

TiO₂ thin films sensitization with natural dyes extracted from *Bactris guineensis* for photocatalytic applications: Experimental and DFT study

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TiO₂ thin films, sensitized by an anthocyanins-rich extract of a common species found in the Colombian Caribbean region (*Bactris guineensis* fruits), were used for the photocatalytic degradation of methylene blue. The sensitization process was verified by diffuse reflectance spectroscopy (DRS). The qualitative and quantitative analyses of the anthocyanins were carried out using high-performance liquid chromatography with photodiode array detection (HPLC-DAD), which provided the total content anthocyanin equivalent to delphinidin chloride (TAEDC) per mL of the extract, of $10.0 \pm 0.8 \mu\text{g TAEDC/mL}$. Here, three main anthocyanins were identified, being cyanidin-3-rutinoside the most abundant constituent (ca. 76%). The interaction of the dyes with a TiO₂ slab model and their adsorption energies were determined through computational simulations. In addition, the molecular modelling evidenced that the sensitization of the semiconductor improved the light absorption in the visible range of the spectrum. As a final point, the photocatalytic test showed that the photocatalytic activity increased 26% for TiO₂/*B. guineensis* thin films under visible radiation respect to bare TiO₂. © 2020 The Authors

Anthocyanin

DFT

Natural sensitizer

TiO₂