

Abstract Submitted
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Mechanisms Leading to Single-Atom Catalysis in Oxide Surfaces

RAJ GANESH PALA, FENG LIU, University of Utah — Recent experiments suggest that few or even a single metal adatom can be catalytically active on oxide surfaces. We propose certain general atomic-level mechanisms that can provide design criteria for these catalytic systems. The adatoms in the oxide surfaces can catalyze chemical reactions by directing reactants' surface diffusion, by altering their structural mode of adsorption and by activating the reactants in its vicinity to create a highly reactive zone with enhanced reactive collisions rate. An important additional criterion is facile removal of the products by desorption or by surface diffusion away from the catalytically active sites. We investigate a model system, CO oxidation by single Au adatom adsorbed on TiO₂ surface, using first-principles calculation to evaluate which of the above criteria are satisfied in this system.

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