

Optimization Of The Electronic And Optical Properties Of TiO₂ For Clean Fuel Production

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Abstract

Among different crystal structures and morphologies of TiO₂, vertically oriented anatase nanotube arrays show the highest activity for solar energy conversion. However, the long-standing bottleneck is the fact that TiO₂ is a wide band gap semiconductor, limiting its activation to the deep-blue and ultraviolet spectral region that contains but a small fraction (5%) of the incident solar energy. Herein, density functional theory (DFT) has been used to compare between density of states of bulk and nanotube forms of TiO₂ by using different concentrations of N atoms. The wave functions were described using two different techniques; linear combination of atomic orbital (LCAO) and plane wave.

Our results showed a shift in the calculated bandgap for bulk TiO₂ only for small concentrations of N atoms as dopant. For TiO₂ nanotube, the bandgap decreases as the concentration of N atoms increases. The effect of the diameter of TiO₂ nanotubes on their optical and structural properties has also been investigated and discussed in details. Our study presents a protocol to fine tune the optical, electronic and structural properties of TiO₂ for energy conversion applications.