# Investigation of heterogeneous molecular structure for

# electrocatalysis applications

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### Abstract

Molecular  $\text{Co}^{2+}$  ions were grafted onto doped graphene in a coordination environment, resulting in the formation of molecularly well-defined, highly active electrocatalytic sites at a heterogeneous interface for the oxygen evolution reaction (OER). The S dopants of graphene are suggested to be one of the binding sites and to be responsible for improving the intrinsic activity of the Co sites. The turnover frequency of such Co sites is greater than that of many Co-based nanostructures and IrO<sub>2</sub> catalysts. Through a series of carefully designed experiments, the pathway for the evolution of the Co cation-based molecular catalyst for the OER was further demonstrated on such a single Co-ion site for the first time. In another demonstration of molecular Ni<sup>2+</sup> based system, We found for the first time that the presence of Fe<sup>3+</sup> ions in the solution could bond at the vicinity of the Ni sites with a distance of 2.7 Å, generating molecularly sized and heterogeneous Ni-Fe sites anchored on doped graphene. These Ni-Fe sites exhibited drastically improved OER activity. It is revealed that the Ni-Fe sites adsorbed HO<sup>-</sup> ions with a bridge geometry, which facilitated the OER electrocatalysis.

## **Author CV**



Prof. Xin Wang received his Bachelor (1994) and Master (1997) degrees in Chemical Engineering from Zhejiang University, and Ph. D (2002) in Chemical Engineering from Hong Kong University of Science and Technology. From 2003 to 2005, he worked as a research fellow at University of California, Riverside, and concurrently, as R&D director for a startup fuel cell company. He joined Nanyang Technological University as assistant professor in 2005 and was promoted to associate professor with tenure in 2010

and full professor in 2016. He has been working on electrocatalysis and electrochemical technology for energy harvesting. His recent research focus includes 1) rational design of functional nanomaterials for electrocatalysis in energy and environmental applications such as fuel cells, CO<sub>2</sub> electro-reduction and water splitting, and 2) electrochemical reactor with cogeneration of electricity and valuable chemicals. He has published ~200 SCI papers with citations over 17000 (Web of Science) and H index of 65. He is a Fellow of Royal Society of Chemistry (FRSC) and Clarivate Analytics Highly Cited Researcher 2018 (Cross-field).

# A Design Strategy Towards Oxygen Electrocatalysts

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In this talk, I am going to summarize our recent progresses towards design of effcient oxygen electrocatalysts for various electrochemical energy conversion and storage applications. The design strategy includes: 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 B.Eng. (1st Class Honors) and M.Eng. degrees in Chemical Engineering from the National University of Singapore, and obtained his Ph.D. degree in Chemical Engineering from University of Minnesota in 2011. Thereafter, he moved to University of California, Berkeley and worked as a postdoctoral researcher in Department of Chemistry during 2011 - 2012 before joining School of Chemical and Biomedical Engineering at Nanyang Technological University as an Assistant Professor in 2012. He is now an Associate Professor at NTU. His main research interests are electrocatalysis, photovoltaics and photoelectrochemistry. information can be found More at http://www.ntu.edu.sg/home/liubin/home.html.



### Synthesis of Hollow Nanostructures for Electrochemical Energy Storage

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## Abstract:

Hollow nanostructures are promising as electrode materials for electrochemical energy storage, including lithium-ion batteries, supercapacitors and lithium-sulfur batteries. In this talk, I will briefly discuss the design, synthesis and electrochemical properties of hollow nanostructures of metal oxides/sulfides. Specifically, we have been able to synthesize different hollow nanostructures of many binary metal oxides such as SnO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub>, and many mixed transition metal oxides/sulfides such as NiCo<sub>2</sub>O<sub>4</sub> and NiCo<sub>2</sub>S<sub>4</sub>. We have also designed many hollow structures to fabricate advanced cathode materials for lithium-sulfur batteries.

#### **Biography**

Dr. David Lou received his B.Eng. (1st class honors) (2002) and M.Eng. (2004) degrees from the National University of Singapore. He obtained his Ph.D. degree in chemical engineering from Cornell University in 2008. Right after graduation, he joined Nanyang Technological University (NTU) as an Assistant Professor. He was promoted to Associate Professor since September 2013, and to Full Professor since September 2015. He is currently the Cheng Tsang Man Chair Professor in Energy. He has published about 310 papers with a total citation of >59,500 (ISI) or >68,000 (Google scholar), and an h-index of 147 (ISI)



and 156 (Google scholar) as of May 2019. Among which, 154 papers are ESI highly cited papers.

His main research interest is on designed synthesis of nanostructured materials for energy applications including batteries, electrocatalysis and photocatalysis. He was listed as a Highly Cited Researcher by Thomson Reuters/Clarivate Analytics for 5 years consecutively in 2014-2018.