356b Nano-Scale Effects in the Reactivity of Pt Clusters toward Co Oxidation

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Platinum supported on oxides is widely used in oxidation catalysis, but many aspects of supported Pt catalysts are still not well understood. For instance, it is only recently that the active phase for CO oxidation is beginning to be elucidated. Nano-clusters of Pt and other metals can now be synthesized on oxide surfaces at precisely defined sizes, which may be realistically modeled and offer a viable platform on which to further our understanding of redox catalysis on Pt. DFT calculations are currently being performed to examine the properties of reduced and partially oxidized Pt clusters. We find that the Pt clusters exhibit markedly different reactivity for oxygen and CO adsorption and for CO oxidation compared to the bulk metal. The calculations provide insight into the coupling between particle size, support, chemical environment, and reactivity toward CO oxidation and complement on-going experiments to explore CO oxidation on supported, well-defined Pt nano-clusters.