Abstract Submitted
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Theoretical Investigation of the Electronic Interaction between Au and TiO2 Nano-systems[1] ANDREW RICE, West Virginia Unversity — The focus of this research is to theoretically study the underlying mechanisms of the enhanced catalytic properties presented by the oxide supported gold nanoparticles. Extensive studies have established that the interaction between the gold nanoparticles and the oxide substrates plays an important role in enhancing the catalytic performance. Several factors, such as geometry, electronic coupling and the charge transfer occurring between Au and TiO2 need to be considered in order to understand the interaction between Au and TiO2. One issue that will be discussed in this study is the bonding character between the Au/ TiO2 nanosystems. Experimentally, geometries on this subject have been researched. However, there is no clear picture of how the Au nanoparticles bonding to TiO2 surfcace in terms of the preference locations along certain orientation of TiO2 (anatase in our study). Using computational approaches, we are aiming to understand the bonding characters and the electronic properties of Au/ TiO2 nanosystems. The spherical shape of Au13 has been established. As for the TiO2 substrate, we considered three anatase nanoparticles with both (101) and (001) surface existence. Along with size increasing, the (001) surface tends to be the dominate surface of TiO2 nanoparticle. The reason we designed the TiO2 nanoparticle in this manner is that we are interested in the preferable locations of Au nanoclusters anchoring to TiO2. In our study, we found Au13 on all three TiO2 substrates showed geometric deformation.

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