University of Louisville
Department of Chemistry

Kinithi Wickramaratne

Literature Seminar

When: October 1, 2020
Time: 2:30 PM
Location: Microsoft TEAMS

Descriptors for Hydrogen Evolution Reaction Electrocatalysis

Abstract

The global energy crisis and adverse effects of climate change are driving forces for exploration of sustainable, renewable, and ecofriendly energy sources. Significant attention has been turned towards molecular hydrogen which has been considered as a clean fuel and one of the most promising energy sources. Electrochemical water splitting is presumed to be a sustainable process for large scale hydrogen production. Therefore, development of a sustainable catalyst that can lower the overpotential for hydrogen generation is important to improve the overall process. Noble metals such as platinum are considered the highly active electrocatalysts for hydrogen generation, but their prohibitive cost and low abundance have become a major obstacle that impedes the applications of hydrogen evolution reaction (HER). Thus, exploring stable, cost effective, and earth abundant electrode materials such as transition metals to replace noble metals have become an important goal. Identification of electrochemical parameters and understanding descriptors of HER are important to the development of highly active catalysts.[1] Hydrogen adsorption and desorption behavior on the catalyst is a major parameter to consider when designing efficient catalysts for HER via orbital modulation.[2] The d orbitals of the transition metals in the catalyst can be influenced by orbital modulation to enhance catalytic performance for HER. Investigating the role of the d band center (an indicator of hydrogen binding) provides a key to a rational catalyst design and thus tuning the position of the d band by varying surface compositional ratio of transition metals is beneficial when understanding catalytic properties of metal electrocatalysts.[3] Given that both water discharge and hydrogen adsorption free energy affect the activity of electrocatalysts for HER, it is critical to balance the adsorption of hydrogen and hydroxyl species.[4] Therefore surface reactivity of the catalyst can be optimized by doping different transition metals with favorable hydrogen adsorption energetics. The electrochemical parameters such as onset potential, Tafel slope, overpotential, and electrochemically active surface area can be optimized for enhanced electrocatalysts with better efficiency towards HER.[5]

References

1. Zhang, Q., et al. (2019). "Trends and descriptors of metal-modified transition metal carbides for hydrogen evolution in alkaline electrolyte." ACS Catalysis 9(3): 2415-2422

2. Li, F., et al. (2019). "Balancing hydrogen adsorption/desorption by orbital modulation for efficient hydrogen evolution catalysis." Nature communications 10(1): 1-7.

3. Wei, C., et al. (2020). "Surface Composition Dependent Ligand Effect in Tuning the Activity of Nickel–Copper Bimetallic Electrocatalysts toward Hydrogen Evolution in Alkaline." Journal of the American Chemical Society 142(17): 7765-7775.

4. Zhang, B., et al. (2019). "Dual-Descriptor Tailoring: The Hydroxyl Adsorption Energy-Dependent Hydrogen Evolution Kinetics of High-Valance State Doped Ni3N in Alkaline Media." ACS Catalysis 9(10): 9332-9338.

5. Zhu, J., et al. (2019). "Recent advances in electrocatalytic hydrogen evolution using nanoparticles." Chemical Reviews 120(2): 851-918.