
Contribution ID: **208** Type: **Poster Presentation**

# Density Functional theory study of optical and electronic properties of (TiO2)n=5,8,68 clusters for application in organic and hybrid organic-inorganic solar cells

*Thursday, 11 July 2019 15:00 (2 hours)*

A range of solution processed organic and hybrid organic–inorganic solar cells, such as dye-sensitized solar cells and bulk heterojunction organic solar cells have been intensely developed in the past two decades. TiO2 is widely employed as electron transporting material in nanostructured TiO2 perovskite-sensitized solar cells and semiconductor in dye sensitized solar cell. Understanding the optical and electronic mechanisms that govern charge separation, transport and recombination in these devices will enhance their power to current conversion efficiencies under illumination to sunlight. In this work, DFT with PBE functional computational approach was used through various computational softwares which are CASTEP, GPAW and AVOGADRO within an atomic simulation environment to explore the optical and electronic properties of three modelled TiO2 brookite clusters which are Ti5O10, Ti8O16 and Ti68O136 for application in organic and hybrid organic-inorganic solar cells. The simulated optical absorption spectrum for (TiO2)5 and (TiO2)8 cluster shows excitation around 200 nm to 400 nm but, (TiO2)8 cluster shows higher absorbance than the corresponding (TiO2)5 cluster. The density of states and the projected density of states of (TiO2)5, (TiO2)8 and (TiO2)68 clusters were computed using GPAW and PBE exchange correlation functional to further understand their electronic structure. The density of states spectrum reveals surface valence and conduction bands separated by a band gap of 1.10 eV, 2.31 eV and 1.37 eV for (TiO2)5, (TiO2)8 and (TiO2)68 clusters respectively. The projected density of states spectrum reveals 2p atomic orbitals contributing mostly to the highest occupied valence band (VB) state, whereas the lowest unoccupied state of the conduction band is mainly dominated by the contributions of titanium 3d atomic orbitals. Our findings generally shows that the optical and electronic properties of TiO2 cluster varies with the size of the cluster.

Keywords: Density Functional theory, Titanium dioxide, optical properties, electronic properties, hybrid solar cells.

## Apply to be<br> considered for a student <br>   award (Yes / No)?

yes

## Level for award<br> (Hons, MSc, <br>   PhD, N/A)?

PhD

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**Session Classification:** Poster Session 2

**Track Classification:** Track G - Theoretical and Computational Physics