Computational Discovery of Catalytic Active Sites for Energy and Environmental Applications

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Nanoscale catalysts find tremendous applications 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 catalysts, their application has heavily relied on trial-and-error experimentation in the lab. This lecture will demonstrate how computational research, blending computational chemistry calculations, multiscale modeling, and machine learning, can help us understand complex catalytic mechanisms, identify active sites on a catalyst surface, design robust, active, and selective catalysts and accelerate catalyst discovery. Examples will include electrocatalysts, such as atomically precise ligand-protected nanoclusters for CO_2 reduction, tungsten oxide bronzes for hydrogen evolution, as well as the design of thermodynamically stable multimetallic nanocatalysts. Overall, this seminar will highlight novel rational catalyst design methodologies that help interpret and guide experimentation.