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Computational Design of Core-shell Nanostructured Materials for Catalysis

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Abstract

Given the crucial role of catalysis science to our society, understanding how to design catalyst structures for desired catalytic activity and selectivity becomes a grand challenge. Core-shell nanostructured materials hold the promise of being active, cost-effective, and stable catalysts. I will demonstrate how we understand the structure -performance correlation at the atomic-scale level through a set of computational approaches and apply it to address the catalyst challenge in the fields of the fuel cell and electrochemical water splitting. Computationally, we designed two classes of novel core-shell nanostructured materials: 1) alloy-core@shell metallic nanoparticles, 2) heterostructured perovskites, which were then experimentally synthesized, characterized and validated. I will also share our insight on the tuning mechanisms of the surface reactivity and activity of these two systems. Finally, I will bridge these two systems and discuss our vision of potential design strategies.

About the Speaker

Dr. Liang Zhang is an assistant professor in the department of chemical and biomolecular engineering at the University of Connecticut. In 2015, He received his Ph.D. degree in Physical Chemistry under the supervision of Prof. Graeme Henekelman at the University of Texas at Austin. After that, he worked with Prof. Jens. K. Nørskov and Prof. Aleksandra Vojvodic at Stanford University and the University of Pennsylvania for his postdoctoral training. In 2018, Dr. Liang Zhang started his professorship at the UCONN. Dr. Zhang's research focuses on the atomistic simulation of chemical reactions, computational design of materials and development of accelerated molecular dynamics methods for energy and environment