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Adsorption of Gold on TiC (001) and ZrC (001) : Au-C interactions and charge polarizations

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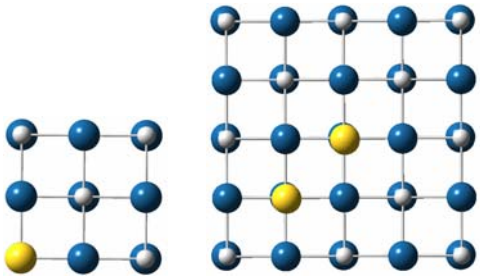
Abstract – The interaction Au, Au_2 with TiC (001) and Zr (001) has been studied in terms of a periodic density functional theory based approach. The bond exhibit between Au, Au_2 and the TiC (001) and Zr(001) surface exhibits very little character ionic, but there is a substantial polarization electron of around Au that effects its chemical properties.

Recently, gold has become the subject of a lot of attention due its unusual catalytic properties when dispersed on some oxide supports [1]. Several models have been proposed for explaining the activation of supported gold especially to the effects of metal ◄► support. What happens when Au is deposited on the other types substrates? A very recent article indicates that Au nanoparticles dispersed on an ultrathin TiC film cam perform the oxidation of carbon oxide at temperatures below 200 K. The unexpected effect of the TiC support on the reactivity of Au nanoparticles opens the way the new Au-based catalysts and also raises fundamental questions on the interaction of Au with TMCs (transition metal transition), the formation of supported Au nanoparticles and their reactivity. In this work, density functional calculations for suitable periodic models within the repeated slab approach were carried out to investigate the bonding of Au, Au_2 on the TiC (001), and ZrC (001) substrate with adatoms on top of C (see Figure 1). The nature interaction has been analyzed through a topological analysis of the electron localization function (ELF) and charge distributions were estimated by the method of Bader [2,3].
For interaction Au with ZrC and TiC, it found that the energies are significantly large indicating a rather strong interaction (see Table I). In fact, the adsorption energies increases in a per Au atom basis due to the effects of Au-Au bonding. After depositing Au on TiC and ZrC surfaces, there is a noticeable charge transfer from the substrate to the adsorbed Au which becomes negatively charged (see Table 1and Figure 2). It can see that Au could be activated after depositing them on surfaces of TiC and ZrC. In these respect, ZrC (001) should be a much better support for gold than TiC (001). The substantial Au negative charge in Au/ZrC (001) should facilitate bonding of adatoms with electron-acceptor molecules (CO, O_2, SO_2, etc)

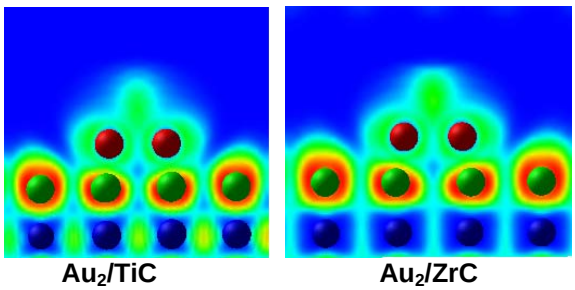
Table 1. Adsorption energies (Eads in eV) and Bader charges (Q_{Au} in a.u.)

Substrate	E_{ads}		Q_{Au}	
	Au_1	Au_2	Au_1	Au_2
TiC	1.94	4.44	-0.20	-0.20
ZrC	2.30	5.09	-0.41	-034



Au_1-Top_C Au_2-Top_C

Figure 1. Adsorption site for Au and Au_2 on the TiC (001) and ZrC (001)



Au_2/TiC Au_2/ZrC

Figure 2. ELF maps for Au_2 adsorption on TiC (001) and ZrC (001)

References

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