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Design of Catalysts and Electrocatalysts for Energy Applications

Abstract

In the current talk we will use two examples to demonstrate the importance of using fundamental studies to identify and design catalysts and electrocatalysts. Our research approaches involve parallel efforts in density functional theory (DFT) calculations, surface science experiments on model systems, and synthesis and evaluation of supported catalysts under thermochemical or electrochemical conditions. We will first use water electrolysis to demonstrate the feasibility of using one atomic layer (monolayer) Pt on transition metal carbides (TMC) to achieve the same activity as bulk Pt. We will present DFT calculations of similar electronic and chemical properties between monolayer Pt/TMC and Pt, synthesis and characterization of monolayer Pt/TMC films, and electrochemical evaluation of the activity and stability of Pt/TMC for water electrolysis. Compared to the state-of-the-art Pt electrocatalyst, monolayer Pt/TMC catalysts represent a significant reduction in Pt loading for water electrolysis.

We will then use the conversion of biomass-derived oxygenates as an example to illustrate the advantages of bimetallic catalysts, which often show unique activity and selectivity over the corresponding parent metals due to the electronic modification and strain effect. We will present our results on the characterization of Ni/Pt bimetallic model surfaces and supported catalysts under in-situ reaction conditions, further highlighting the importance of using the combined approaches of DFT calculations, surface science experiments, and reactor evaluation for catalyst discovery.

Bio - Dr. Jingguang Chen is the Thayer Lindsley Professor of chemical engineering at Columbia University. He received his PhD degree from the University of Pittsburgh and then carried out his Humboldt postdoctoral research in Germany. After spending several years as a staff scientist at Exxon Corporate Research he started his academic career at the University of Delaware in 1998, serving as the director of the Center for Catalytic Science and Technology and the Claire LeClaire Professor of chemical engineering. He moved to Columbia University in 2012. He is the co-author of 20 US patents and 300 journal articles with over 10,000 citations. He received many awards, including the 2015 George Olah award from the American Chemical Society (ACS).