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Density functional theory study of Cyanidin (Cy) dye molecule adsorbed on (100) TiO2 anatase surface for application in DSSCs

The dye sensitized solar cells have attracted more attention due to their low cost, transparency and flexibility. These types of solar cells use the dye molecule adsorbed on TiO2 semiconductor in nano architectural form with the role of absorbing photo catalytic properties only in the ultraviolet region of solar spectrum. TiO2 absorbs light in the ultraviolet spectrum but can be photosensitized by the adsorption of organic and/or inorganic dye molecules to absorb the light in visible and near infrared regions. In the this study, density functional theory was used to investigate the geometric, electronic and optical properties of cyanidin dye adsorbed on (100) anatase TiO2 surface. Our results show a redshift absorption of cyanidin dye adsorbed on (100) anatase TiO2, with a shift of Valence band towards the conduction band which is the reduction of band gap The adsorption results show a spontaneous electron injection followed by efficient regeneration of the oxidized dye molecules by the electrolyte and strong binding ability to the TiO2 surface.

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

yes

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

MSc

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