

**Special Session:** Electrolysis process and Membrane transport

**Session Description:**

The electrolysis process has a good application prospect in power generation, hydrogen production, water treatment and even air dehumidification, especially when high-performance membranes are used. This technology is also suitable for using renewable energy sources such as solar or biomass energy. The transport phenomena (heat, mass, momentum and energy transport) at different scales from molecular to macros determines the electrolysis performance and energy efficiency. This session aims to look for the research related to the modeling, material development and performance improvement of electrolysis or photocatalytic process, with priority given to research that occurs in membranes. Topics include, but are not limited to, multiscale modeling of transport phenomena, numerical simulation, system thermodynamics, transport enhancement, system optimization and energy utilization improvements.

**Session Organizers:**

**Professor Ronghui Qi** received her Ph. D degree in 2013, and was appointed as postdoctoral in 2013-2016 from the Hong Kong Polytechnic University. She joined the South China University of Technology in 2016 and was promoted to the professor on Sep, 2019. Prof. Qi's main research interests are advanced air dehumidification technologies (e.g. electrolytic and desiccant absorption/adsorption dehumidifiers), heat&mass transfer enhancement mechanism and solar energy utilization. As the first or corresponding author, she has published more than 60 international peer-reviewed papers, including 40 SCI papers. She has received the Distinguished Young Scholar from National Natural Science Foundation. She has in the editorial board of <International Journal of Green Energy>, used to be a guest editor of <Heat Transfer Engineering> and <Polymers>.



**Professor Chuanshuai Dong** received his Ph. D. from the Department of Building Environment and Energy Engineering, the Hong Kong Polytechnic University, Hong Kong, China. He is currently an Associate Professor in South China University of Technology. Dr. Dong's research focuses on the basic heat/mass transfer of phase change materials and multiphase flows. He has developed several constitutive equations for multiphase flow analysis. Dr. Dong has also authored more than 30 SCI journal papers in well-known journals, such as Physics of Fluids, Energy, and International Journal of Multiphase Flow, etc. As PI, Dr. Dong has presided over several research projects supported by National Natural Science Foundation, National Natural Science Foundation of Guangdong, and China Postdoctoral Science Foundation, etc.



## Stable and high-performance microgenerator formed by TiO<sub>2</sub>/Co-based hydrogel films utilizing ambient air humidity

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### Abstract:

Utilizing humidity gradients to drive electron motion in nanomaterials and generate usable electricity is promising especially for self-powered electronics and sensors. In this paper, a novel humidity gradient-driven microgenerator (HGMG) was developed that employs TiO<sub>2</sub> nanoparticles coated with Co hygroscopic hydrogel films. The prepared TiO<sub>2</sub> slurry was scraped on a hydrophilic frosted polyethylene (PET) membrane to form the power layer rich in nanochannels, and Co hydrogels were coated on the bottom of the generator to form the stable humidity gradient. SEM, FTIR, Raman, XRD and XPS spectra have been conducted for physical and chemical characterizations. Results showed that by putting in a 25°C, 60% room environment, a single unit of generator can achieve a 0.95 V of the open-circuit voltage and 60 μA of short-circuit current, i.e. 5.78 μW/cm<sup>2</sup>, a significantly improvement compared to previous studies (<1 μA on a single unit). The performance can maintain stable with less than 5% attenuation over 100 hours. Besides, these microgenerators are suitable for use in series, 5 of them can power a calculator, and 7 of them can light an LED for more than a week. The mechanism of humidity gradient-induced power generation was analyzed by numerical simulation. It was found that the hygroscopic hydrogel within the nanomaterial channels can absorb moisture from the air, leading to the separation of positive and negative ions due to the combined effect of electric double layer. Since only a small part of positive ions could move to the upper electrode, the concentration of positive and negative ions across the electrodes were polarized, creating an electrical current in microgenerators. This work provides a brand-new power generation method that can utilize ambient air humidity and have a great application prospect.

### Short bio:

Professor Ronghui Qi received her Ph. D degree in 2013, and was appointed as postdoctoral in 2013-2016 from the Hong Kong Polytechnic University. She joined the South China University of Technology in 2016 and was promoted to the professor on Sep, 2019. Prof. Qi's main research interests are advanced air dehumidification technologies (e.g. electrolytic and desiccant absorption/adsorption dehumidifiers), heat&mass transfer enhancement mechanism and solar energy utilization. As the first or corresponding author, she has published more than 60 international peer-reviewed papers, including 40 SCI papers. She has received the Distinguished Young Scholar from National Natural Science Foundation. She has in the editorial board of <International Journal of Green Energy>, used to be a guest editor of <Heat Transfer Engineering> and <Polymers>.



## Performance intensification and anti-fouling of the two-phase flow enhanced direct contact membrane distillation for seawater desalination

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### Abstract:

Membrane distillation is a promising approach to the fresh water crisis due to the low operating temperature and pressure, and high rejection of non-volatile components. However, it suffers a lot from the polarization effect and membrane fouling, especially in the membrane distillation of high-salinity sea water or waste water. Thus, this paper aims at developing a novel two-phase flow enhanced direct contact membrane distillation (TP-DCMD) system and investigating the effect of two-phase flow behaviors on the heat and mass transfer and membrane fouling comprehensively. First, a novel experimental system of TP-DCMD is developed and well validated using the mass and energy conservations between the hot feed liquid and cold permeate liquid. Then, the effect of flow parameters, such as the superficial gas and liquid velocities, and void fraction on the transmembrane permeate flux and permeate flux multiplier are discussed. The results clearly indicate that the introduction of gas could effectively improve the membrane distillation performance as high as 27 % by increasing the flow turbulence. Third, the relationship between the performance enhancement of the membrane distillation and the two-phase flow regimes is discussed in detail. Both permeate flux and multiplier clouds are proposed based on the two-phase flow regime map. The slug flow demonstrates superior enhancing effect to the other flow regimes due to the low possibility of gas penetration and high flow turbulence of the liquid. Finally, the effect of two-phase flows on the membrane fouling is investigated. The two-phase flow demonstrates excellent anti-fouling effect in the DCMD system, especially in the treatment of high-salinity sea water or waste water. After 420 minutes of accelerating fouling test, the transmembrane permeate flux dropped by 38.2 % in the conventional DCMD system, while it just decreases by 6.6 % in the two-phase flow enhanced DCMD system.

### Short bio:

Professor Chuanshuai Dong received his Ph. D. from the Department of Building Environment and Energy Engineering, the Hong Kong Polytechnic University, Hong Kong, China. He is currently an Associate Professor in South China University of Technology. Dr. Dong's research focuses on the basic heat/mass transfer of phase change materials and multiphase flows. He has developed several constitutive equations for multiphase flow analysis. Dr. Dong has also authored more than 30 SCI journal papers in well-known journals, such as *Physics of Fluids*, *Energy*, and *International Journal of Multiphase Flow*, etc. As PI, Dr. Dong has presided over several research projects supported by National Natural Science Foundation, National Natural Science Foundation of Guangdong, and China Postdoctoral Science Foundation, etc.



## Developing novel multifunctional electrodes for high-efficient water splitting

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### Abstract

Sustainable energy resources, including solar, wind, and tide etc., generate electricity intermittently, which lead to the challenges to supply continuous power to the current electrical grid. Therefore, a high-efficiency and robust electrochemical energy storage or conversion system coupled with the sustainable energy resources to accommodate seasonal, daily or even hourly changes becomes critical. Proton exchange membrane electrolyzer cells (PEMECs), which act as a reverse proton exchange membrane fuel cell, have been regarded as a very promising energy storage method for hydrogen production from water splitting. To reduce the loading and improve the utilization rate of the noble metal electrocatalysts for oxygen evolution reaction (OER), several methodologies have been proposed and demonstrated. In this study, iridium (Ir) catalysts are proposed on novel titanium thin/tunable liquid/gas diffusion layers (TT-LGDLs) for serving as anode gas diffusion electrodes (GDEs) in high-efficiency PEMECs or Ir-based catalyst is deposited onto Nafion membrane to form a patterned electrode. Our previous studies revealed that the triple-phase boundary significantly affects the OER sites on catalyst layer in a PEMEC, and there is a large portion of catalysts is not effectively utilized. Therefore, a novel thin/tunable GDE is developed by depositing the catalyst on a tunable pattern that is observed to be active for the OER. The Ir loadings of the novel thin GDEs are varied from 0.027 to 1.307 mg/cm<sup>2</sup>, and their *in-situ* electrochemical properties are comprehensively investigated in a PEMEC. The PEMEC performance and efficiency can be improved with higher Ir loading, while the Ir catalyst mass activity increases for the sputter deposited GDEs and decreases for the electroplated GDEs with higher Ir loading. An electroplated GDE with lower Ir loading of only 0.208 mg/cm<sup>2</sup> exhibits a high Ir mass activity of about 2.602 A/mg at 1.6 V. The stability of the GDEs is also examined and analyzed, and the lowest degradation rate that has been obtained is about 24.4  $\mu$ V/h. The novel thin GDEs and the novel patterned electrode can remarkably improve the catalyst mass activity with an acceptable PEMEC performance by improving the catalyst efficiency with a very simple fabrication process and low cost. In addition, the novel thin GDEs significantly reduce thickness from hundreds of micrometers to only 25 $\mu$ m. This concept shows promise for the future electrodes development in low temperature and high efficiency PEMECs, which will help to greatly reduce the cost, thickness, and weight of the electrode itself and the system as a whole.

**Keywords:** water splitting, hydrogen production, catalyst mass activity, OER, HER

### Short bio:

Zhenye Kang is currently a full professor in School of Chemical Engineering and Technology at Hainan University, China. He received his Ph.D. from The University of Tennessee, Knoxville (UTK), U.S. at 2018 (Supervisor: Dr. Feng-Yuan Zhang), and did his postdoc at National Renewable Energy Laboratory (NREL) U.S. from 2018-2021 (Supervisor: Dr. Guido Bender). He joined Hainan University as an associate professor since Apr. 2021 and has been promoted to professor position in Oct. 2021. His research is focused on hydrogen production, water electrolysis technology and application, micro/nano-scale fluidics and heat transfer, additive manufacturing, novel multifunctional materials, and micro/nano electro-mechanical systems. He has published more than 40 papers in high impact journals, including Energy & Environmental Science, Science Advances, Nano Energy, Applied Energy, etc. He has joined several projects from Department of Energy (DOE), U.S., and has received research grants from National Natural Science Foundation of China, Hainan Province Science and Technology Special Fund, Start-up Research Foundation of Hainan University.



## Exploiting MnO<sub>2</sub> -based Bifunctional Oxygen Catalytic Electrode with Tailored Catalytic Activity for Rechargeable Zn-Air Batteries

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### Abstract

Metal-air batteries, as highly effective clean energy devices, play an important role in current sustainability development. Zn-air batteries are of great interest in future power devices due to eco-friendly, superior safety, cheap and high theoretical energy density. Currently, it remains a significant challenge to exploit low-cost, high-efficient and strong durability bifunctional catalysts to boost the various reactions for Zn-air batteries. 2x2 tunnels  $\alpha$ -MnO<sub>2</sub> as classic electro-catalyst with unique orthorhombic unit cell structure shows higher oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) activity than other-phase MnO<sub>2</sub>. In this work, a bifunctional oxygen catalytic self-supported MnO<sub>2</sub>-based electrode is well designed, which displays superior oxygen reduction/evolution reactions (ORR/OER) performance ( $\Delta E = E_{(j=10)} - E_{1/2}$ : 0.69V) over noble metal electrodes. In addition, the as-synthesized NiCo<sub>2</sub>O<sub>4</sub>@MnO<sub>2</sub>/CNTs-Ni foam self-supported electrode can be directly used as the oxygen electrode without externally added carbon or binder and shows decent battery performances with high peak power density of 226 mW cm<sup>-2</sup> and long-term charge-discharge cycling lifetime (5mA for 160h). As expected, the quickly oxygen catalytic intrinsic kinetics and high battery performances of NiCo<sub>2</sub>O<sub>4</sub>@MnO<sub>2</sub>/CNTs-Ni foam electrode should be originated from the following points: i) the unique 3D hierarchical structure effectively promotes mass transfer; ii) CNTs combined with Ni foam form a unique "meridian" conductive structure that enables rapid electron conduction; iii) the abundant Mn<sup>3+</sup> active sites activated by bimetallic ions shorten oxygen catalytic reactions distance between the active sites and reactant, and reduce the surface activity of MnO<sub>2</sub> for O, OH, and OOH species. This work provides an effective method to achieve MnO<sub>2</sub>/CNTs materials with tailored catalytic activity by anchoring different metal oxides, and reveals great potential in the field of high specific energy batteries for portable electronics, electrical vehicles, and wearable devices.

**Keywords:** Zinc-air battery; Bimetallic activation, Self-supported electrode, Heterojunction, Hierarchical structure

### Short bio:

Dr. Nengneng Xu received his PhD degree from Donghua University. From July 2019 to July 2021, Dr. Xu worked as a postdoctoral fellow and then assistant professor in University of Louisiana at Lafayette. Now, Nengneng Xu is an Associate Professor of the College of Environmental Science and Engineering, Donghua University, China. His current research focuses on the development of nanostructured catalysts for rechargeable metal-air batteries, methane oxidation and solid oxide fuel cells.



## Constructing optimal Triple-Phase Boundaries for an efficient water electrolysis system

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### Abstract

Most renewable energy is a type of process energy which should be converted and stored with an energy carrier. Water splitting is a process that combined energy conversion and mass transformation. The chemical reaction that occurs at the triple-phase boundary is influenced by many factors such as mass flow and exchange rate, electric potential and surface chemical properties. Reducing mass-transport resistance is crucial for improving performance of water electrolysis. In a PEM electrolyzer, a porous transport layer (PTL) is required to ensure efficient the gas/water transport and the electric charges transfer. As the direction of water and gas transfer in a PEM electrolyzer is opposite, favorable mass transport channels for both water and gas are essential. A micron scale water/gas dual-channel porous transport electrode was designed which can greatly reduce mass transfer losses. For an efficient energy conversion in the triple-phase boundary, durable electrocatalysts for hydrogen and oxygen evolution reactions is also a major challenge. We developed a novel hybrid nanostructure with RuCo nanoparticles (NPs) embedded in a N doped carbon nanotube with hollow polyhedron structure. The optimized Ru@Co-N/C show attractive OER and HER activities higher than that of commercial RuO<sub>2</sub> || Pt/C. We also investigated the effect of metal and non-metal substitution in NiFe-based catalysts on the reaction at the three-phase boundary. The incorporation of high-valence cations into NiFe improves the adsorption capacity with active intermediates in the liquid phase, inhibit the transformation of active phase  $\beta$ -NiOOH to inactive phase  $\gamma$ -NiOOH, and thus improve the activity for water oxidation.

**Keywords:** PEM electrolysis; Triple-Phase Boundaries; Mass transfer; Electrocatalysts.

### Short bio:

Dr. Jinzhan Su is currently a professor in Xi'an Jiaotong University. He received his BSc degree in Physics (2005) and Ph.D. degree in Thermal Engineering (2011) at Xi'an Jiaotong University. From Oct. 2008 to Sep. 2010, he worked as a visiting scholar in the Pennsylvania State University, PA, United States. His current research focuses on photoelectrochemical/photoelectrolysis and mass flow properties of catalyst/electrolyte interface and its charge transfer kinetics for the application of fuel cell and water electrolysis. He has published about 90 papers in SCI-indexed internationally peer review journals with more than 3800 citations.



## The kinetics regulation of photo-generated carriers in g-C<sub>3</sub>N<sub>4</sub> by bulk/surface engineering towards high-efficiency photocatalytic H<sub>2</sub> production

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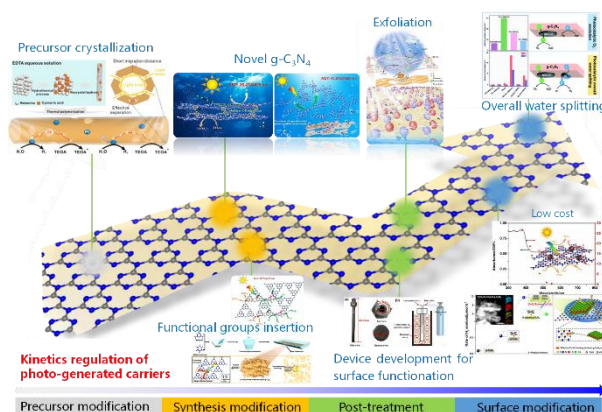
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### Abstract

Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) has been extensively studied as a metal-free and visible-light-responsive photocatalyst in the realm of solar catalysis for H<sub>2</sub> production. The unique merits of low cost, good physicochemical stability, regulable electronic band structure and non-toxicity make g-C<sub>3</sub>N<sub>4</sub> have significant advantages for the potential industrial application. However, it still remains great challenge to achieve critical breakthrough in H<sub>2</sub>-production efficiency due to the low utilization of photo-generated carriers in g-C<sub>3</sub>N<sub>4</sub>. Herein, we make a summary of our previous works about the bulk/surface engineering of g-C<sub>3</sub>N<sub>4</sub> to adjust the kinetics of photo-generated carriers for promoting photocatalytic H<sub>2</sub> production, including precursor recrystallization, functional groups insertion, novel g-C<sub>3</sub>N<sub>4</sub> development, nanosheets exfoliation designation, device development for surface functionalization, surface reactive sites adjustment towards low-cost photocatalysis and overall water splitting. We demonstrate a series of research strategies and theories in the understanding of the structure-carriers-photocatalysis relationship of g-C<sub>3</sub>N<sub>4</sub>, which could provide a meaningful reference for developing highly efficient g-C<sub>3</sub>N<sub>4</sub> photocatalytic systems towards solar energy conversion and industrial application.

**Keywords:** Graphitic carbon nitride; Hydrogen; Photo-generated carriers; Photocatalysis; Water splitting



### Short bio:

Dr. Jinwen Shi is currently an associate professor at Xi'an Jiaotong University. His research interest is focused on conversion and utilization of renewable energies, new energy materials, and photocatalysis, especially the development of novel photocatalysts and photocatalytic systems for water splitting under visible-light irradiation. He has published over 100 SCI-indexed papers in international journals and was granted over 10 China invention patents.



## Sustainable Fuel Production from Ambient Moisture via Semiconductors: Solar-Driven Catalysis System

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### Abstract

The major drawbacks associated with the state-of-the-art electrocatalytic and photoelectrochemical water-splitting systems reported so far are the requirement for huge volumes of liquid electrolyte (sea or wastewater) and electrical energy that is required to do water splitting. Continuous research is being carried out with a view of reducing the amount of energy required for achieving overall and complete water splitting process. Here, we have realized a special set of hybrids  $\text{BaTiO}_3@Cu_2O$ ,  $\text{BaTiO}_3@BiVO_4$ , and  $\text{BaTiO}_3@MoS_2$  that can perform efficient water oxidation and reduction, respectively. Combining them with an in-house developed and versatile super-hygroscopic hydrogel that harvests enormous amounts of moisture together, we have developed an artificial-photosynthetic system that absorbs the moisture from the ambient air and converts it into hydrogen and oxygen, thereby realizing two benefits – zero-energy dehumidification and energy/fuel (hydrogen) generation from ambient humid air. The application scenarios are low storey, tropics, moist places, and storage box, where a substantial amount of energy is being spent on air-conditioning to maintain thermal comfort. In lieu of this, we have proposed the atmospheric moisture splitting process to achieve maximum thermal comfort by reducing relative humidity and concurrently produce sustainable fuels at zero energy expense.

**Keywords:** humidity, hydrogel, semiconductor, moisture splitting, dehumidification

### Short bio:

Dr. YANG Lin is an associate professor at the Chongqing University, China. He received his Ph.D at this University in 2018 in Department of Physics. His research interests are Atmospheric water harvesting via super hygroscopic hydrogel, Water splitting via photo/electrocatalysis, and Photoelectrochemical interfacial mass transfer. At present, he has published over 40 research papers in Nat. Common., Joule, Adv. Mater., ACS Nano, Energy Environ. Sci., Nano Energy, et. al.

