

## Rationale for the High Reactivity of the Interfacial Sites in Methanol Oxidation on Au/TiO<sub>2</sub>\*

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The role of perimeter/interfacial sites of titania supported gold nanoparticles have recently been the subject of discussion in several experimental and theoretical studies because of their high activity in various reactions. We have carried out density functional theory based calculations to find that the high activity of these active sites in Au/TiO<sub>2</sub> towards methanol reaction originates from the charge transfer induced Coulomb interaction among gold, reactant, and reducible TiO<sub>2</sub> through the formation of ionic O-Au bond between gold atoms and methoxy in the active sites. A direct result of such charge transfer induced repulsion is tilting of the methoxy axis, which leads to facile reaction of methoxy with bridge oxygen atoms readily available from the reducible support through C-H scission. We will present details of the charge density redistributions, projected electronic density of states and calculated activation energy barriers and reactions paths which may control the selectivity of the reaction towards the formation of formaldehyde and compare them with experimental data from the Chen group [1].

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[1] D. A. Chen *et al.*, to be published.