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Operando Computations for Discovery in Heterogeneous Catalysis

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Computational methods have had a profound impact on the science of heterogeneous catalysis. One of the challenges in making these models more rigorous, for instance to establish quantitative relationships between experimental observations and models, is to properly account for the influence of the catalytic reaction environment on the state of a catalytic material and on mechanism. "Operando" experiments interrogate catalysts at the conditions at which they are functioning. In the same way, by incorporating statistical mechanical and dynamics models, it is in principle to model a catalyst "operando" from first principles. In this presentation I describe our recent efforts to apply these concepts to catalysis within the pore of a zeolite, a catalytic environment of practical relevance and sufficiently well-defined to lend itself to a complete description from first principles. Specifically, I discuss these ideas in the context of the selective catalytic reduction (SCR) of NO_x by Cu-exchanged zeolites. We find that it is possible to predict with quantitative accuracy the structure and evolution of Cu catalytic sites within a zeolite as a function of reaction conditions, that site dynamics are important to catalytic function, to infer from this information catalytic mechanisms, and ultimately to use this information to guide catalyst design.

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Bill Schneider's expertise is in chemical and engineering applications of density functional theory (DFT). After receiving his Ph.D. from the Ohio State University in 1991, he began his professional career in the Ford Motor Company Research Laboratory working on a variety of problems related to the environmental impacts of automobile emissions. There he developed an interest in the catalytic chemistry of NOx for diesel emissions control, and he has published extensively on the chemistry and mechanisms of NOx decomposition, selective catalytic reduction, trapping, and oxidation catalysis. In 2004 he joined the Chemical and Biomolecular Engineering faculty at the University of Notre Dame as an Associate Professor. At Notre Dame he has continued his research into the theory and molecular simulation of heterogeneous catalysis, with particular emphasis on reaction environment effects on catalytic materials and their implications for mechanism and reactivity. He was promoted to Professor in 2010 and was recently recognized as a Fellow of the American Association for the Advancement of Science. He has co-authored more than 140 papers and book chapters and is a Senior Editor of the *Journal of Physical Chemistry*. He makes his home in Granger, Indiana with his three children, Justin, MiMi, and Meredith.