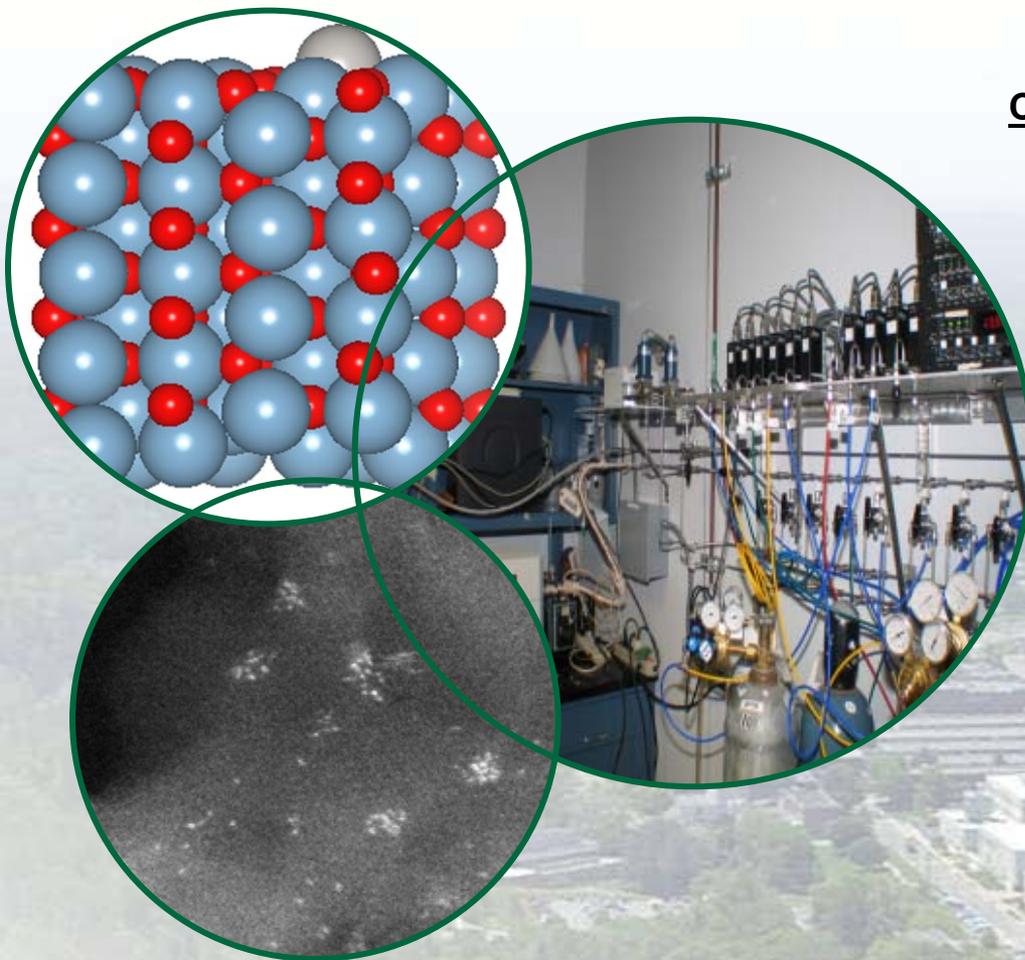


Catalyst by Design - Theoretical, Nanostructural, and Experimental Studies of Emission Treatment Catalyst

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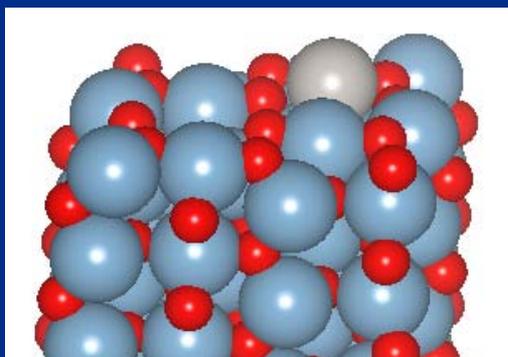
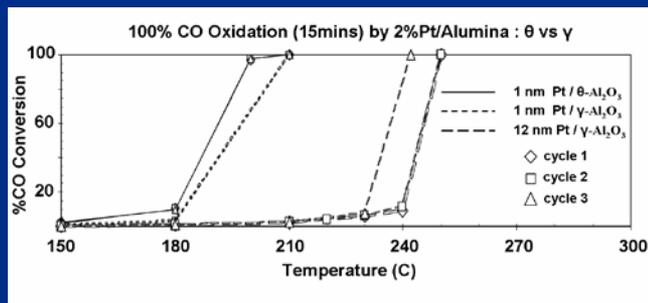
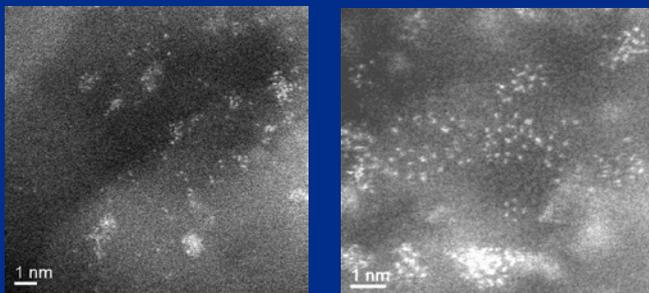
Physical Chemistry of Materials, Materials Science and Technology Division



Poster Location: P-8

August 27, 2010

Catalyst by Design - Theoretical, Nanostructural, and Experimental Studies of Emission Treatment Catalyst



- **Pt/θ-Al₂O₃ is a better model for Pt-γ-Al₂O₃ than Pt/α-Al₂O₃**
- **Nanostructure for both**
 - Single Pt atoms
 - 10-20 atom agglomerates with no Pt-Pt bond
- **CO oxidation for both**
 - Starts and complete at identical temperatures
- **DFT studies on Pt/θ-Al₂O₃ suggest that Pt is in zero oxidation state**
 - Alternate CO oxidation mechanisms possible
- **The energetics of Pt-Pd clusters suggest that Pd does not stabilize Pt against coarsening when particles are in sub-nanometer range**