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DFT STUDY OF SELECTED NEAR INFRARED (NIR) FREE METAL DYE MOLECULES FOR APPLICATION IN DYE SENSITIZED SOLAR CELLS

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

Dye-sensitized solar cells (DSSCs) have attracted considerable attention in recent years as they offer the possibility of low-cost conversion of photovoltaic energy. DSSCs use the dye molecules adsorbed on the TiO₂ semiconductor in nano architecture with the role of absorbing photon from the sun. The electronic structure and excitation properties of dye sensitizer determine the efficiency of the DSSCs. The dye molecule is sensitizer that absorbs the photon from the sun and inject an excited electron on the TiO₂ semiconductor. The study focuses on the understanding of different properties (electronic optical properties) of NIR-dye molecules employing density functional theory (DFT) calculations. The calculations are based on the determinations of Absorption spectrum, UV-Vis spectrum and Light Harvesting Efficiency of the dye molecules. The results obtained shows that NIR-dye molecules can improve the efficiency of DSSCs as there is a shift of absorption to the near infrared, which increase the absorption range from visible on the solar spectrum.

Keywords: Dye Sensitized Solar Cells, Dye,Efficiency

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