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Excited States of Cyanidin as Dye Sensitizer on Small TiO_2 Nanoclusters Used as Photocatalyst in Hydrogen Production: A DFT Study

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ABSTRACT

Based in prior work within our research team, we use anthocyanidin molecule cyanidin as a pigment water soluble widely distributed in plants interacting with $(TiO_2)_n$ nanoclusters. Using our prior results with nanostructures formed with pristine cyanidin and $(TiO_2)_n$ we gathered data about ground states. Using these basis we carry out a study involving these same nanostructures to compute excited state energies, as well as absorption wavelength using Time Dependent-Density Functional Theory (TDDFT) for both nanostructures in its pristine form and also for the different variants formed by one out of four nanoclusters, in particular, when there is interaction with cyanidin. All calculations were developed using DFT theoretical methods performed at the Gaussian09 programs suite. Ground states calculations for pristine nanoparticles, including geometries, atomization energies, HOMO-LUMO and other properties, were obtained using B3LYP/6311+G(d, p). For the emission wavelength, the excited state geometry optimization was carried out with Hartree–Fock Configuration Interaction Singles (HF/CIS). Our theoretical results are new data related to the geometry as well as to the spectral absorption/emission properties of the proposed nanostructures. These cluster variants present features interesting for solar technology and optical applications. Our work generates data to learn more about the interaction of cyanidin with $(TiO_2)_n$ nanostructures which is a topic of interest for the application of natural dyes in solar cells and photocatalysis.

Keywords: Titanium dioxide nanoclusters, cyanidin, photocatalysis, hydrogen generation