

# HIGHLANDS IN CHEMISTRY SEMINAR SERIES



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### “Elucidating and Controlling Catalytic Sites and their Environments for the Selective Reduction of CO<sub>2</sub> and Oxygenates into Chemicals and Fuels”

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Future strategies for sustainable energy and chemicals production will undoubtedly require the design of catalysts that actively and selectively convert natural resources such as biomass as well as waste such CO<sub>2</sub> into chemicals and fuels. While enzymes elegantly integrate highly active centers together with adaptive nanoscale environments to exquisitely control catalytic transformations, they are limited industrially by their durability and stability. The design of robust heterogeneous catalytic materials that can mimic the activity and selectivity of enzymes, however, has been hindered by our understanding of how such transformations proceed over inorganic materials and complex environments. Advances in theory, simulations, spectroscopy and characterization begin to allow us to track the molecular transformations and how they proceed in heterogeneous catalytic systems at specific sites and within particular environments. This information can enable the design of unique atomic surface ensembles and nanoscale environments that can efficiently catalyze different molecular transformations. Herein we briefly discuss the development and application of theoretical and computational methods that can examine electrocatalytic and heterogeneous catalytic systems. Computational simulations are used along with experimental results to analyze the selective reduction of CO<sub>2</sub> into chemical intermediates and to compare and contrast electrocatalytic systems which occur at metal/solution interfaces with those for gas phase systems which occur at metal/support interfaces. The differences in the catalytic sites and the local environment that form under reaction conditions ultimately dictate the catalytically intermediates and the resulting products. Many of the same interfacial sites that drive CO<sub>2</sub> reduction translate into the selective hydrogenation and hydrogenolysis of oxygenate intermediates such as acids derived from biomass over supported metal catalysts to specific products. We discuss the similarities between the different interfacial sites and environments across these different reaction systems and how they drive and control the selective formation of products.