Contribution ID: **218** Type: **Poster Presentation**

COMPUTATIONAL STUDY OF ELECTRONIC AND OPTICAL PROPERTIES OF THE CROCONATES DYE MOLECULES FOR APPLICATION IN DYE SENSITIZED SOLAR CELLS.

Tuesday, 4 July 2017 17:10 (1h 50m)

Currently the dye sensitised solar cells have attracted more attention due to its low cost, transparency and flexibility. These types of solar cells uses the dye molecules adsorbed on the TiO₂ semiconductor in their architecture with the role of absorbing photon from the sun. The electronic structure and excitation properties of dye sensitizer determine the efficiency of the dye sensitised solar cell. The sensitizer absorbs the photon from the sun and then inject an electron on the TiO₂ semiconductor. In the current work the DFT calculations were employed to study the geometric, electronic and optical properties of two croconate dye molecules. The calculations are based on conjugate length, charge transfer distance and absorption bands. The analysis of the excited state properties and free energy changes for electron injection support that the croconates dye molecules can improve the efficiency of DSSCs as they can absorb on the near infrared, which increase the absorption range on the solar spectrum. The increase of absorption towards the infrared gives more probability of high photon absorption and electron transport on the large band gab TiO₂.

Keywords: Dye Sensitized Solar Cells, Dye, Croconate, Efficiency

Apply to be
 considered for a student
   award (Yes / No)?

Yes

Level for award
 (Hons, MSc,
   PhD, N/A)?

MSc

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

Primary author: Mr RANWAHA, Tshifhiwa Steve (University of Venda)

Co-authors: Mrs ELEGBELEYE, Ife Fortunate (University of Venda); Dr MALUTA, Nnditshedzeni Eric (University of Venda); Dr MAPHANGA, Rapela (University of Limpopo)

Presenter: Mr RANWAHA, Tshifhiwa Steve (University of Venda)

Session Classification: Poster Session 1

Track Classification: Track F - Applied Physics