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Multifunctional Bi₂Se₃-TiO₂ Nanostructures for Rapid Photocatalytic Degradation of Anticancer Drugs and Enhanced Photoelectrochemical Water Splitting

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Abstract: Anticancer drugs (ACDs) are among the most toxic pharmaceutical pollutants and are increasingly detected in hospital effluents, where they pose a serious risk to aquatic environments. Three-dimensional Bi₂Se₃ topological insulators, with a narrow bulk band gap (~0.3 eV) and an oxidized state band gap of ~0.8 eV, offer strong IR-visible absorption and favorable band alignment for photocatalysis and photoelectrochemistry. In this work, Bi₂Se₃ nanoparticles were prepared by electrochemical exfoliation, while TiO₂ nanotube arrays and TiO₂ nanowires-on-nanotubes films were grown on Ti by anodic oxidation. Bi₂Se₃/TiO₂ nanostructured films with controlled Bi₂Se₃ loading were fabricated and characterized structurally, morphologically, and compositionally. Their photocatalytic activity toward eight representative ACDs (IF, CY, GEM, CAP, MET, DOX, IRI, 5-FU) was quantified by LC-MS/MS, with optimized architectures achieving apparent first-order rate constants up to ~2.4–2.7 × 10⁻¹ min⁻¹ for 5-FU and ~1.5–3.5 × 10⁻¹ min⁻¹ for several other drugs, enabling rapid removal in both model solutions and real hospital wastewater, with stable performance over at least five reuse cycles. Additionally, Bi₂Se₃ hexagonal nanosheets-TiO₂ nanoparticle nanocomposites obtained via hydrothermal synthesis showed markedly enhanced photoelectrochemical water-splitting currents under UV-Vis and Vis illumination, owing to improved IR-Vis light harvesting and more efficient separation of photogenerated carriers at Bi₂Se₃-TiO₂ heterointerfaces. These results identify Bi₂Se₃-TiO₂ nanostructures as promising dual-function materials for pharmaceutical wastewater remediation and solar-driven hydrogen production.

Keywords: Bi₂Se₃-TiO₂, Anticancer Drugs, Photoelectrochemical (PEC) water splitting, LC-MS/MS

