

### **356c Heterogeneous Catalysis by Gold: Dft Investigations of O<sub>2</sub> Interactions with Oxide Supported Gold Materials**

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Gold nano-particles supported on metal oxides are active in a number of heterogeneous catalytic processes such as low temperature CO oxidation, propylene epoxidation, hydrogenation reactions, the reduction and decomposition of NO and N<sub>2</sub>O. The unique catalytic activity of Au nano-clusters has stimulated an intense debate about the fundamental factors that cause this behavior. Possible explanations include quantum size effects, strain, charging of gold particles by interaction with defect sites of oxide supports, a cooperative action of oxide supports and metal nano-particles, the effect of metal-insulator transitions, the effect dominated by low-coordination of Au atoms in nano-particles, possible formation of Au nano-oxides, etc. It has also been observed that Au nano-particles adsorbed on reducible oxide supports (TiO<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, CeO<sub>2</sub>) are more reactive in a number of oxidation reactions than the Au particles dispersed on irreducible oxide supports (Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>) at identical external conditions and for gold nano-particles of equal size. Experimental evidence suggests that the activation of molecular oxygen at Au/oxide interface sites governs the catalytic activity of Au/oxide catalysts. We have employed Density Functional Theory (DFT) calculations to investigate oxygen adsorption and dissociation at interface sites of Au and multiple reducible and irreducible oxides. These studies have revealed mechanistic insights into the support-sensitive catalytic activity of various Au/oxide systems. We have also investigated the behavior of the Au/oxide systems as a function of gas-phase oxygen pressure and temperature.