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# DENSITY FUNCTIONAL STUDY OF CYANIDIN DYE MOLECULE ADSORBED ON TiO2 SEMICONDUCTOR

The performance improvement of Dye-sensitized solar cells (DSSCs) have been the centre of research in recent years as DSSCs are of low-cost conversion of photovoltaic energy. DSSCs uses the dye molecules adsorbed on the TiO2 semiconductor for the photon absorptions. The electronic structure and excitation properties of dye sensitizer determine the efficiency of the DSSCs. The current work discusses the computational study of selected cyanidin dye adsorbed to TiO2 semiconductor using the density functional theory. The electronic and optical properties of dye molecule and TiO2/dye complex, and the electron injection between the dye molecule and the TiO2 semiconductor are discussed in detail. The results obtained shows that there is a spontaneous electron injection between the dye molecules and TiO2 semiconductor with strong light harvesting efficiency, this feature can improve the efficiency of DSSCs as they cause a red shift of absorption to the near infrared, which increase the absorption range from visible solar spectrum.

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