

ABSTRACT

In this research, Ag (3 and 6 wt. %) and carbon sphere (CS) (3 wt. %) were successfully incorporated into Fe_2O_3 using a co-precipitation approach. This study aimed to degrade the methylene blue (MB) dye and investigate the bactericidal effect of doping-dependent Fe_2O_3 . The pristine sample has good stability and is less toxic; however, it showed poor degradation potency. To enhance the catalytic activity (CA), CS was introduced as it increases Fe_2O_3 adsorption capacity and improves metal oxide properties. Ag was incorporated into CS- Fe_2O_3 , which created additional active sites and might generate reactive oxygen species (ROS). XRD patterns revealed the tetragonal and monoclinic structure of Fe_2O_3 , and crystallinity was enhanced with dopants (Ag and CS). FTIR was performed to identify vibrational and rotational modes and functional groups of samples. SAED pattern represented the polycrystalline structure of Fe_2O_3 and (3 & 6 wt.%) Ag/CS- Fe_2O_3 . UV-vis spectroscopy depicted that absorption decreased with the increasing amount of Ag/CS and increased band gap energy (E_g). PL spectra of doped Fe_2O_3 represent the reduction in recombination rate, resulting in enhanced CA. EDS spectra exhibited the presence of Fe, O, Na, Au, and C, which confirmed the elemental composition of pristine and doped samples. TEM images indicate nanorods (NRs) of Fe_2O_3 , and HRTEM provides interlayer d-spacing increased upon doping. The nanostructures exhibited excellent CA for the degradation of MB dye in an acidic medium, around 99.44%. Ag/CS- Fe_2O_3 (6 wt. %) nanostructures have shown a significant increase in the inhibition zone (3.65 mm) against *Escherichia coli* (*E. coli*) at high-level doses. This study suggests that (3 & 6 wt.%) Ag/CS- Fe_2O_3 nanostructures revealed superior catalytic and antibacterial activity for wastewater treatment. First-principles calculations indicate that the adsorption energies show a relatively strong interaction between MB and (3 & 6 wt.%) Ag/CS- Fe_2O_3 .