Theoretical and Experimental Investigations of Propylene Epoxidation on TiO_2 Supported Gold Nanoparticles

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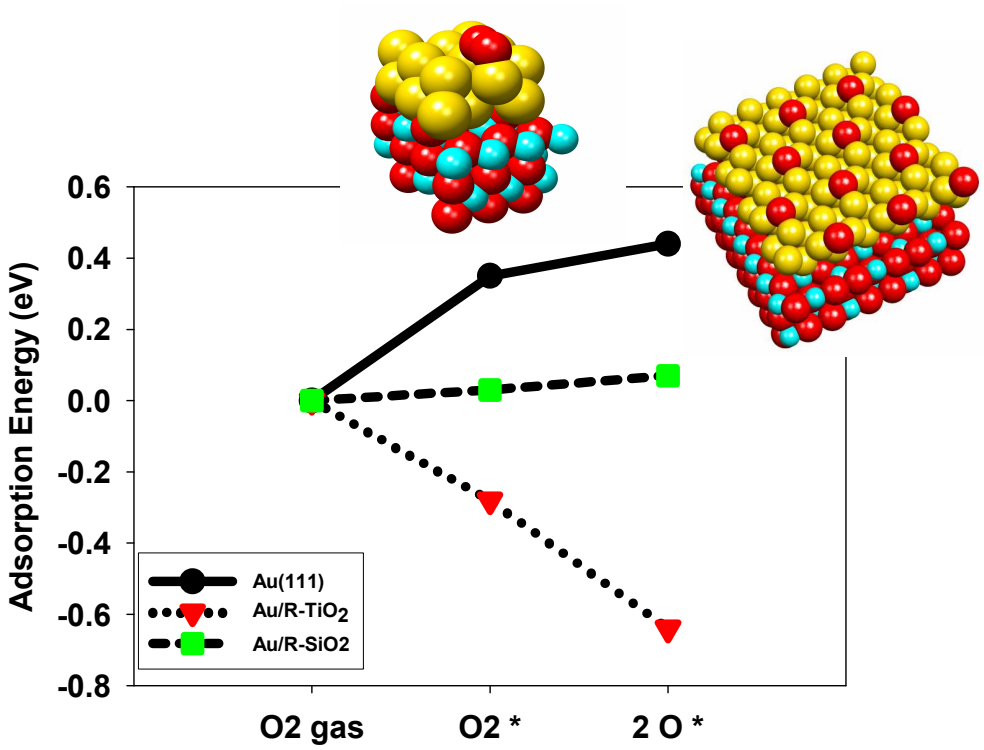

• We have studies the interactions of oxygen with oxide-supported Au nano-structures

•Density Functional Theory (DFT) quantum calculations show that oxygen interacts more strongly with Au supported on oxides (TiO_2 and SiO_2) or unsupported Au

• We find that on oxygen-vacancy-rich oxide supports, charge transfer from the vacancy to Au enhances the chemical activity of Au towards the O_2 dissociation reaction

• We also find that there are special sites at the metal/oxide interface that exhibit an unusual chemical activity.

• Some if these findings are reported in: Siris Laursen and Suljo Linic, "Oxidation catalysis by oxide-supported Au nanostructures: The role of supporters and the effect of external conditions", *Physical Review Letters*, 97, 026101, 2006.