



Contribution ID: 128

Type: Oral Presentation

Computational study of dye adsorption in nano TiO_2 film for the applications in dye sensitized solar cells using different computational techniques

Wednesday, 13 July 2016 12:15 (20 minutes)

Abstract content
 (Max 300 words)
Formatting &
Special chars

The theoretical and computational studies of dye sensitized solar cells (DSSCs) can contribute to a deeper understanding of these types of solar cells. In the current study the density functional theory and the finite element methods are used to understand the factor affecting the dye adsorption and electronic properties of the TiO_2 semiconductor as the main element of DSSCs. The light adsorption occurs in dye molecules adsorbed on a highly porous structure of TiO_2 film. The processes followed experimentally for dye uptake is by dipping the TiO_2 semiconductor electrode into the dye solution for periods of several hours to several days. To understand the process of dye adsorption on the surface of TiO_2 , the DFT calculations was carried out to study the electronic structure of the ruthenium doped brookite TiO_2 surface. The factors controlling the dye uptake process are also investigated, using a simple model based on the Langmuir isotherms. Our computational modelling results show that the adsorption of dye into the TiO_2 nanotubes film is controlled by the diffusion coefficient, the adsorption-desorption ratio and the initial dye concentration.

Keywords: Solar Cells, Dye Sensitized, Dye, Surface Coverage, Langmuir

Primary author: Dr MALUTA, Nnditshedzeni Eric (University of Venda)

Co-authors: Mrs MULAUDZI, Sophie (University of Venda); Prof. SANKARAN, Vaith (University of Venda)

Presenter: Dr MALUTA, Nnditshedzeni Eric (University of Venda)

Session Classification: Parallel Track B

Track Classification: Material and Nano Sciences