Engineering Molecular Transformations over Supported Catalysts for Sustainable Energy Conversion

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Future strategies for energy production will undoubtedly require processes and materials that can efficiently convert sustainable resources into fuels and chemicals. While nature’s enzymes elegantly integrate highly active centers together with adaptive nanoscale environments in order to exquisitely control the catalytic transformation of molecules to specific products, they are difficult to incorporate into large scale industrial processes and limited in terms of their stability. The design of more robust heterogeneous catalytic materials that can mimic enzyme behavior, however, has been hindered by our limited understanding of how such transformations proceed over inorganic materials. The tremendous advances in ab initio theoretical methods along with high performance computing that have occurred over the past two decades provide unprecedented ability to track these molecular transformations and how they proceed at specific sites and within particular environments. This information together with the unique abilities to follow such transformations spectroscopically is enabling the design of unique atomic surface ensembles and nanoscale reaction environment that can efficiently catalyze specific molecular transformations. This talk presents the advances that have occurred within chemistry and chemical engineering that have enabled this evolution of molecular engineering and discuss its applications to energy conversion strategies as well as chemical syntheses. More specifically, we will discuss the applications to selective oxidation and hydrogenation over supported metals for biomass conversion, zeolite catalyzed C-C bond formation and electrocatalytic oxidation over metal particles.