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**Understanding the Chemical Structure and Properties of Alumina Based
Catalysts Through Synergism Between Theory and Experiment***

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An atomic-level understanding of catalytic systems would be a very powerful tool to aid the selection of catalytic materials and optimize their properties. At present, however, there is very limited information on the atomic configurations of the active sites, their electronic structure, and activation barriers for surface and subsurface diffusion, oxidation and reduction. Without such information, atomistic mechanisms are largely a matter of speculation, and their development is mostly empirical. Here we demonstrate atomic-scale description of catalysts, through a combination of Z-contrast imaging of atomic configurations and first-principles studies of bulk and surface properties. This combination of techniques delivers an atomic scale description of catalytic activity that can form the basis for the rational design of new catalysts and the optimization of their properties.

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