Simulation of natural dyes adsorbed on TiO2for photovoltaic applications

Gomez T.

Jaramillo F.

Schott E.

Arratia-Pérez R.

Zarate X.

The study of the electronic structure and optical properties of natural pigments using state of the art time-dependent first-principles calculations is presented to highlight their usefulness for photo electrochemical devices. Ground state geometries, UV?vis spectra and photovoltaic properties are reported. In the family of chosen anthocyanidins, it is observed that the frontier molecular orbitals (FMOs) are mainly localized over the whole molecule with exceptions noted for Delphinidin and Petunidin, while in the anthocyanins all the FMOs are localized over the three rings of the molecule, without any contribution of the glycoside motifs. Conversely, the interaction between Cyanidin and Cyanidin 3,5-diglucoside with TiO2as the semiconductor in its cluster and surface form was also studied using periodic density functional calculations for suitable supercell models representing the systems of interest. For the Cyanidin 3,5-diglucoside/TiO2system the results showed that its highest occupied molecular orbital (HOMO) is located in the TiO2bandgap and its lowest unoccupied molecular orbital (LUMO) is close to the TiO2conduction band minimum (CB) leading to greatly enhanced visible light absorption.

Dye-sensitized solar cell

Optical spectra

TD-DFT

Calculations

Dye-sensitized solar cells

Dyes

Electronic structure

Ground state

Light absorption

Molecular orbitals

Molecules

Optical properties

Electronic structure and optical properties

First-principles calculation

Frontier molecular orbitals

Highest occupied molecular orbital

Lowest unoccupied molecular orbital

Optical spectra

Photo-electrochemical device

TD-DFT

Titanium compounds

adsorption

dye

electrical conductivity

optical property

photovoltaic system

physicochemical property

pigment

solar power

spectrum

titanium