**Accelerated Catalyst Discovery: The interplay between surface site stability and catalytic behavior**

Metal nanoparticles find tremendous applications as catalysts in modern industry, facilitating the production of fuels and chemicals, while reducing the energy cost and environmental impact associated with chemical conversion processes. Despite the wide use of metal nanoparticles, their application as catalysts has heavily relied on trial-and-error experimentation in the lab. This lecture will demonstrate how computational research, blending first-principles calculations, multiscale modeling, and machine learning, can identify the active sites on a catalyst surface and accelerate catalyst discovery. Generalized models describing nanoparticle stability, adsorption, and catalytic behavior as a function of nanoparticle size, shape and metal composition will be presented effectively screening the tremendous materials space of bimetallic nanoparticles. Additionally, steps towards addressing complexity arising from reaction conditions will be introduced. Examples include changes on the surface site distribution of metal nanoparticles at elevated temperatures under thermochemical transformations, as well as the generation of active sites on ligand-protected nanoclusters in the presence of an applied potential, under electrocatalytic CO2 reduction conditions. Overall, this seminar will demonstrate a strong interplay between thermodynamic stability of active sites and catalytic activity, unlocking novel rational catalyst design methodologies to guide experimentation.