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Modelling TiO2 supported Au cluster photocatalyst using DFT and SCC-DFTB approaches

Photocatalysis, which exploits the use of clean and infinite solar energy, has the potential to be one of the most influential solutions to green and sustainable chemistry. Titanium dioxide-based catalysts have shown great capability in photocatalysis due to its non-toxic, stable and highly active properties. However, the reaction efficiency is still too low for practical applications. To address this issue, co-catalysts can be introduced to the photocatalysis system. Nobel metal nanoparticles supported on semiconductors can provide reaction sites, take part in charge separation and transportation thus significantly improving the photo-reactivity. Metal clusters have recently been shown to also act as co-catalysts in photocatalytic systems. Metal clusters can have completely different physical and chemical properties due to their size effects; they have higher surface-area-to-volume ratio than normal metal materials and have demonstrated ability to lower activation barriers by enabling new reaction pathways for reaction. Thus, metal clusters have great potential as co-catalysts in photocatalytic systems.

Density Functional Theory (DFT) is used to investigate the structure and photocatalytic activities of binary photocatalysts made up of Au clusters supported on TiO2. Compared to ab initio quantum mechanical methods, DFT is more effective when performed carefully with proper benchmarking . However, in order to simulate realistic Au cluster-TiO2- photocatalysts, an extraordinary large model, which is beyond the capability of DFT needs to be simulated. This poster will present early results work utilizing Self-Consistent Charge Density Functional Tight-Binding (SCC-DFTB) calculations. DFTB parameters are developed for the Au-TiO2 photocatalytic system using automatic DFTB parameterization code. A comparison will be made between DFT calculation and DFTB of structural and energy properties.

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