

Improvement of the photocatalytic activity of TiO₂ using Colombian Caribbean species (*Syzygium cumini*) as natural sensitizers: Experimental and theoretical studies

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Natural dyes composed by anthocyanins extracted from natural Caribbean species *S. cumini*, were employed to evaluate their effects on the photocatalytic properties of TiO₂ thin films. The qualitative and quantitative analyses of the anthocyanins were carried out using high-performance liquid chromatography with photodiode array detection (HPLC-DAD). From the chemical characterization of the *S. cumini* extract three main anthocyanins were identified and the most abundant compound was delphinidin-3,5-diglucoside (44%). The total anthocyanin content expresses as delphinidin chloride (TAEDC) per mL of the extract was equal to $124 \pm 5 \mu\text{g TAEDC/mL}$. After the identification, a sensitization process was performed and verified by infrared spectroscopy (IR) and absorption diffuse reflectance. Afterwards, the Methylene Blue photodegradation process was studied under visible light irradiation on the *S. cumini*-sensitized TiO₂ material (TiO₂/*S. cumini*). The results indicated that the photocatalytic activity of the sensitized material TiO₂/*S. cumini* was 3 times greater than unmodified TiO₂ thin films, which let us to propose that the extract from Caribbean Colombian *S. cumini* could have a great potential as source of photosensitizers for photocatalytic applications. Finally, the electronic structure of each anthocyanin found in the extract (delphinidin-3,5-diglucoside, malvidin-3-5-diglucoside and petunidin-3-5-diglucoside) and their

interaction with a TiO₂ model was studied by means of the density functional theory (DFT). © 2017

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