Electronic Supplementary Information

Bandgap-Engineered In_2S_3 Quantum Dots Anchored on Oxygen-Doped g-C_3N_4: Forging a Dynamic n-n Heterojunction for Enhanced Persulfate Activation and Degradation of Metronidazole

1. Synthesis of g-C_3N_4 and O@g-C_3N_4

A facile thermal polymerization method produced pure g-C_3N_4 using melamine as the precursor. In a perfect world, 5 g of melamine would be burned for 4 hours at a temperature of 550 °C with a ramp rate of 20 °C/min. After allowing the yellow product to cool naturally to room temperature, it was evenly crushed into powder.

Similarly, 1 g of oxalic acid dihydrate and 5 g of melamine were crushed and calcined for 4 hours at the same temperature to create O@g-C_3N_4. When the final goods had naturally cooled to room temperature, they were uniformly crushed into powder.

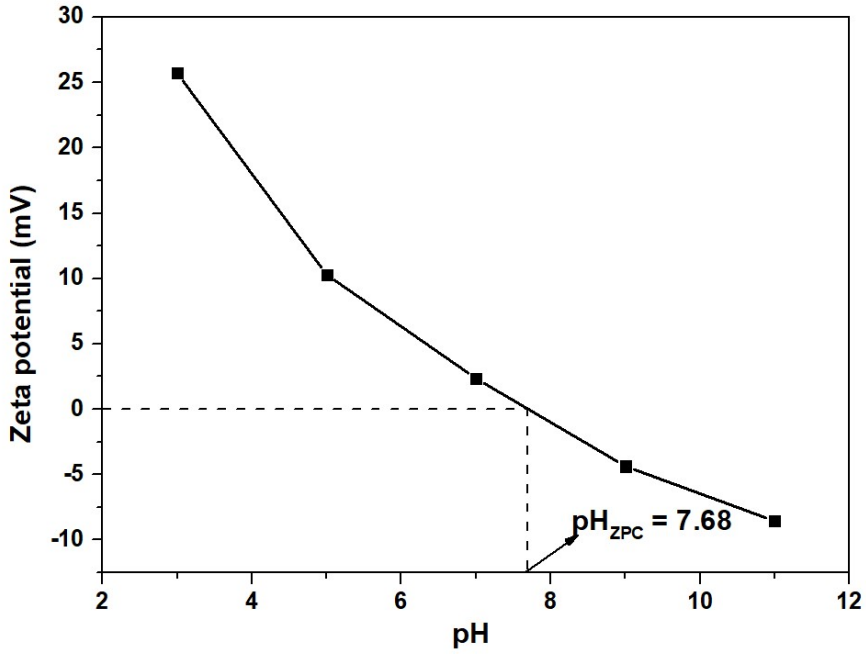
2. Synthesis of In_2S_3

3 mmol of thioacetamide and 2 mmol of indium chloride tetrahydrate were added to a 100 mL beaker containing 40 mL of distilled water and 10 mL of ethanol. Before being moved to a Teflon container within a stainless-steel autoclave, the solution was stirred for 30 min at 600 rpm in a magnetic stirrer at room pH. The sealed autoclave was maintained at 160 °C in a hot air oven for about 12 hours. The resultant material was centrifuged, thoroughly washed with distilled water, and dried at 65 °C overnight to obtain the required In_2S_3 nanoparticles.

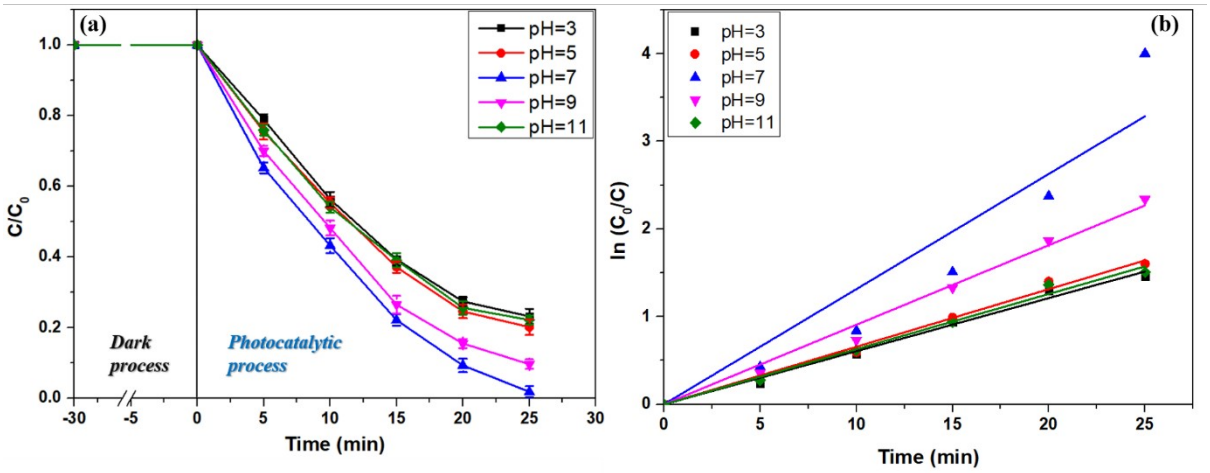
3. Characterization details

Using the PANalytical X'PERT powder X-ray diffractometer, the X-ray diffraction (XRD) spectra of the produced In_2S_3 nanoparticles, O@g-C_3N_4, and In_2S_3/O@g-C_3N_4 nanocomposite were obtained. The surface functional groups of all the produced materials were evaluated

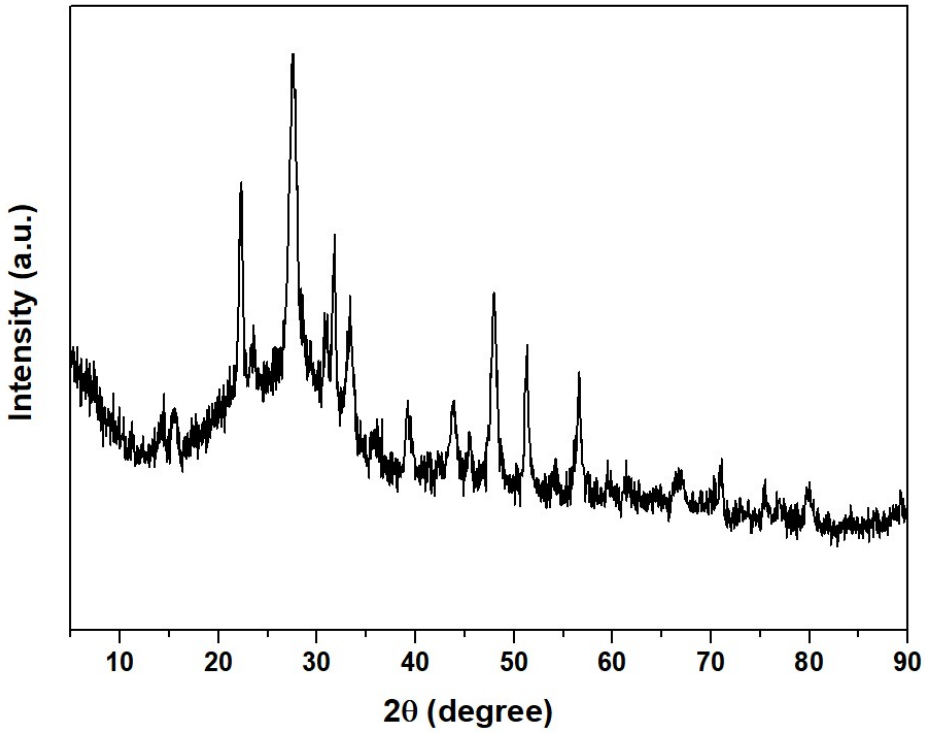
using Fourier transform infrared spectroscopy (FT-IR, Niagoli IS50, USA) over a wavelength range of 500–4000 cm^{-1}. SAED patterns and high-resolution transmission electron microscopy (HRTEM) pictures were acquired using a JOEL JEM 2100 apparatus. The PHI 5000 Versa Probe III spectrometer recorded the nanocomposite's X-ray photoelectron spectra (XPS). The energy dispersive X-ray (EDX) data and FE-SEM pictures were recorded using an FEI quanta FEG 200 high-resolution scanning electron microscope (SEM). The intermediate products of MDZ degradation were measured using the mass spectra obtained with a Xevo XS QTof mass spectrometer. Using a Hach Dr 6000 UV-Vis spectrophotometer, the ultraviolet-visible diffuse reflectance spectra (UV-DRS) data were collected. The absorbance spectra of the liquid samples were captured using a GENESYS 10S UV-visible spectrophotometer with a 1 cm quartz cell and a scan rate of 600 nm/min.



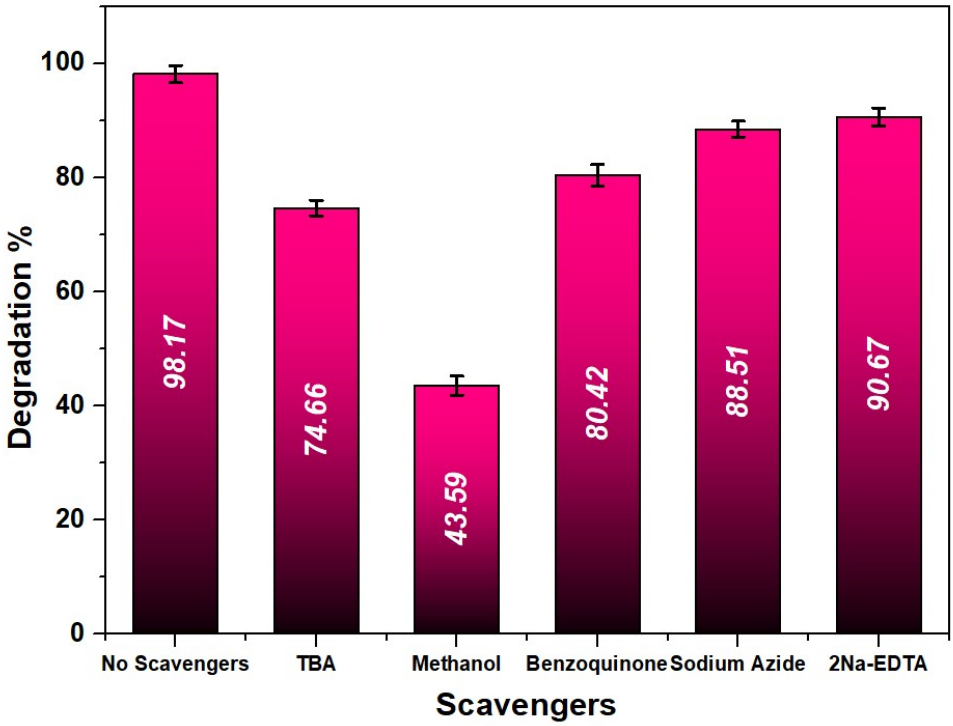
Supplementary Figure 1: *Zeta potential of In_2S_3/O@g-C_3N_4.*



Supplementary Figure 2: *a) Degradation profile and b) degradation kinetics for the effect of pH.*



Supplementary Figure 3: *XRD analysis of the fabricated material after seven cycles.*



Supplementary Figure 4: *Role of scavengers in the degradation of MDZ.*