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DENSITY FUNCTIONAL STUDY OF ELECTRONIC, OPTICAL AND ADSORPTION PROPERTIES DYE ON ANATASE AND BROOKITE TIO2 SURFACES FOR APPLICATION IN DYE SENSITIZED SOLAR CELLS

Monday, 4 December 2017 13:30 (30 minutes)

Theoretical and computational studies of doped TiO2 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 TiO2 film [1-2]. 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 TiO2 as photon absorption [3]. Transition metal doping is one of the most effective approaches to extend the absorption edge of TiO2 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 TiO2 to some degree [3-5].

In the current study, electronic density of states and optical properties of doped and undoped, Anatase and Brookite surfaces were performed using the first-principles calculations based on Density Functional Theory (DFT) using a plane-wave pseudopotential method. The generalized gradient approximation (GGA) was employed in the scheme of Perdew-Burke-Ernzerhof (PBE) to describe the exchange-correlation functional. All calculations were carried out with CASTEP (Cambridge Sequential Total Energy Package) code in Materials Studio of Accelrys Inc [6]. The results confirm that the mixing of the dopants induced states with the original Ti 3d and O 2p valence band and conduction band attributes to the band gap, hence the shifting of the absorption edge of TiO2 from UV to visible spectrum. The light harvesting efficiency of the dye molecules were calculated and compared to the experimental values.

Keywords: Dye sensitized solar cells, Density Functional theory, Bandgap, Optical and Electronic Properties.

References

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First-principles calculations based on Density Functional Theory (DFT) using a plane-wave pseudopotential method. The generalized gradient approximation (GGA) was employed in the scheme of Perdew-Burke-Ernzerhof (PBE) to describe the exchange-correlation functional. All calculations were carried out with CASTEP (Cambridge Sequential Total Energy Package) code in Materials Studio of Accelrys Inc [6]

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