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Au-Nano-particle Deposition on oxide surfaces to tune a novel material for catalytic application – a first principle study

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It has been found that nanometer size gold particles on different oxide supports can act as catalysts. Suggestions include quantum size effects, availability of low coordinated sites, and strain or combined effects of the gold particles and the oxide support. From photo dissociation spectroscopy and theory it has been inferred that the 2D / 3D structural transition transition occurs between five and seven atoms depending on charge state ~neutrals and singly positively charged ions.

Some DFT-based local properties, e.g. Fukui functions and local softness, have already been used for the reliable predictions in various types of electrophilic and nucleophilic reactions[1]. We have compared the Ag bonding to Pd over hydroxylated/clean alumina (100) surface to study deposition and correlated the activity of Ag and Pd binding over alumina surface[2]. Here we will look into the interaction of gold particles over different sites of the metal-oxide surface to tune the catalytic activity of the novel material using first principle periodic calculations and compare them with the reactivity index to formulate a priori rule for metal cluster interaction. Figure 1 and 2 depicts two such optimized structure with alumina (100) clean surface to monitor the transition between 2D and 3D structures.

References

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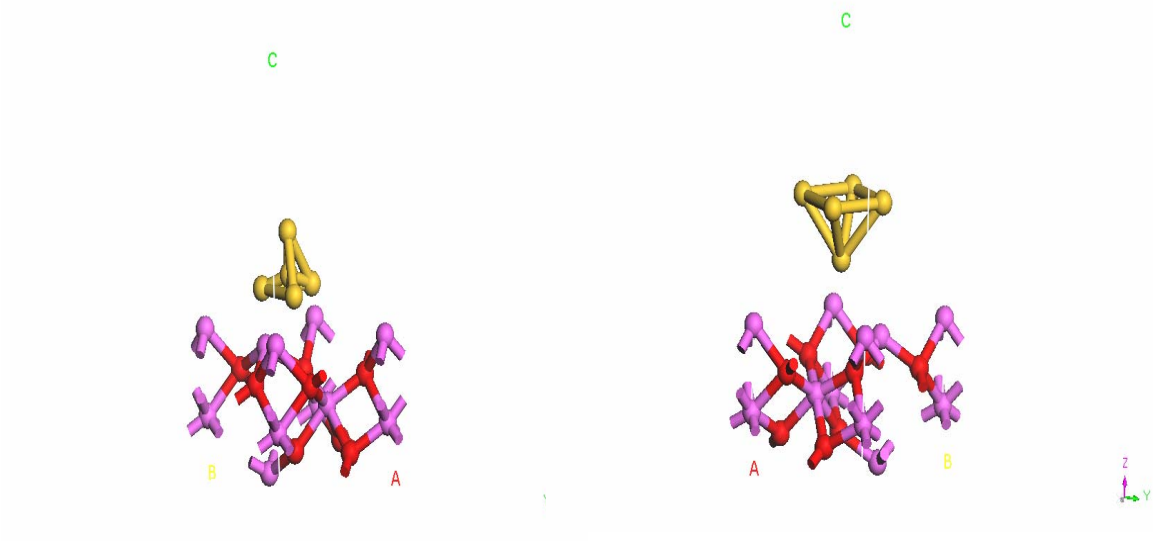

Fig. 1 **Interaction of 3D cluster with alumina (100) surface**

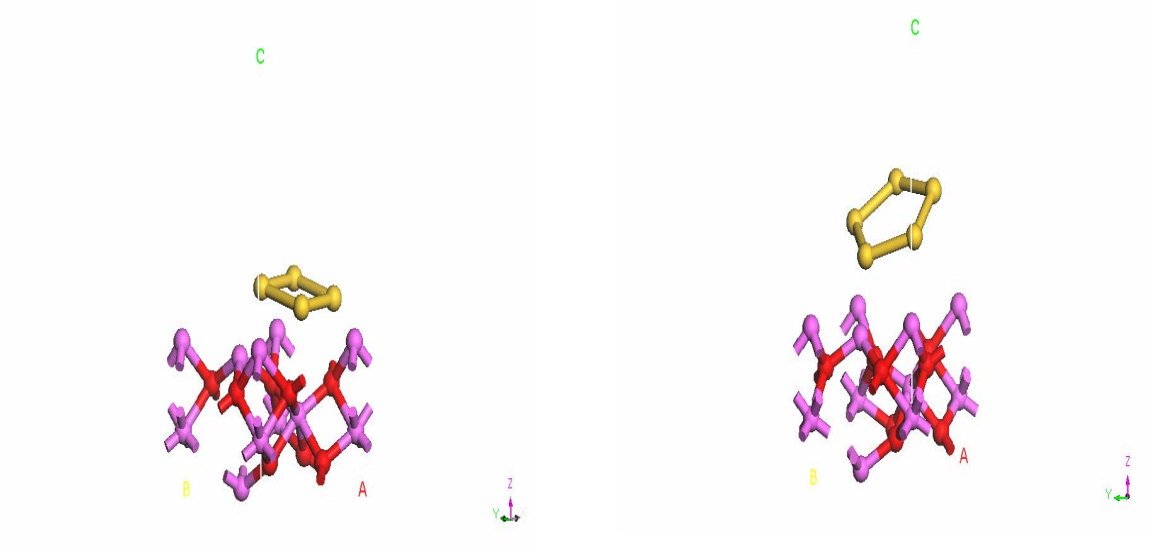

Fig. 2 Interaction of 2D cluster with alumina (100) surface