Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering. This journal is © The Royal Society of Chemistry 2023

Supporting Information

For

Electrocatalytic and Photocatalytic Activity of CuTiO₃ Perovskites for Complete

Degradation of Methylene Blue under Sunlight Irradiation

Sanakousar. F. M¹, Vidyasagar. C. C^{1*}, Shikandar. D. B^{2*}, Mounesh³, Viswanatha. C. C⁴, Swapna S Chigari¹

¹Department of PG Studies and Research in Chemistry, Rani Channamma University, Belagavi-591156 Karnataka, India.

²Department of Chemistry, K.L.E. Institute of Technology, Hubli-580030, Karnataka, India.

³Centre for Nano and Materials Sciences, Jain (Deemed-to-be University) Global Campus, Jakkasandra, Kanakapura, Bangalore-562112, Karnataka, India.

⁴Department of Chemistry, J.S.S Arts, Science & Commerce College, Gokak-591307, Karnataka, India

(Email: vidya.891@gmail.com Cell No.: +91-9742885912)

X-ray fluorescence (XRF)

The results of an X-ray fluorescence (XRF) chemical investigation of the CuTiO₃ perovskites of 0.10 M CuTiO₃, 0.15 M CuTiO₃, and 0.12 M CuTiO₃ perovskites are given in **S. Fig. 1 a-c**. Energy dispersive X-ray spectroscopy (EDX) examinations confirmed the compositional analyses shown of 0.10 M CuTiO₃, 0.15 M CuTiO₃, and 0.12 M CuTiO₃ perovskites in **S. Fig. 1 d-f**. The existence of Ti, O, and Cu from components was verified by the EDS and XRF spectra of CuTiO₃ perovskites. In XRF spectra the oxygen peak was very low.



Fig. S1. Shows the XRF and EDX data of (a & d) 0.10 M CuTiO₃, (b & e) 0.15 M CuTiO₃, and (c & f) 0.20 M CuTiO₃ perovskites.

Copper-leaching test

In the water filtration systems, secondary water pollution could result from a potential copper leaching from the 0.20 M CuTiO₃ during dye degradation from dye-contaminated water. To look into this potential problem, 0.15 g of 0.20 M CuTiO₃ was added to 100 mL of deionized water with a pH of 7.0 and a temperature of 25 °C while being shaken at 150 rpm for 24 h. The contents were separated by centrifugation, and the filtrate was examined using an atomic absorption spectrometer to determine whether any copper had leached from the 0.20 M CuTiO₃ into the aqueous medium. It was found that the 0.20 M CuTiO₃ leached 0.02 mg/L of copper concentration. This copper leached out of the 0.20 M CuTiO₃ because most of the copper formed a chemical bond with the titanate, while some of the copper could not bond strongly with the titanate due to their restricted availability, any of the aggregation in nanoparticles upon compounding with the 0.20 M CuTiO₃, all of which can result in weak bonding of copper at certain places in the composite, resulting in leaching of some copper contents into a test water bath.¹ According to the World Health Organization (WHO) and the U.S. Environmental Protection Agency (EPA), the maximum Cu (II) concentration in aqueous systems should be 1.3 mg/L and 3 mg/L, respectively,² and the amount of Cu that was leaking in our study was less than that (0.02 mg/L). The chance of secondary contamination is significantly reduced by the very small concentration of 0.02 mg/L of copper that was leached from 0.15 g of 0.20 M CuTiO₃ (0.15 g CuTiO₃ contains 63.5 mg of Cu), confirming the material's strong impregnation with Cu. Additionally, the leaching profile confirms the 0.20 M CuTiO₃ composite's stability and applicability for usage in water treatment and other possible environmental applications.

Calculation of Valence band and Conduction band

The valence band potential (E_{VB}) and conduction band potential (E_{CB}) of the 0.20 M CuTiO₃ perovskites photocatalyst were determined using the equations below.

$$E_{CB} = \chi - E_e - 1/2 E_g \tag{1}$$

$$E_{VB} = E_{CB} + E_g \tag{2}$$

Where ' χ ' represents the semiconductor's absolute electronegativity, which is determined using the geometric mean of each atom's electronegativity, valence band potential is represented by E_{VB} , E_{CB} represents the conduction band potential, E_e is the hydrogen scale's (4.5 eV) free electron energy and the band gap energy of the photocatalyst is E_g . absolute electronegativity and the bandgap energy of 0.20 M CuTiO₃ perovskites, were determined to be 5.789 eV and 3.24 eV, respectively. The estimated valence band potential (E_{VB}) and conduction band potential (E_{CB}) for 0.20 M CuTiO₃ perovskites are 2.909 eV and -0.331 eV, respectively.³

References

- 1 A. Ayub, Z. A. Raza, M. I. Majeed, M. R. Tariq and A. Irfan, *Int. J. Biol. Macromol.*, 2020, **163**, 603–617.
- 2 Y. Liu, H. Wang, Y. Cui and N. Chen, Int. J. Environ. Res. Public Health, , 2023, 20, 3885.
- 3 V. Jayaraman, C. Ayappan, B. Palanivel and A. Mani, *RSC Adv.*, 2020, **10**, 8880–8894.



Fig. S2. Shows the absorbance spectra of MB dye without catalyst (a) in dark (b) under sunlight irradiation (self-photolysis), and adsorption of (c) MB dye with 0.10 M CuTiO₃ perovskite (d) MB dye with 0.15 M CuTiO₃ perovskite, and (e) MB dye with 0.20 M CuTiO₃ perovskite in dark.



Fig.S3. Shows the shorter time interval UV-visible absorbance spectra for photocatalytic degradation of MB dye using (a) 0.20 M CuTiO₃ perovskites with 05 mg catalyst using 10 ppm MB dye solution at natural pH. (b) 0.20 M CuTiO₃ perovskites with 20 mg optimized catalyst using 10 ppm MB dye solution at natural pH. (c) 0.20 M CuTiO₃ perovskites with 20 mg optimized catalyst using 20 ppm MB dye solution at natural pH. (d) 0.20 M CuTiO₃ perovskites with 20 mg optimized catalyst using 20 ppm MB dye solution at natural pH. (d) 0.20 M CuTiO₃ perovskites with 20 mg optimized catalyst using 20 ppm MB dye solution at natural pH. (d) 0.20 M CuTiO₃ perovskites with 20 mg optimized catalyst using 20 ppm MB dye solution at pH 7.