Anthocyanins are pigments obtained from plants that may appear in different colors and because of this, they have become a subject of great interest [1-6]. We use delphinidin 3-glucoside ($C_{21}H_{21}O_{12}$)$^+$, known as delphinidin, as a sensitizer on four small ($TiO_2$)$_n$ nanoclusters with (n=2-5) used in prior research within our team [7-9]. Results within the literature are compared with our results for the individual particles.

Our contribution relies in the study of the interaction between delphinidin and the nanoclusters aimed to understand their electronic structure for applications in hydrogen generation employing photocatalysis.

Delphinidin is known for its blue-red colors in some flowers and fruits and may benefit ($TiO_2$)$_n$ nanoclusters properties for solar technology applications. DFT theoretical calculations were performed in the Gaussian09 programs suite [10]. Delphinidin as a (+1) cation initial structure as well as ($TiO_2$)$_n$ nanoclusters were relaxed using B3LYP/6311+G(d, p). DFT calculations include geometry, vibrational frequencies and atomization energies and HOMO-LUMO parameters for the individual delphinidin and nanoclusters. Conceptual DFT was used for individual particles to calculate ionization potential, electronic affinity, softness, hardness, and Fukui functions. Four nanostructures were formed with delphinidin and a particular variant out of four ($TiO_2$)$_n$ nanoclusters. This work intends to generate data so we learn more about the feasibility of using ($TiO_2$)$_n$ sensitized with delphinidin for the application in photocatalysis when used within a hydrogen generation process.

Keywords: Titanium dioxide nanoclusters, Delphinidin pigment, Hydrogen generation

References:


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