MAR08-2007-000188

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Investigating the Molecular Level Details of Catalytic Oxidation Reactions[1]

GRANT JOHNSON, Pennsylvania State University

Gas-phase cluster reactivity studies are providing significant insight into the molecular level mechanisms of oxidation reactions occurring on catalytic surfaces. Our experimental approach, employing tandem mass spectrometry, uses mass selected metal oxide clusters to model specific catalytic active sites. This technique enables investigation of the influence of factors such as size, stoichiometry, charge state, and elemental composition on the reactivity of catalytic materials. Particular emphasis is on identifying species with enhanced activity for the selective oxidation of simple hydrocarbons and atmospheric pollutants. Recent findings pertain to the kinetics of ethylene oxidation in the presence of vanadium oxides and the oxidation of carbon monoxide in the presence of gold and iron. Through a combination of experiments and theoretical calculations we establish structure-reactivity relationships and propose general reaction mechanisms for these catalytic processes.

[1]Financial support provided by the U. S. Department of Energy, Grant No. DE-FG02-92ER14258.