Theoretically exploring feature-performance relationships of electrocatalysts for hydrogen production

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Abstract: The discovery of high-performance electrocatalysts, which is traditionally a crapshoot, holds a key for many Australian urgently needed clean energy applications, such as hydrogen production via water splitting. However, the industrial electrocatalysts for hydrogen evolution reactions (HERs) and oxygen evolution reactions (OERs) in water splitting devices often use expensive and scarce platinum group metal (PGM) based materials, e.g. Pt, RuO_2 and Ir/C. Therefore, the electrocatalysis for massive hydrogen productions faces high materials cost. Thus, it is of vital importance to discover low-cost high-performance materials to replace PGM based electrocatalysts. Stability, selectivity and activity are three of most essential parameters in evaluating overall performances of low-coast and earth-abundant electrocatalysts, which are largely dependent on their intrinsic features. To this end, the understanding of feature-performance relationships of electrocatalysts can greatly accelerate the discovery of novel high-performance materials for hydrogen production. Yet, the interplay of structural, chemical, and environmental degrees of freedom introduces a very high complexity to identify the accurate and holistic feature-performance relationships of electrocatalysts. In this talk, we will use some examples based on our recent first-principles computational results in combination with the experimental data to elucidate the feature-performance relationships of some electrocatalysts for HERs and OERs at the atomic level. Finally, we will show how to exploit such feature-performance relationship to rationally design novel materials and new chemical reaction processes, and guide the controllable synthesis of highly active electrocatalysts with desired features and improved performances.

Biographical Statement of speaker: Dr Yun Wang is a lecturer at Griffith University. His previous postdoctoral training was completed at the University of Texas at Austin in the USA, and the University of Sydney. He received his PhD degree from Fudan University. He also briefly worked at Shanghai Jiao Tong University, China. Dr Wang has published more than 90 refereed articles in high-impact journals including Nature and Nature Energy. His current h-index is 25. Dr Wang's research aims at the rational design of novel functional materials involving two green chemistry areas: heterogeneous catalysis and renewable energy. The outcomes will advance fundamental understanding of the operational principles for green chemistry technologies. The developed solid knowledge and insights will lead to improved device design to enable higher performance of functional materials.

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