Catalysis by Design – Theoretical and Experimental Studies of Model Catalysts for Lean NO_x Treatment

C.K. Narula*, L.F. Allard, D.A. Blom, M. Moses, Y. Xu, W. Shelton,
Oak Ridge National Laboratory, Oak Ridge, TN 37831
W. Schneider, University of Notre Dame, Notre Dame, IN 46556

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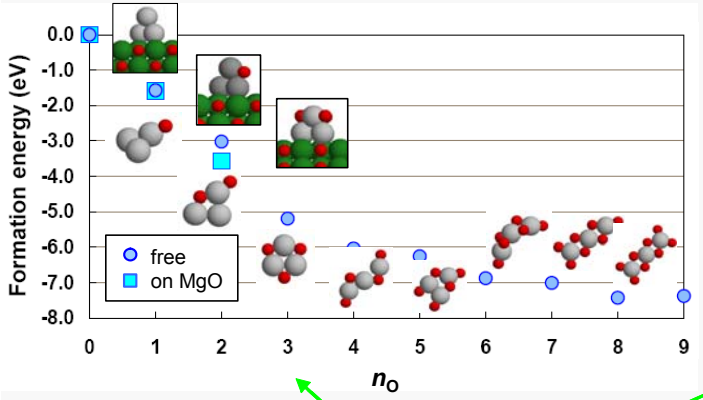
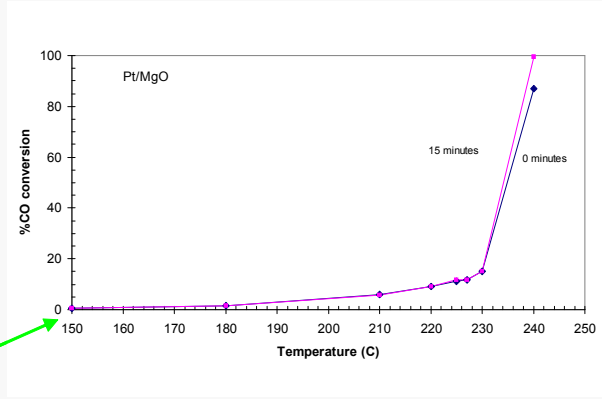
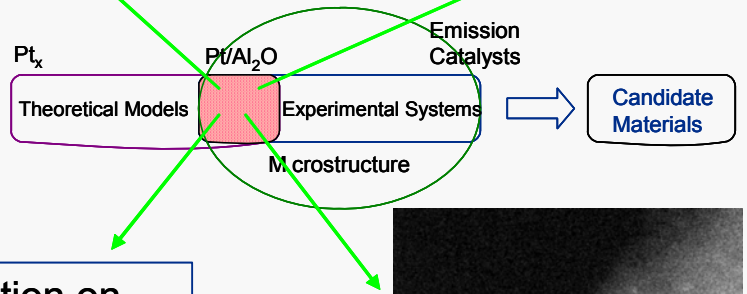
Catalysis by Design





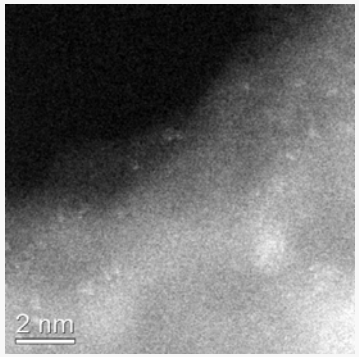


Candidate Materials

Combinatorial Screening

Optimum Catalyst Materials

Pt deposition on single crystal particles of MgO by solution methods



Lean NO_x Catalysts

- Studies on model catalysts, Pt/MgO, suggest that oxidation energetics and morphologies of free Pt nanoclusters is preserved on a relatively inert surface.
- The adsorption energies of CO rises monotonically with cluster size, and the energy profile of CO oxidation on nanoclusters differs from bulk Pt.
- The experimental observation on 2%Pt/γ-Al_2O_3 clearly shows differences between nanoclusters and large particles.
- We have initiated efforts to employ “catalyst by first principles’ protocol to design a lean NO_x catalyst with broad operating window.