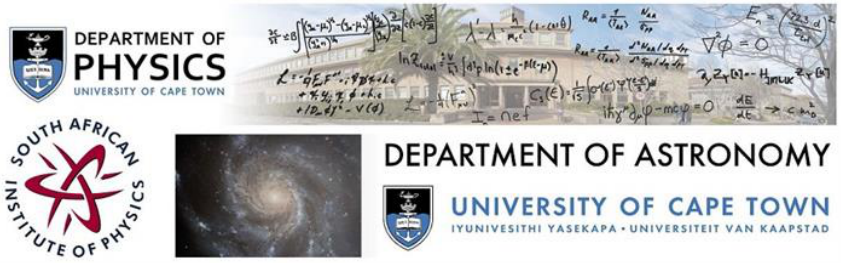

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Computational study of TIO2 Brookite (1 0 0) surface doped with Ruthenium for application in dye sensitised solar cells

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Abstract content
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Recently, there has been a renewed interest in TiO2 brookite as charge transfer layer in dye-sensitized solar cells (DSSCs). In this work, the structural optimizations, band structure, and electronic density of states of doped and un-doped TiO2 (100) surfaces were performed by using the first principles calculations based on DFT using a plane-wave pseudopotential method. The generalized gradient approximation (GGA) was used in the scheme of Perdew-Burke-Ernzerhof (PBE) to describe the exchange-correlation functional. All calculations were carried out with CASTEP (Cambridge Sequential Total Energy Package) code in Materials Studio of Accelrys Inc. The calculations showed that band gap of Ru-doped TiO2 decreases with an exception of the case when Ru is placed at a distance 2.0 Å from the top layer. The overlap among the Ru 3d, Ti 3d, and O 2p states enhances photocatalytic activity in the visible light region. TiO2 brookite (100) surface doped with Ru at a distance of 2.0 was found to have the highest band gap amongst the different displacements considered in this study and it also has the highest negative total energy of -2.24480572 eV. For the structures of TiO2 brookite (100) doped with Ru, whereby one Ti atom was replaced with Ru, total energy of doped structures shows that they are energetically favourable, with the band gap being reduced to 0.223 eV compared to 2.376 eV of the pure structure.

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