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### **Environmental Catalysis from First Principles**

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Innovation in environmental catalysis—catalysis related to sustainable production and consumption of energy and materials—is one of the most pressing societal needs of the day. Fuel cells, fuel reforming, hydrogen generation, emissions control, and many other processes all rely on effective catalysts to facilitate the transformation of chemicals into more desirable forms. Historically these heterogeneous catalysts, most often consisting of active transition metal particles dispersed on a high surface area support, have advanced in a largely evolutionary fashion. Today, the increasing demands for more capable catalysts have dovetailed with a revolution in experimental and computational techniques available for preparing and studying these materials at the nanoscale to create the potential for unprecedented advances in catalyst research and discovery. Three central questions have emerged in nanoscale environmental catalysis: First, how does the structure and catalytic function of transition metal catalysts evolve as particles decrease in size from the micro to the nanoscale? Second, how do these particles interact and communicate with supports, and what are the effects on structure and catalytic function? Third, how does the particle/support system respond to realistic and dynamic reaction environments? Density functional theory (DFT) simulations provide a means to interrogate these questions independently and have proved a powerful complement to experiment in the investigation and development of nanocatalysis. In this talk we will review recent progress in studying these questions using DFT methods, with a particular emphasis on the connection between oxidation environment, catalyst composition, and activity for CO and NO oxidation with Pt and Ru catalysts.