Structure-property relationships at the atomic scale: Understanding next-generation heterogeneous catalysts

Joaquin Resasco
Postdoctoral Fellow
University of California, Santa Barbara

Abstract: Modern society’s reliance on fossil resources as a feedstock for fuels and chemicals has created issues for public health and the health of our environment. Alleviating these problems will require new technologies that decrease our reliance on fossil fuels, and improved processes that reduce the impact of using fossil fuels. Catalysis is key to both of these advances. Catalysts composed of Platinum (Pt) currently represent the state of the art for both renewable technologies (e.g. biomass conversion, water electrolysis, fuel cells) and technologies that reduce the harmful effects of fossil fuel use (e.g. refining, catalytic converters). This has motivated the search for new classes of materials that enhance the performance and metal usage efficiency of Pt. One such class is atomically dispersed catalysts, where single Pt atoms are dispersed on a support. In these materials, unlike conventional catalysts, every Pt atom is exposed and participates in catalysis. However, the behavior of these materials as catalysts has been difficult to rationalize, and relationships between the local coordination of the Pt atoms and their performance are lacking.

In this talk, I will describe the framework we have developed for understanding the behavior of this new and exciting class of materials. I will discuss the synthesis and characterization of sinter-resistant catalysts composed of isolated Pt atoms in well-defined locations on oxide nanoparticle supports. Through a combination of in-situ spectroscopy and in-situ atomic resolution microscopy supported by density functional theory calculations we demonstrate that the local coordination of the most stable Pt species depends on the composition of the oxide, and that these changes strongly influence both stability and reactivity. I will further show how the most stable Pt structure on a given support depends on the chemical potential of the environment the catalyst is exposed to. Finally, I will show how these insights can be applied to predict the behavior of Pt catalysts for both the oxidation of carbon monoxide, a reaction important for catalytic converters, and the hydrodeoxygenation of cresol, a representative reaction for biomass upgrading to fuels.

Educational Development and training: These studies show that building understanding of fundamental surface chemistry can help design next-generation catalytic materials.

Biosketch: Joaquin Resasco completed his B.S in Chemical Engineering at the University of Oklahoma, and his Ph.D. in Chemical Engineering at the University of California, Berkeley under the guidance of Professor Alexis Bell. His doctoral research elucidated the effects of electrolyte ions on the kinetics of electrochemical CO2 reduction. Joaquin was the recipient of the UC Berkeley Chancellor’s Fellowship and NSF GRFP. He was also selected to the Forbes 30 under 30 list in Science. Joaquin is currently a postdoctoral scholar in the Department of Chemical Engineering at the University of California, Santa Barbara working with Professor Phillip Christopher. His postdoctoral work focuses on developing relationships between the dynamically evolving structure of atomically dispersed catalysts and their reactivity.