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DFT Study of the (210) TiO_2 Brookite Surface Doped with V and Zr for Application in DSSCs

Dye-sensitized solar cells (DSSCs) present a promising photovoltaic technology due to their cost-effectiveness, high efficiency, and flexible device design. DSSCs generally use titanium dioxide (TiO_2) as a photoanode material. Brookite TiO2 phase provides special electrical characteristics fit for maximum solar energy conversion. However, the broad bandgap of bulk TiO_2 limits its absorption in the visible light range.
In this work, density function theory has been used to explore the properties of (210) TiO_2 brookite surface doped with vanadium (V) and zirconium (Zr). Generalized gradient approximation was used to define the exchange-correlation function within the scheme of Perdew-Burke Ernzerhof, as implemented in Material Studio. The results show that doping greatly lowers the energy bandgap of TiO_2 Brookite (210) surface, therefore improving the visible light absorption. Also, doped surfaces show less reflectance, desired for light harvesting. From computation of formation energies, the stability of the doped systems is verified as V and Zr dopants efficiently integrate into the TiO_2 surface without sacrificing structural integrity. The study reveals that Vand Zr doping enhances the optical and electrical characteristics of the TiO_2 Brookite (210) surface, therefore offering a suitable material for effective DSSC uses.
Keywords: Semiconductor, band gap, density functional theory, dye-sensitized solar cells, TiO2 brookite.

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Primary authors: RANWAHA, Tshifhiwa (University Of Venda); DIMA, Ratshilumela Steve (CSIR); MALUTA, Eric (University of Venda); MAPHANGA, Regina (Council of Scientific and Industrial Research (CSIR))

Presenter: RANWAHA, Tshifhiwa (University Of Venda)

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