
Contribution ID: **298** Type: **Poster Presentation**

# Electronic and Optical Properties of Ru and Pt Doped TiO2 Brookite Surfaces Using Density Functional Theory

*Thursday, 11 July 2019 15:00 (2 hours)*

The electronic structures and optical properties of brookite TiO2 (210) surfaces doped with transition metals (Ru and Pt) have been investigated by first-principles calculations based on the density functional theory employing generalized gradient approximation (GGA). The modelled surface structures were constructed from an optimized brookite bulk structure. TiO2 surfaces were doped with transition metals, with one Ti atom replaced by a transition metal atom. The results indicate that both transition metals doping can narrow the band gap of TiO2, leading to the improvement in the photo reactivity of TiO2. The metal dopants shift the absorption to high wavelengths and improves optical absorbance in visible and near-IR region.

## Apply to be<br> considered for a student <br>   award (Yes / No)?

yes

## Level for award<br> (Hons, MSc, <br>   PhD, N/A)?

PhD

**Primary author:** Mr RATSHILUMELA STEV, DIMA (CSIR/UNIVEN)

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

**Presenter:** Mr RATSHILUMELA STEV, DIMA (CSIR/UNIVEN)

**Session Classification:** Poster Session 2

**Track Classification:** Track A - Physics of Condensed Matter and Materials