Quantum Mechanical studies of catalytic effects on water splitting

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Fossils are the world's outstanding fuel source. As the world's population increases, fuel usage is also increased. The problem is fossil fuel is not renewable. Also the combustion of fossil fuel produces pollutants like CO_2, which increases environmental pollution. Even though there are alternative energy sources like wind, hydropower, geothermal and solar; it is essential a produce clean and renewable energy source. Hydrogen is considered as the fuel for the future as it is environmental friendly and clean. Numerous studies have been developed to produce hydrogen by splitting water after Fujishima and Honda first showed photocatalytic water splitting in the presence of a TiO_2 catalyst[1] in 1972.

Experiments have shown that H_2 evolution is 1.9 times more efficient when TiO_2 is absorbed on a graphene oxide (GO) sheet than from pure TiO_2.[2] This is because TiO_2 can form a p-n heterojunction with GO for visible light absorption. ZnO also can form a p-n heterojunction with GO[2]. ZnO is a semiconductor, which has a wide band gap (3.4 eV).

This study is mainly focused on density functional theory calculations of water splitting on GO-ZnO surface. Initial studies were carried out using $(ZnO)_n$, with n=1, 2 and 3, ZnO monolayer and (ZnO)3 cluster absorbed on Graphene Oxide.Preliminary calculations of the structures were optimized with density functional theory (DFT) using the B3LYP exchange functional and STO-3G and 3-21G basis sets in the GAUSSIAN 09 quantum chemistry package, to be followed by calculations on larger clusters adsorbed on a sheet of graphene oxide with more accurate basis sets at the DFT and MP2 levels.

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