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Density functional theory study of Porphyrin dye molecule adsorbed on TiO2 (010) Anatase surface.

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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 nanoarchitecture with the role of absorbing photons from the sun. In this study, Density functional theory (DFT) has been used to study the geometric, electronic, and optical properties of Pheophytin dye and its adsorption behaviour on (010) TiO2 anatase surface. The generalized gradient approximation (GGA) was used in the scheme of Perdew-Burke Ernzerhof to describe the exchange-correlation function as implemented in the CASTEP package in the material studio of BIOVIA. The results obtained show that Pheophytin dye molecules can improve the efficiency of DSSCs as they show an absorption shift to the near-infrared region, which increases the absorption range on the visible solar spectrum.

Key words: DSSC, DFT, Porphyrin Dye

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

YES

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

MSc

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