Overview of Mechanisms for catalytic selective oxidation and ammoxidation
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Over the last decade there have been significant advances in developing Mixed Metal Oxide catalysts: MoVNbTaTeOx effective at selectively ammoxidation Propane directly.

Propane (CH3-CH2-CH3) + O2 + NH3 \rightarrow acrylonitrile (CH2=CH-CN)

Patents: here are held by Mitsubishi, BP, and perhaps others.
We want to describe the bulk and surface phases of mixed (VNbTa)Mo(TeSb) oxides and the interfaces between phases, including amorphous phases
Typical catalyst may have a variety of surface sites with a variety of defect structures and may be affected in a variety of ways by the coupling to the support

We want to treat all these sites and phases simultaneously to describe how the catalytic processes change with external conditions of Temperature, pressure, surface preparation etc.
It is very difficult to include all of these situations into a high quality QM calculation.
On the other hand we need to use QM to describe the reaction mechanisms.
Strategy:
1. use QM to explore fundamental reaction steps: compare with experiments where possible
2. Develop Reactive Force Field (ReaxFF) to capture QM results
3. Use ReaxFF for realistic consideration of complex reactive system

This talk will summarize the mechanism for propene ammoxidation developed at MSC (with Yun Hee Jang, Janet Allison). The following talk by Kimberly Chenoweth will discuss our new ReaxFF and the results of applying it to the initial steps in propene activation.

A first step will be to examine the active sites proposed by Grasselli and coworkers and to determine