Understanding Functional Materials for Catalysis

De-en Jiang

Department of Chemistry, University of California, Riverside, USA

Activation and conversion of small molecules require efficient catalysts. Although many insights have been obtained into catalysis by transition metals, there have been relatively few general trends guiding our understanding of catalysis by transition-metal oxides. On one hand, this is due to the complexity of electronic structure associated with many transition-metal oxides; on the other hand, their complicated surface chemistry and reconstruction also hamper the surface-science studies. Our recent computational efforts aim to correlate the structural, energetic, and electronic features of typical transition-metal oxides and their surfaces to activation energies and catalysis. We will show that a simple geometric descriptor can be used to describe the activity of lattice oxygen sites on transition-metal oxides. We further extend the lattice-site mechanism to CO_2 reduction via lattice hydride in 0D materials. If time allows, we will also discuss 0D and 2D materials for water splitting and N_2 reduction.