel Cells

Session Description:

Climate change mitigation and environmental issues require developing a new sustainable energy solution. As an energy conversion device that converts the chemical energy of fuels and oxidants directly into electricity, fuel cells are widely accepted as promising substitutes for the present non-renewable energy system due to their high energy efficiency, zero-emission capability, high reliability, and low noise operation. To further improve fuel cell performance, various advanced electrocatalysts, materials, and systems have been under intensive research and development. This special session will focus on the latest development for fuel cells, ranging from fundamental materials to hydrogen evolution, oxygen reduction reaction (ORR) catalysts, and real lifetime evaluation of fuel cell power systems.

Session Organizers:

Yunqi Li (Beihang University)   Jing Tang (East China Normal University)

Session Contents:

Topic 1: Materials Space-Tectonics: A Conceptual Paradigm for Creating Second-Generation Porous Materials

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Abstract

Different types of inorganic nanomaterials have been designed using various methods, including sol-gel, electrochemical/chemical reduction, calcination, hydrothermal reaction, etc. The dimensionality of these nanomaterials (x, y, z) can be classified as zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), or three-dimensional (3D), respectively. Accordingly, for 0D nanomaterials, dimensions are measured on the nanoscale (< 100 nm for each dimension). 0D nanomaterials, for example, nanoparticles (or sometimes nanocrystals), most commonly have isotropic morphologies where the usually thermodynamically stable planes of lower reactivity are exposed at the nanoparticles' surfaces. For 1D nanomaterials, a single dimension is extended beyond the nanoscale. This class of nanomaterials includes nanotubes, nanorods, and nanowires.

In contrast to 0D and 1D nanomaterials, 2D nanomaterials have recently attracted great interest for the next generation. However, such 2D materials are often formed by stacking/assembly, processes that vastly reduce their active surface areas and negatively affect their performance in potential applications. Despite recent and significant advances in inorganic nanomaterials of different dimensionalities, we remain active in making substantial efforts to develop new nanomaterials to help address energy- and environmental-related issues. Our group is fully aware of the serious limitations of the currently available materials' designs. The continued use of the current nanomaterials design paradigm based on traditional 0D, 1D, 2D nanomaterials obscures the innovative approaches required to address the aforementioned serious issues. Therefore, we have developed a new conceptual paradigm "materials space-tectonics" which is defined as the creation of novel mesoporous/nanoporous materials with precisely controlled internal space (or pore size), composition, and morphology with the assistance of nanomaterials informatics to optimize their functional applications (Figure 1).

The overarching aims are to:

- <u>Control and enhance the "space-tectonics" of conductive nanoporous materials (carbons, metals, sulfides, phosphides, *etc.*):</u> (i) large increase in accessible surface area, (ii) selection of exposed crystal facets (*e.g.*, facet selection, chirality), (iii) generation of catalytically ultra-active sites on kinks and step sites (*e.g.*, high index facets), and (iv) increased diffusion rates of guest molecules (reactants) inside the components, especially in the case of 2D materials.

- <u>Connect nanoporous components in hybrid nanoarchitectures:</u> development of methodologies for the hybridization of novel nanoporous conductive materials with precisely controlled building blocks (like Lego®) for hybrid architectures to bring out many advantages beyond what is currently known, such as (i) unlimited increases in the interface between different components (e.g., hetero-junctions, charge-separation), (ii) maintaining high diffusion rates of guest molecules (reactants) inside the hybrid materials through the introduction of multiple and hierarchical pore structures, and (iii) formation of gradient potential energy or polarization within assembled materials (e.g., one-directional electron/energy transfer, light-harvesting, up-conversion, multi-electron reduction).

- <u>Combine "machine learning (MI)" with inorganic synthetic techniques:</u> this will accelerate the optimization of synthetic parameters for target nanomaterial design and enable selection of the optimal combinations of parameters for each inorganic building block for effective integration of the materials.

Increasing demand for sustainable energy and environmental remediation has accelerated research of various technologies, such as energy storage and conversion (*e.g.*, fuel cells, water splitting, secondary battery). These technologies rely heavily on the catalyst (or electrode) materials, which can significantly increase the efficiency of chemical reactions by reducing their activation energy or by modulation of the reaction mechanism. Although traditional porous materials (including mesoporous silicas, zeolites and coordination polymers) have been extensively studied, the poor electrical conductivity of those materials has restricted their utilization in future potential applications, *esp.* electrochemical-based applications. Therefore, our main target is to establish a platform for the synthesis of the second generation of highly conductive materials. We strongly believe that our new synthetic concept of "second-generation porous materials" can be considered to have significant potentials for the further development of secondary battery electrodes, (electro)catalysts, optical or electronic sensors, *etc.* Today, we will present several important examples from our on-going projects.
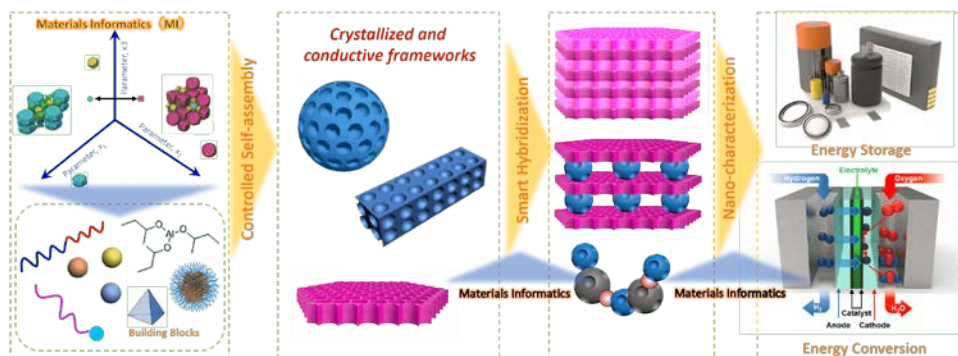

Fig. 1. Concept of "materials space-tectonics" for achieving precise control of the design

of conductive nanoporous materials towards energy and environmental applications.

Prof. **Yusuke Yamauchi** received his Bachelor's degree (2003), Master's degree (2004), and Ph.D. degree (2007) from the Waseda University, Japan. After receiving his Ph.D., he joined the National Institute of Materials Science (NIMS), Japan, to start his own research group. At the same time, he started to serve as an adjunct professor to supervise Ph.D. students at the Department of Nanoscience and Nanoengineering, Waseda University. After being granted the ARC Future Fellowship, in May 2016, he joined the Institute for Superconducting & Electronic Materials (ISEM), the Australian Institute for Innovative Materials (AIIM), the University of Wollongong (UOW) as a Professor. In 2018, he moved to the University of Queensland (UQ). Presently, he is a Senior Group Leader at the Australian Institute for Bioengineering and Nanotechnology (AIBN) (on secondment from the School of Chemical Engineering until 2026), a Professor at the School of Chemical Engineering, and a Director at the Australian Materials nanoTectonic Centre. He concurrently serves as an ERATO Research Director at the JST-ERATO Yamauchi Materials Space-Tectonics, a Group Leader at the Mesoscale Materials Chemistry Group, the International Center for Materials Nanoarchitectonics (WPI-MANA), the National Institute for Materials Science (NIMS), a Visiting Professor at the Waseda University, an Advisory Board Member of prestigious journals (Small, Small Structures, ChemCatChem, J. Inorg. Organomet. Polym. Mater., etc.), and an Associate Editor of the Journal of Materials Chemistry A published by the Royal Society of Chemistry (RSC) and Chemical Engineering Journal (Elsevier).

He has published more than 850 papers in international refereed journals (>10 Nature's and Science's sister journals, >20 J Am Chem Soc, >10 ACS Nano, >10 Chem Sci, >30 Angew Chem Int Ed, >25 Chem Mater, >10 Mater Hor, etc.) with > 50,000 citations (h-index > 115, Google Scholar; h-index > 100 Web-of-Science). **He is selected as one of the Highly-Cited Researchers in Chemistry in 2016, 2017, 2018, 2019, and 2020 and in Materials Science in 2020.** He has received many outstanding awards, such as the NISTEP Award by the National Institute of Science and Technology Policy (2016), the Chemical Society of Japan (CSJ) Award for Young Chemists (2014), the Young Scientists' Prize of the Commendation for Science and Technology by MEXT (2013), the PCCP Prize by the Royal Society of Chemistry (2013), the Tsukuba Encouragement Prize (2012), the Ceramic Society of Japan (CerSJ) Award (2010), and the Inoue Research Award for Young Scientists (2010). **Recently, he was selected as one of Australia's Top 40 Researchers of Research Report published by The Australian in 2019 and 2020.**

Topic 2: Application of Carbon-Metal Hybrid Electrocatalyst in Hydrogen Evolution

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Abstract

As a new energy with high energy density and environmental protection, hydrogen energy is regarded as the most potential renewable clean energy carrier. Hydrogen production from electrolyzed water is an important way to obtain high purity hydrogen and realize the effective storage of intermittent renewable energy such as solar energy and wind energy. However, the activity, stability and cost of the catalyst have become one of the bottlenecks restricting its development.

In this report, we will introduce three strategies for the construction of high-efficiency carbon-metal hybrid materials for the hydrogen evolution reaction (HER). 1. We propose a facile anisotropic surface modification and etching strategy for the synthesis of hollow structured ZIF-67 nanoframes. Our strategy relies on the structural and compositional distinctions between each crystallographic facet of truncated rhombic dodecahedrons ZIF-67 (tZIF-67 RDs) and the moderate coordinating and etching effects of cyanuric acid (CA). 2. Inspired by binary cooperative complementary materials in nature, we successfully apply redox units of polyaniline (PAni) to cooperatively in situ assemble Ru nanoclusters in a hierarchically-ordered carbon electrode. 3. We develop a new class of Co-C-N complex bonded carbon for HER with self-supported and three-dimensional porous structure, which shows an unexpected catalytic activity with low overpotential and long-term stability.

Keywords: hydrogen energy; water electrolysis; HER catalysts

Dr. **Zhong-Li Wang** received his Ph.D. degree from Changchun Institute of Applied Chemistry (CIAC), Chinese academy of Science (CAS) in 2010. After graduation, he worked as an assistant professor at CIAC. He became an associate professor in 2012 at CIAC. In 2015, he joined Prof. Yusuke Yamauchi's group as JSPS international research fellow in NIMS, Japan. Currently he is a full Professor at School of Chemical Engineering and Technology, Tianjin University. His research interests are advanced carbon and inorganic functional materials for electrochemical energy storage and conversion.He has published over 60 peer-reviewed journal papers (23 of them are ESI hot papers) with more than 9000 citations (Google Scholar, H-Index 37).

Topic 3: Electrosynthesis promoted hydrogen evolution/hydrogenation reaction

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Abstract

Oxygen evolution reaction (OER), the anodic reaction of both electrocatalytic water splitting and hydrogenation reaction, is a kinetically slow process which needs large overpotential to drive and results in much increased energy consumptions. Moreover, the produced oxygen can be obtained from the air, therefore is of poor value. Additionally, the produced oxygen will not only lead to the possible formation of degradable reactive oxygen species but also may be mixed with hydrogen produced at the cathode, implying the potential explosion risk. Here, the coupling of electrosynthesis by biomass electrooxidation with hydrogen evolution/CO_2 hydrogenation reaction have been advocated, in which OER is replaced by kinetically favorable biomass oxidation reactions. Thus, not only the energy consumption can be lowered, but also hydrogen/CO_2 reduction products and high value biomass oxidation products can be obtained concurrently.

Keywords: electrosynthesis; hydrogen evolution; CO_2 hydrogenation reaction

Dr. Lisong Chen received his Ph.D. degree in Materials Physics and Chemistry under the supervision of Prof. Jianlin Shi from Shanghai Institute of Ceramics, Chinese Academy of Sciences (SICCAS) in 2016, Since then he joined East China Normal University (ECNU). Currently he is an associate professor at School of Chemistry and Molecular Engineering, East China Normal University, China. He has published over 40 papers in peer-reviewed journals, including Nature Communications, Angewandte Chemie International Edition et.al. His research interest is focused on the System design and catalysts development for efficient hydrogen electrocatalysis, including hydrogen evolution and hydrogen oxidation reactions.

Topic 4: Transient Performance Loss of Pt/C Fuel Cell Catalyst Hindering High Efficiency Operation

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Abstract

The continuous decay of Pt/C ORR catalyst, commonly referred as "transient performance loss", is studied at 0.8 V by chronoamperometry under membrane electrode assembly (MEA) testing conditions. Based on the results from the time-resolved cyclic voltammetry (CV), surface oxidation was identified as the primary cause of the transient loss at small time scales. The reduction of surface oxide was observed to occur at 0.6 V, and the recovery of cathode performance can hence be achieved at equal or lower potentials. In addition, the effect of operating temperature and cathode humidity was also studied. The coverage of Pt surface oxides and the extent of the transient loss both were significantly reduced as temperature decreased. The benefit of a lower operating temperature however came with the cost of slower recovery kinetics. In terms of the impact of humidity, the presence of liquid water was identified to be the critical factor leading to much severer performance loss over time.

Keywords: Fuel Cell Catalyst, Transient Performance Loss, Recovery
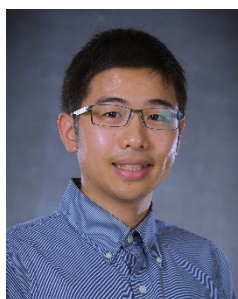
Dr. **Yung-Tin (Frank) Pan** is an assistant professor at the Department of Chemical Engineering, National Tsing Hua University (NTHU). He received his PhD. degree in Chemical Engineering from the University of Illinois Urbana-Champaign, USA. Before joining NTHU Chemical Engineering, he worked as a postdoc researcher at Los Alamos National Laboratory and is the major contributor to the US-DOE 2019 Annual Merit Review Awards wining project in Fuel Cell R&D. He started off his profession career at NTHU by receiving the Young Scholar Award from the Ministry of Science and Technology of Taiwan, and has been granted research funds from Industrial Technology Research Institute (ITRI) and industrial sources. His current research focus lies in the development of active and durable catalyst materials for polymer electrolyte membrane (PEM) reaction systems such as fuel cell (PEMFC), water electrolysis (PEMWE), and other gas phase electrochemical reactions.

Topic 5: Lifetime Evaluation Methods for Vehicle Fuel Cells and Analysis of Key Influencing Factors

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Abstract

Lifetime is one of the key factors that restrict commercialization of vehicle fuel cell. It is of great significance to study the lifetime evaluation methods and the key influencing factors of lifetime under different application scenarios of fuel cells for promoting the wide application of vehicle fuel cells. When the fuel cell is used as a fixed power source, its lifetime can reach 30000~50000 hours, while when it is used as a vehicle power source, its lifetime is only about 10000 hours. The frequent load change is the main reason that leads to its lifetime attenuation. In this report, we present the recent research results on the lifetime evaluation methods for vehicle fuel cells, and the judgement of internal state of fuel cells based on the internal gas and liquid transfer process and mechanism.

Keywords: Proton Exchange Membrane Fuel Cells, lifetime evaluation, internal gas and liquid transfer, gas starvation

Dr. **Huicui Chen** received her PhD degree from School of Vehicle and Mobility, Tsinghua University in July 2015 and joined School of Automotive Studies, Tongji University as an assistant professor in the same year. She has been devoted to the research on the core technologies of vehicle fuel cell engines, including the degradation mechanism of vehicle fuel cell dynamic process, fuel cell durability evaluation method and high-durability vehicle fuel cell control strategy, etc. She has presided over several major scientific research projects such as the National Key Research and Development Program and Project supported by the National Natural Science Foundation of China. In the past five years, she has published 23 SCI/EI papers, including 17 SCI papers, 4 ESI highly cited papers Top 1%, and 2 papers won the Applied Energy 2018 highly cited research paper award. She won the Science and Technology Special Award of China Transport Association in 2020 and was selected in the Sailing Program of Shanghai Youth Science and Technology Talents in 2018.

Topic 6: Graphene Nanomesh as An Effect Electrocatalysts for Oxygen Reduction in Acid Media

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Abstract

Two-dimensional (2D) materials usually exhibit extraordinary performance in lots of applications. Although graphene nanomesh is quite attractive as a member of 2D carbon materials, general synthetic routes to produce functional graphene nanomesh on a large scale are complex and tedious. Here, we elaborately design a simple two-step dimensional reduction strategy for exploring nitrogen-doped graphene nanomesh by thermal exfoliation of crystal- and shape-modified metal-organic frameworks (MOFs).

MOF nanoleaves with 2D rather than 3D crystal structure are used as the precursor, further thermally unraveled into nitrogen-doped graphene nanomesh by using metal chlorides as the exfoliators and etching agent. The prepared nitrogen-doped graphene nanomesh shows a unique ultrathin two-dimensional morphology, high porosity, rich and accessible nitrogen-doped active sites, and defective graphene edges, contributing to an unprecedented catalytic activity for oxygen reduction reaction (ORR) in acid electrolytes. This approach is suitable for scalable production and is probably universal for the synthesis of thousands of novel low-dimensional functional carbon materials by breaking the dimensional limitation of traditional three-dimensional MOFs and further executing thermal exfoliation.

Keywords: two-dimensional (2D); graphene nanomesh; ORR; exfoliation

Dr. **Wei Xia** received his Ph.D. degree in Materials Chemistry from the Nanjing University of Aeronautics and Astronautics in 2020. Currently, he is a postdoctoral researcher at East China Normal University. In 2019, he worked at National Institute for Materials Science (NIMS), Japan as a visiting scholar and made contributions in the areas of fuel cells, Metal-air batteries, electrocatalysis and computational modeling. He has published over 40 peer-reviewed journal papers (2 of them are ESI hot papers), as well as the reviewer for more than 10 international academic journals.