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## Title

### ***Cyanobacterial pigment adsorbed on TiO<sub>2</sub> thin films***

## Abstract

The rise in toxicity related to cyanobacterial bloom in freshwater is a current problem that perturbs the trophic chain and risks the ecosystems and human health. Currently, the use of biomass as a potential source of value-added bio-products is an important goal to be achieved in the scope of a sustainable bio-economy. Thus, taking advantage of such bacteria is needed. In the present work, we studied the use of cyanobacterial biomass coming from the Malambo swamp in Colombia as a source of Phycocyanobilin (C-PC) and Chlorophyll-a (Chla) which were used as natural pigments for TiO<sub>2</sub> thin films. The concentration obtained of C-PC and Chla extracted were 215 µg/mL and 0.417 µg/mL, respectively. We modeled the natural dye adsorption kinetics on TiO<sub>2</sub> thin films through three different models. The Langmuir model showed the best fitting, indicating that the pigment extracted from cyanobacterial biomass can sensitize thin TiO<sub>2</sub> film through the formation of a monolayer. Furthermore, the TiO<sub>2</sub> films present higher adsorption of C-PC (25.8 mg/g) than Chla (23.3 mg/g). Finally, the adsorption modes were assessed using periodic DFT approximations, which is a remarkable method for studying the structure and properties of solid materials. In terms of binding energies, it was found that the dye shows the strongest interaction with TiO<sub>2</sub> through the titanium atom. Thus, the main contribution of this work is directed to explore in deep the natural dye adsorption on TiO<sub>2</sub> from both experimental and computational point of view. © 2024 Elsevier B.V.

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