NITheCS
National Institute for Theoretical and Computational Sciences

NITheCS Colloquium
Monday, 16 August 2021, 16h00

Dr Eric Maluta (University of Venda)

"Theoretical Studies of Brookite TiO_2 as a Material for Dye-Sensitized Solar Cells"

ABSTRACT

Theoretical and computational studies of doped TiO_2 polymorphous can contribute to a deeper understanding of dye sensitized solar cells. These solar cells represent a promising approach to a direct conversion of sunlight into electrical energy at low cost and with high efficiency. The light adsorption occurs in dye molecules adsorbed on a highly porous structure of TiO_2 film. The problem encountered with the TiO2 is its wide band gap which is about 3.4 eV and show photocatalytic activity under UV light irradiation that accounts for only a small portion of solar energy, in contrast to visible light which has a major part of solar energy. Harnessing and effectively utilizing sunlight is the most challenging subject for the extensive application of TiO_2 as photon absorption. Transition metal doping is one of the most effective approaches to extend the absorption edge of TiO_2 to visible light region, which either inserts a new band into the original band gap, or modification of the conduction band (CB) or valence band (VB) improving the photocatalytic activity of TiO_2 to some degree. In this presentation, theoretical studies on understanding the interactions of dopants and dye molecules with brookite surfaces and nanoclusters will be discussed focusing mainly on electronic and optical properties.

BIOGRAPHY

Nnditshedzeni Eric Maluta was born in the Mafukani village in the rural Mutale region of Limpopo. He attended the University of Limpopo (Turfloop Campus) where he graduated with an honors degree in physics. He completed a master's degree through the renewable energy (physics) program at the University of Venda. In 2007, Eric was awarded a sponsorship to further his studies at the University of Bath in the UK and completed a PhD within three years. His research topic was 'Simulation of Dye Sensitized Solar Cells.'

Since joining the University of Venda full time, he has volunteered to support projects that improve the physical sciences curricula in rural SA secondary schools under Vuwani Science Resource Centre. He also participated in the Kagiso Trust teachers upgrading projects, SA National Science Week, and regional & national science fairs. He holds the education portfolio as a council member of the South African Institute of Physics (SAIP).

"I am interested in computational studies of different energy material (theoretical studies of materials for solar energy conversion) to improve the efficiency of different renewable energy technologies. Apart from the computational studies of energy materials, my other research focus involves the analysis of solar radiation and renewable energy hybrid systems that will provide a sustained supply of energy to rural regions that aren't on the electrical grid. By supplementing the supply in rural communities, it will no longer be necessary to practice load-shedding in SA cities."

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