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Adsorption of natural dye (Porphyrin and Pheophytin) molecules on TiO2 (101) anatase surface for improved light harvesting efficiency in dye-sensitized solar cells

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Dye-sensitized solar cells (DSSCs) have gained popularity in recent years due to their ability to convert sunlight to photovoltaic energy at a low cost. DSSCs use dye molecules adsorbed on TiO2 semiconductors in nanoarchitecture to absorb photons from the sun. In this study, density functional theory was utilized to investigate the geometric, electrical, and optical features of pheophytin and porphyrin dye, as well as its adsorption behaviour on the (010) TiO2 anatase surface. Generalized gradient approximation (GGA) was used to define the exchange-correlation function within the scheme of Perdew-Burke Ernzerhof (PBE), as implemented in the material studio of the BIOVIA CASTEP module. Pheophytin experienced lower photon absorbance in both the visible and near-infrared regions, resulting in lower efficiency. However, when methanol, ethanol, and water solvents were added to the molecule, the blue shift to the visible region and more photon absorption at a higher oscillating strength increased the visible region's efficiency. The results showed that pheophytin and porphyrin dye molecules can improve DSSC performance by shifting absorption to the near-infrared region, improving visible solar spectrum absorption.