### 63<sup>rd</sup> ANNUAL CONFERENCE OF THE SA INSTITUTE OF PHYSICS



Contribution ID: 350

Type: Poster Presentation

### DFT study of Modifications of Pt-doped TiO2 using N, for application in DSSCs

Thursday, 28 June 2018 15:00 (2 hours)

Doping has found to be one of the most promising method to in increasing photocatalytic activity of various materials. The location and nature of the doping elements strongly affect the structural, electronic and optical properties of TiO2. To tailor the band structure and modify the photocatalytic activity of TiO2 brookite (210) surface, a pair of dopants is selected. Platinum and Nitrogen atoms are inserted in the TiO2 network as substitutional and N was also doped through absorption on the surface. The main objective behind the different locations and methods of the dopant elements are to banish the isolated unoccupied states from the forbidden region that normally annihilates the photogenerated carriers. Pt replaced Ti, N replaced O and N was also absorbed and bond with 2 coordinated O in the TiO2 brookite (210) surface network. N absorbed Pt\N TiO2 provided a suitable configuration of dopant atoms in terms of geometry and band structure. Moreover, the optical properties showed a notable shift to the visible regime. Individual dopants either introduced isolated unoccupied states in the band gap or disturbed the Fermi level and structural properties. Furthermore, the other co-doped configurations showed no remarkable band shift, as well as exhibiting a suitable band structure. Resultantly, comparing the band structure and optical properties, it is argued that Pt (at Ti) and N absorbed (at O) doped would strongly improve the photocatalytic activity of TiO2 brookite (210) surface.

### Please confirm that you<br>have carefully read the<br>abstract submission instructions<br>under the menu item<br>"Call for Abstracts"<br><b/(Yes / No)</b>

yes

## Consideration for<br>student awards<br><b>Choose one option<br>from those below.</b><br>N/A<br>Hons<br>MSc<br>PhD

PhD

# Supervisor details<br><b>If not a student, type N/A.</b><br>Student abstract submision<br>requires supervisor permission:<br>please give their name,<br>institution and email address.

Eric Maluta, University of venda, eric.Maluta@univen.ac.za

Primary author: Mr DIMA, Ratshilumela Steve (University of venda)

Co-authors: Dr MALUTA, Nnditshedzeni Eric (University of Venda); Dr MAPHANGA, Rapela (CSIR)

Presenter: Mr DIMA, Ratshilumela Steve (University of venda)

### Session Classification: Poster Session 2

Track Classification: Track F - Applied Physics