



BERKELEY CATALYSIS CENTER

Distinguished Lecture Series Seminar

December 6, 2005 The McCollum Room
775A Tan Hall
2-3:30

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“Theoretical Insights into Acid Catalysis over Polyoxometalates”

ABSTRACT:

Acid catalysis is at the heart of many hydrocarbon conversion processes including catalytic cracking, isomerization, oligomerization and alkylation. Of these processes, alkylation is predominantly carried out using homogenous HF and H₂SO₄ which are highly corrosive acids and lead to waste disposal and catalyst separations issues. Despite the nearly 30 years of research, there are still very few if any solid acid alternatives. Catalyst deactivation remains one of the foremost challenges in finding acceptable solid acid replacements. A more complete understanding of the fundamental structural and electronic catalyst features that control acidity, selectivity and the potential modes of deactivation could considerably advance our efforts toward the design of new materials. While there have been a number of studies devoted to elucidating the mechanisms that control solid acid catalyzed conversion processes, our understanding is still fragmented and rather incomplete. Much of our understanding is based on assumed analogies with solution phase chemistry. Over the past decade, however, theoretical efforts have helped to establish fundamental concepts of solid acidity in zeolites and their influence on catalytic cracking. Herein we will review some of these general features and how they apply to alkylation over heteropolyacids. More specifically we examine potential mechanisms that control the alkylation of isobutane with n-butene and potential deactivation of HPAs by the loss of water.