Hydrogen electrocatalysis: from mechanistic study to advanced catalyst development

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My research interests are centered on addressing challenges in renewable energy research, and mainly focused on electrochemical energy storage and conversion applications such as electrolyzers, fuel cells, flow batteries, and electrochemical synthesis of high-value chemicals. I aim to bridge the fundamental understanding in electro-catalysis and surface science constructed on model electrode systems to the design and development of high-performance nano-scale materials and structures for clean energy applications.

One of the intriguing topics in renewable energy research is the utilization and generation of hydrogen energy. Hydrogen oxidation and reduction reactions (HOR/HER) are two of the key components in low-temperature fuel cells and electrolyzers. The pH values of the electrolytes have a great impact on the reaction kinetics such that the HOR/HER on the state-of-the-art Pt catalyst in alkaline media decreases by two orders of magnitude than that in acids. The slower HOR kinetics on Pt is projected to impose an additional overpotential (~130 mV at 1.5 A/cm^2_{MEA} with a Pt loading of 0.05 mg_{Pt}/cm^2_{MEA}) in alkaline or alkaline membrane fuel cells (AFCs/AMFCs), thus the use of Pt catalyst at the anode in AFCs/AMFCs requires a higher catalyst loading.[1, 2] With the development of many non-precious metal catalysts for the oxygen reduction reaction in both acid and alkaline electrolytes, showing comparable activity to Pt, the demand for highly active and cost-effective HOR catalyst in alkaline medium is arising and becomes one of the crucial challenges to make AFCs/AMFCs more practical.

Rational design of highly efficient HOR/HER catalysts requires identification of the reaction descriptor for the HOR/HER in alkaline electrolyte. It is shown that the HOR/HER exchange current density in alkaline media on a wide range of monometallic surfaces follows a volcano type of relationship with the calculated hydrogen binding energy (HBE) of the metals with Pt having the optimum HBE value.[3] This discovery indicates that HBE values can serve as the designing principle for developing efficient electrocatalysts for the HOR/HER in base. Motivated by this finding and the fact that Ni exhibits certain HOR/HER activity in base, we calculated the HBE of NiMo bi-metallic and CoNiMo multi-metallic surfaces and found that they have similar HBE values as Pt. We subsequently synthesized NiMo and CoNiMo alloys by electrodeposition and performed HOR/HER tests in 0.1 M KOH at different temperatures. The results show that the HOR/HER on CoNiMo outperforms electroplated Ni by 20 times.[4] At sufficient catalyst loading, this promising material will alleviate the catalyst cost issue raised by higher Pt loading in alkaline electrolytes, and will facilitate the development of the AFCs/AMFCs technology.

References:

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