Zn(II)-tetracarboxy-phthalocyanine-Sensitized TiO_2Thin Films as Antimicrobial Agents under Visible Irradiation: A Combined DFT and Experimental Study

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Abstract
In this article, we studied the antimicrobial activity of TiO2 sensitized by the Zn(II)-tetracarboxy-phthalocyanine (TcPcZn) complex using TiO2-Degussa P25 as a semiconductor source. The TiO2 thin films were deposited by the doctor blade method and were sensitized by the chemisorption process. The obtained compounds were characterized using Fourier transform infrared spectroscopy, UV-vis spectrophotometry, Raman spectroscopy, diffuse reflectance spectroscopy, and scanning electron microscopy. Furthermore, we studied the stability of the adsorbed sensitizer on the semiconductor surface by using the density functional theory (DFT). Additionally, we determined the antimicrobial activity of TcPcZn-TiO2 against methicillin-resistant Staphylococcus aureus (MRSA). The Raman and optical results confirmed the sensitizing process. The TcPcZn-TiO2 thin films showed radiation absorption in the visible range of the electromagnetic spectrum (600-750 nm), and the dye anchored on the TiO2 surface had a band gap of 1.58 eV. The DFT study showed that TcPcZn supported on any phase of Degussa P25 is stable, making them suitable to act as catalysts in the proposed reactions. Finally, the TcPcZn-TiO2 thin films reached 76.5% of inhibition activity against MRSA. ©