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Density Functional Theory Study of Azo Dye Molecules Adsorbed onto Anatase TiO2 (112) Surface for Application in Dye-Sensitized Solar Cells

The escalating costs of fossil fuels and the finite nature of accessible reserves the indispensable need of studying alternative energy sources. Organic solar cells present a practical and economical technology for capturing solar energy, utilizing materials that are often both accessible and recyclable. Conventional silicon solar cells demonstrated significant reliability; however, their costs remain a barrier. Dye-sensitized solar cells (DSSCs) present a compelling alternative at a significantly reduced cost. In this study, density function theory has been used to explore the adsorption behavior of synthetic dye on the surface of (1 1 2) TiO2 anatase polymorph. Generalized gradient approximation was used to define the exchange-correlation function within the scheme of Perdew-Burke Ernzerhof as implemented in the Material Studio.The effectiveness of the dye-sensitized solar cell is dependent upon the electronic configuration of the dye-sensitizer and its excitation properties. Our results show the UV-Vis absorbance of Azo dye 1, Azo dye 2, Azo dye 3 and Azo dye 4 at 570 nm, 428 nm, 439 nm, and 648 nm, respectively, along with a calculated light harvesting efficiency of 51.3%, 29.5%, 50.58%, 74.8%, respectively. Among the computed four Azo dyes, the results indicate that Azo dye 4 has a stronger sensitization capability relative to the others, with a small HOMO-LUMO gap. Furthermore, the band gap of the anatase is reduced after Azo dye adsorption. The calculated adsorption energies are found to be negative, implying that Azo dyes molecules are electron-donating substituents, and strongly bind strongly to the anatase surface.
Keywords: Azo dyes, semiconductor, band gap, density functional theory, Dye-sensitized solar cells, TiO2

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