

## The generation of charge carriers in semi conductors – A theoretical study

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### ABSTRACT:

A systematic study of electronic and optical properties of titanium dioxide under visible light was simulated using the first principles calculations. Both electronic and optical properties were studied. The findings support the application of TiO<sub>2</sub> in photo energy generation after experimentally modifications. Our calculations were done using DFT with the GGA+U approach to mimic the experimental results and avoid underestimation of DFT. A theoretical band gap of 3.15 eV complimented the experimentally obtained band gap of 3.2 eV. Finally, our results revealed that upon protonation there is charge generation and this has the potential for application in photo energy generation.