



Machine Learning-assisted Optimization of TiO₂/CuO Nanocomposites for Enhanced Energy Storage Performance

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ABSTRACT

Optimizing nanocomposites for energy storage requires precise control of structural, optical, and electrochemical properties. In this research TiO₂ and CuO nanoparticles were synthesized by hydrolysis and precipitation. They were integrated into a TiO₂/CuO nanocomposite. Structural and morphological features were examined using X-ray diffraction and scanning electron microscopy, while photoluminescence analysis assessed the optical behavior. Machine learning (ML) models, including Support Vector Regression (SVR), artificial neural networks, multilayer perceptron and hybrid fuzzy logic were employed to predict band gap, crystallite size, charge transfer resistance, and energy storage performance, respectively. CuO incorporation decreased the band gap from 3.0 eV at 0% to 2.1 eV at 30%, and minimized charge transfer resistance from ~16.8 Ω to ~5.8 Ω at 15% CuO. The crystallite size stabilized at 20.74 nm, with SVR demonstrating highest predictive accuracy ($R^2 = 0.927-0.956$). These results indicate that the TiO₂/CuO nanocomposite offers enhanced charge transfer and energy storage capability. The study validates the integration of ML and fuzzy logic in nanocomposite optimization, highlighting its potential for high-performance supercapacitors, batteries, and flexible electronic devices.

Keywords: Nanocomposites; Band gap; Charge transfer; Machine learning; Photoluminescence; Energy storage.

1. INTRODUCTION

Recent breakthroughs in science and technology necessitate the fabrication of increasingly advanced and intelligent nanocomposite materials. This encompasses the incorporation of nanostructures and nanocomposites for effective energy storage applications, including supercapacitors, batteries, and fuel cells. Ozankaya *et al.* (2023) predicted the tensile strength and failure load of the nanocomposites using machine learning (ML) models, including adaptive neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) that showed least error in prediction. Three modeling approaches, ANFIS, ANN and response surface methodology (RSM) were employed to understand the relationships between input variables and photocatalytic degradation performance. Low predictive accuracy was observed for ANFIS compared to ANN and RSM, with R^2 values of 0.9159 for ANN and 0.9876 for RSM (Rezvanasab *et al.* 2025). Al-doped ZnO films with varying thickness were investigated for their electrical and optical properties. The films showed an increase in crystallite size and a decrease in electrical resistance as

the thickness increased. The study also observed that doping influenced the optical band gap and improved the transmittance and structural properties of the material (Niyom and Rattanasakulthong, 2023).

ZnO nanoparticles were doped with Ag and Cu for energy storage applications. The doped nanoparticles showed a decrease in optical band gap and an increase in crystallite size. The Cu-doped ZnO nanoparticles demonstrated high specific capacitance, excellent cyclic stability, and good electrochemical properties for supercapacitor applications (Jostar *et al.* 2026). CeO₂ nanoparticles were doped with Ni²⁺, Cd²⁺, and Nb⁵⁺ to study their structural, optical, and photocatalytic properties. The doping led to changes in band gap energy, crystallite size, and surface area. Ni²⁺ doping enhanced photocatalytic degradation efficiency, particularly for methylene blue, making it a promising material for photocatalysis (Jayakumar *et al.* 2024). Cobalt doping in SnO₂ nanoparticles influenced the crystal phase, optical, and magnetic properties. The doping induced ferromagnetic behavior and it modified optical band gap from 3.79 eV to 3.62 eV. The study found that increasing

Co doping enhanced magnetic interactions, contributing to the ferromagnetic properties of the material (Priyadharsini *et al.* 2021).

Vanadium doping in CeO₂ thin films affected the crystallite size, surface morphology, and optical properties. Doping led to a decrease in band gap energy from 3.19 eV to 3.08 eV and increased surface roughness. The optical properties, such as refractive index and dielectric constant were also significantly altered with increasing V doping (El-Habib *et al.* 2021). The LaFe_{0.4}Co_{0.6}O₃/rGO nanocomposites were synthesized using a sol-gel method, which were investigated as catalysts for thermal decomposition of ammonium perchlorate (AP). The LaFe_{0.4}Co_{0.6}O₃/rGO (6:1) composite reduced the thermal decomposition peak of pure AP from 324°C to 308°C. The material was characterized using IR, UV-Vis, X-ray diffraction (XRD), and Raman analyses, with FE-SEM confirming uniform nanoparticle distribution. Artificial neural networks predicted activation energy and TG curves with low MSE values (Likhariya and Dave, 2026).

Çakan *et al.* (2026) synthesized Co-TPA@g-C₃N₄ nanocomposites by modifying graphitic carbon nitride with cobalt-exchanged tungstophosphoric acid for photocatalytic degradation of methylene blue. The ANFIS outperformed ANN and RSM, achieving superior predictive accuracy. Mohanty *et al.* (2026) investigated a triboelectric nanogenerator incorporating an ethylene-vinyl acetate-SrBi₂Nb₂O₉ composite film. The device demonstrated the capability to power a calculator. In addition, an ANN model was employed to predict finger force for real-time hand motion recognition, highlighting its potential applications in smart rehabilitation, prosthetics, and human-machine interfaces (Girimurugan *et al.* 2024).

Kumar *et al.* (2026) fabricated Ni_{0.03}Mn_{0.03}Ce_{0.94}O₂ nanocomposite based on carbon nanofibers for supercapacitor electrodes. The composite exhibited high specific capacitance (613 Fg⁻¹), energy density (196.5 Whkg⁻¹), and power density (1441 Wkg⁻¹), with excellent cycling stability, retaining 89% of capacitance after 5000 cycles. Polypyrrole (PPY) and PPY@CuO-NiO nanocomposites were synthesized for electrochemical pseudocapacitor electrodes. The PPY@CuO-NiO electrode exhibited a high specific capacitance of 702 Fg⁻¹ and excellent cycling stability (86.25% retention after 5000 cycles), demonstrating improved electrochemical performance due to the synergistic interaction between the conducting polymer matrix and metal-oxide components (Lad *et al.* 2026). In a study, MIL-53(Fe)-derived α -Fe₂O₃ was coupled with CuO to form an α -Fe₂O₃/CuO nano-heterostructure. The composite showed ~99% mineralization of ibuprofen and a hydrogen evolution rate of 133 μ molg⁻¹h⁻¹ under visible light, demonstrating efficient charge migration

and photocatalytic performance for both environmental remediation and green hydrogen generation (Sahoo *et al.* 2026). A TiC@C-TiO₂/polyaniline (PANI) nanostructure was synthesized for anode surface modification to enhance microbial fuel cell (MFC) power generation. The incorporation of PANI increased power density by 55% to 435 mW/m², with improved electrochemical performance, including reduced charge transfer resistance. The nanostructure showed great potential as a high-performance material for MFC applications (Dehghanian *et al.* 2026).

The present study introduces a novel TiO₂/CuO nanocomposite for energy storage applications by integrating experimental synthesis with advanced machine learning and a carefully tuned fuzzy logic framework, where membership functions were optimized to accurately capture nonlinear relationships between synthesis parameters and material properties. By adjusting the membership functions, the model precisely predicted structural, optical, and electrochemical behavior, enabling a more reliable and interpretable correlation between composition and performance. This approach not only enhances charge transport and energy storage capabilities but also provides a reproducible and scalable predictive framework, offering a robust strategy for design of high-efficiency nanocomposites for supercapacitors, batteries, and flexible electronics, representing a significant advancement in data-driven material optimization.

2. MATERIALS AND METHODOLOGY

Titanium dioxide nanopowder was manufactured using titanium tetrachloride (TiCl₄), sodium hydroxide (NaOH) and deionized water (DI). Copper oxide (CuO) nanopowder was synthesized utilizing copper(II) nitrate (Cu(NO₃)₂) or copper(II) acetate (Cu(CH₃COO)₂), ethanol (C₂H₅OH), hydrogen peroxide (H₂O₂), sulfuric acid (H₂SO₄), potassium permanganate (KMnO₄), and DI. All chemicals utilized were of analytical quality and had not been subjected to additional purification.

2.1 Methods

To prepare TiO₂ nanopowder, 0.3 mol/L of TiCl₄ was first combined with deionized water. Subsequently, 0.3 mol/L of NaOH was gradually added to the solution, maintaining continuous agitation. The mixture was thereafter subjected to mechanical agitation for four hours at temperature from 55°C to 60°C. Following agitation, suspension was allowed to remain undisturbed for 12 hours, resulting in the formation of a gel-like material. The gel was then rinsed many times with solution of DI water and ethanol to eliminate any remaining contaminants. The resultant product were further dried in an oven at 65°C to 70°C for four hours to

eliminate any residual moisture. Finally, the desiccated substance was meticulously pulverized with a ceramic pestle and mortar to get the final TiO₂ nanopowder.

Copper oxide nanopowder was synthesized using copper(II) nitrate as the precursor. Initially, an aqueous solution of Cu(NO₃)₂ was prepared using DI water. Subsequently, NaOH solution was added dropwise under continuous stirring until a blue precipitate was formed. The mixture was stirred for 2–3 hours at room temperature, followed by heating at 60–80 °C to facilitate the conversion of Cu(OH)₂ into CuO. The resulting black precipitate was collected by centrifugation at 3500 rpm for 20–25 minutes and washed several times with DI water and ethanol to remove impurities. Finally, the purified product was dried in an oven at 80–100 °C for 10–12 hours and ground using a ceramic mortar and pestle to obtain CuO nanopowder.

To synthesize the CuO-doped TiO₂ nanocomposite, an ultrasonic homogenizer was utilized to disperse 0.2 g of CuO and 2 g of TiO₂ in a mixed solvent of DI water and ethanol (1:1 volume ratio). The

suspension was sonicated for 2 hours at 25 °C to ensure uniform dispersion. The sonicated mixture was then transferred into a Teflon-lined stainless-steel autoclave and subjected to hydrothermal treatment at 180–190 °C for 20 hours. After completion of the reaction, the autoclave was allowed to cool naturally to room temperature. The obtained product was collected by centrifugation at 3500 rpm for 20–25 minutes and washed several times with deionized water and ethanol to remove impurities. The purified sample was then dried in an oven at 80 °C for 8 hours. Finally, the dried material was ground using a mortar and pestle to obtain a fine TiO₂/CuO nanocomposite powder. All syntheses were conducted utilizing precursors and rigorously regulated hydrothermal conditions to guarantee repeatability (Zhang *et al.* 2026). Each experiment was conducted in triplicate, yielding consistent optical and structural properties. Minor variations arising due to fluctuations in temperature, precursor concentration, or CuO dispersion influence XRD peak broadening and photoluminescence (PL) intensity. Figure 1 illustrates the schematic representation of the synthesis process.

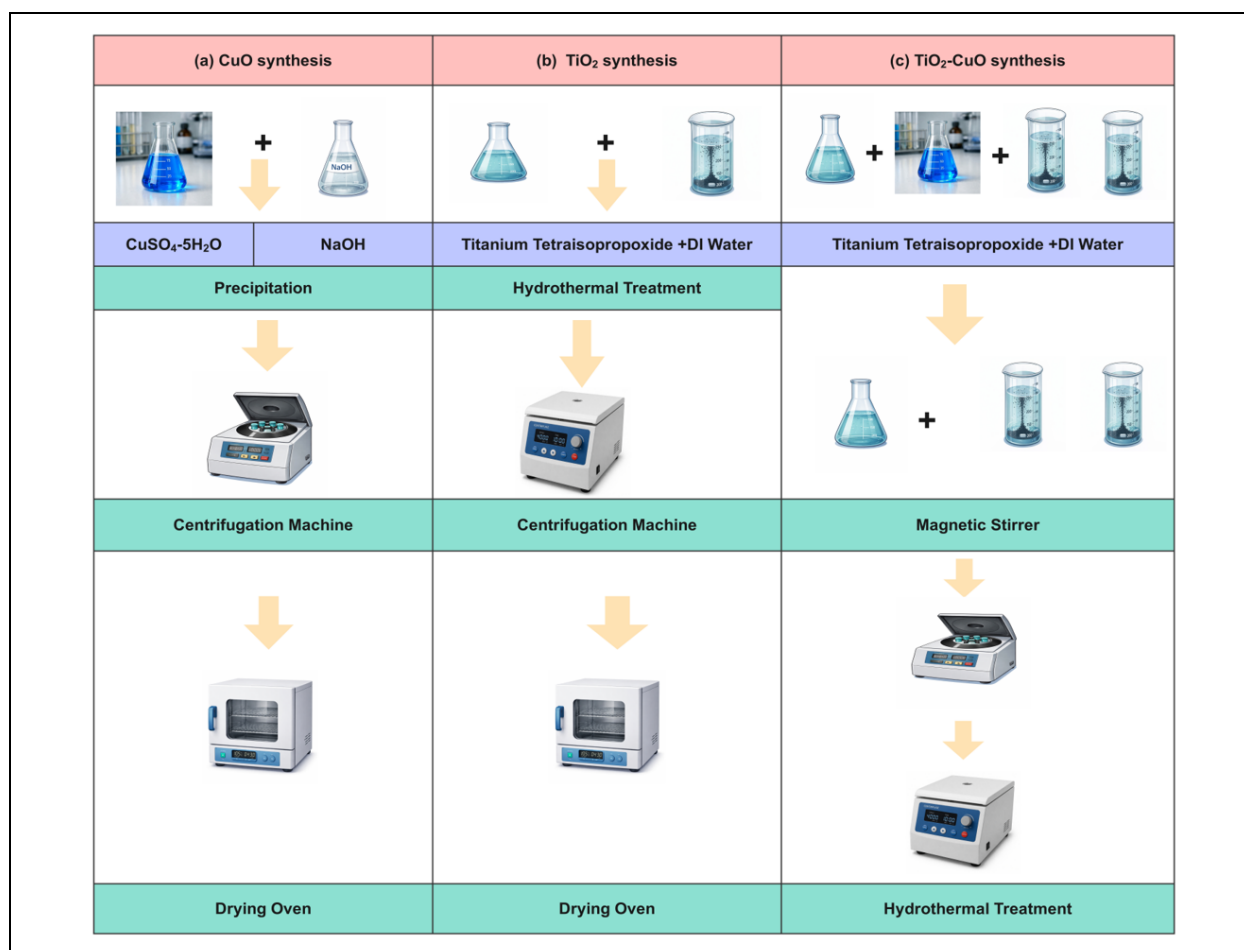


Fig. 1: (a) CuO synthesis process (b) TiO₂ synthesis process and (c) TiO₂-CuO synthesis process

2.2 Characterization

The crystalline structure of the material was studied with a Bruker D8 Advance, operating at 2θ angle of 10° to 80° using $\text{Cu-K}\alpha$ radiation, to assess X-ray diffraction peaks (Kumar and Pallavi, 2026). Surface morphology was analyzed by Field Emission Scanning Electron Microscope (ZEISS, Gemini) and Energy-dispersive X-ray spectroscopy (EDS), functioning at accelerating voltage of 15 kV. The functional groups of the material was analyzed using Fourier Transform Infrared (FTIR) spectroscopy with a PerkinElmer RXI spectrometer (Shelton, CT, USA) at room temperature, within a scanning range $4000\text{--}400\text{ cm}^{-1}$ (Utami *et al.* 2026). Photoluminescence spectroscopy was conducted with a Horiba Jobin Yvon Fluorolog-3 spectrofluorometer, employing 450 W xenon lamp as excitation source. The PL spectra were obtained at ambient temperature within a detection range 200–800 nm, yielding high-resolution insights into the emission and defect features of the nanomaterials while functioning in steady-state mode (Khaerunnisa *et al.* 2026).

2.3 Fuzzy Analysis

The fuzzy logic tool was utilized for computations, data visualization, and intricate analysis (Esmaeili *et al.* 2023). Simulations utilizing this technology fulfill several functions, such as understanding intricate systems, confirming ideas, predicting future conditions, and enhancing performance. This study assessed the band gap, peak intensity wavelength, and crystallite size of the nanocomposites utilizing a fuzzy logic-based approach. The fuzzy logic tool employed input ranges and membership functions that ascertain the degree of membership for each input value, ranging from 0 to 1. The input ranges were obtained from experimental data and published values. Triangular functions, in accordance with Mamdani model, was utilized to depict input-output linkages. The selected input factors, reflecting the standard synthesis conditions for TiO_2/CuO nanocomposites, were TiO_2 (10%–90%), CuO percentage (10%–90%), and molarity (0.1–1 M). Investigation focused on synthesizing

samples including 90 wt.% TiO_2 and 10 wt.% CuO , whereas the wider input ranges were chosen to represent compositions often examined in analogous studies, facilitating interpolation within feasible synthesis parameters.

3. RESULTS AND DISCUSSION

The fuzzy logic model for the TiO_2/CuO nanocomposite system was constructed by selecting TiO_2 and CuO concentrations as the primary input variables, along with molarity, owing to their significant influence on the structural and physicochemical properties of the nanocomposite. As illustrated in Fig. 3(a–c), triangular membership functions were employed to define the input–output relationships, ensuring smooth transitions between linguistic variables. The output parameters, namely crystal size, band gap, and wavelength, were each categorized into three linguistic levels: low, medium, and high. Specifically, the crystal size ranged from 10 to 30 nm, band gap varied between 1.8 and 3.2 eV, and the wavelength spanned from 400 to 700 nm, with the medium membership functions centered around the dominant peak values observed in the system. The fuzzy inference mechanism was developed using a Mamdani-type framework, where a set of rule-based conditions govern the interaction between input variables and corresponding outputs. The membership functions and rule sets were defined using the fuzzy logic toolbox interface, enabling precise modeling of nonlinear relationships between composition and material properties. This structured approach ensured accurate representation of the experimental trends and enhanced the predictive capability of the fuzzy system. Experimental results yielded output ranges of wavelength (375–500 nm), band gap (2.1–3.1 eV), and crystallite size (15–20 nm). These output ranges were subsequently used in the fuzzy logic visualization interface to establish the membership functions and rule-based prediction framework. Figure 2 illustrates the fuzzy inference system architecture employed for the TiO_2/CuO nanocomposite.

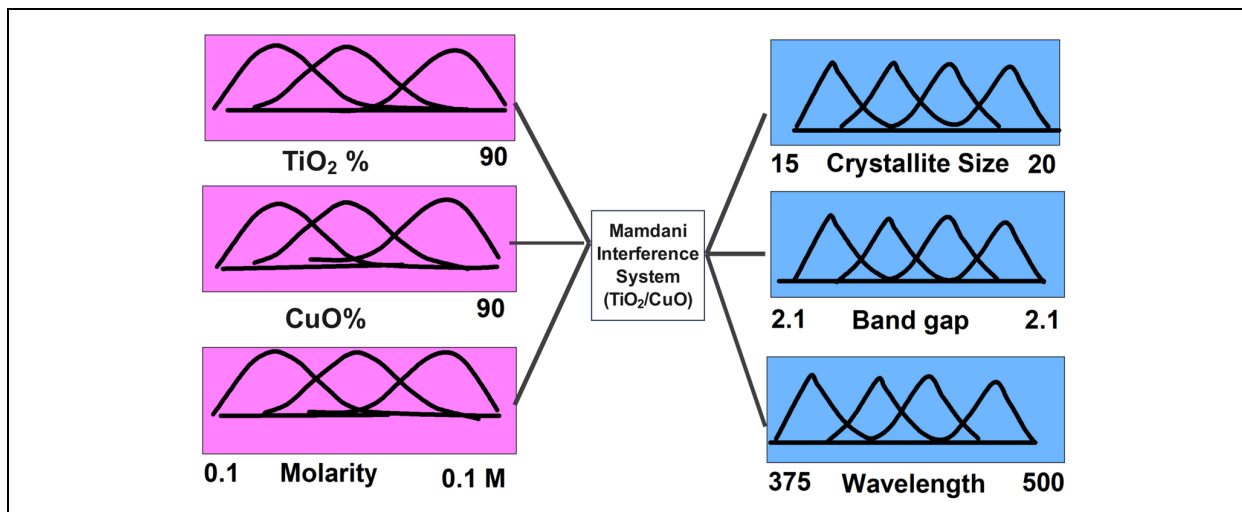


Fig. 2: Fuzzy inference system architecture for TiO₂/CuO nanocomposite

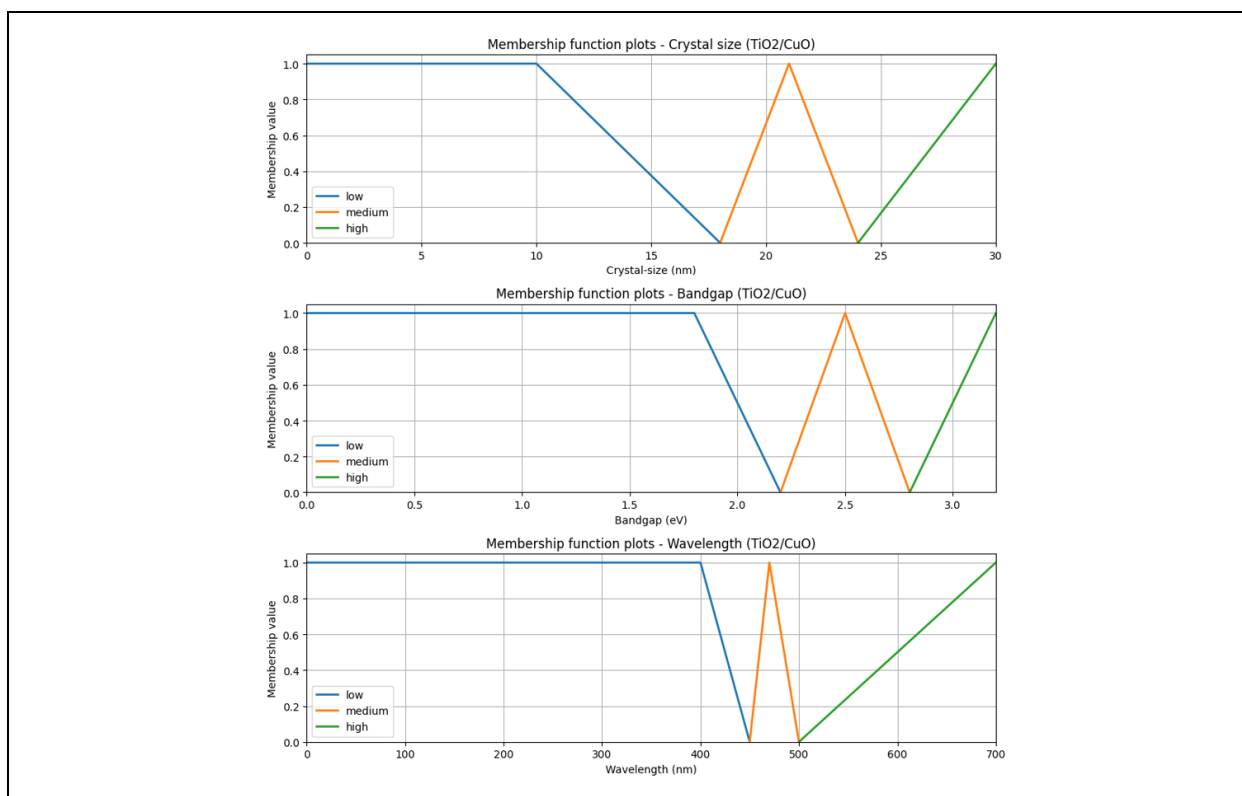


Fig. 3: Fuzzy logic membership functions for crystal size, band gap and wavelength

Figures 4(a) and (b) illustrate the variation in band gap and wavelength as a function of TiO₂ concentration in the TiO₂/CuO nanocomposite system. As observed, the band gap remains nearly constant at approximately 2.55 eV over a wide TiO₂ composition range (60–90 wt.%) indicating a stable electronic structure within this region. However, a sharp decrease in the band gap to around 2.30 eV is evident beyond 90 wt.% TiO₂, suggesting a significant alteration in the electronic interactions due to reduced CuO influence. In contrast, the wavelength exhibits minimal variation

(approximately 460–462 nm) up to 90 wt.% TiO₂, followed by a sudden increase to about 565 nm at higher TiO₂ concentrations. This abrupt shift indicates a strong correlation between composition and optical response, likely due to changes in defect states and band structure. These trends, derived from the fuzzy logic model demonstrate its capability to capture nonlinear relationships between composition and optical properties. The results further support the effectiveness of the Mamdani fuzzy inference system in predicting material behavior based on compositional variations. In

comparison, ZnO–CuO– CeO₂ ternary hybrid nanocomposites were synthesized by Hameed *et al.* (2026) using a simple and inexpensive hydrothermal method. The nanocomposites exhibited increased

crystallinity, with average crystallite sizes of 19, 23, and 28 nm at annealing temperatures of 400, 600, and 800 °C, respectively.

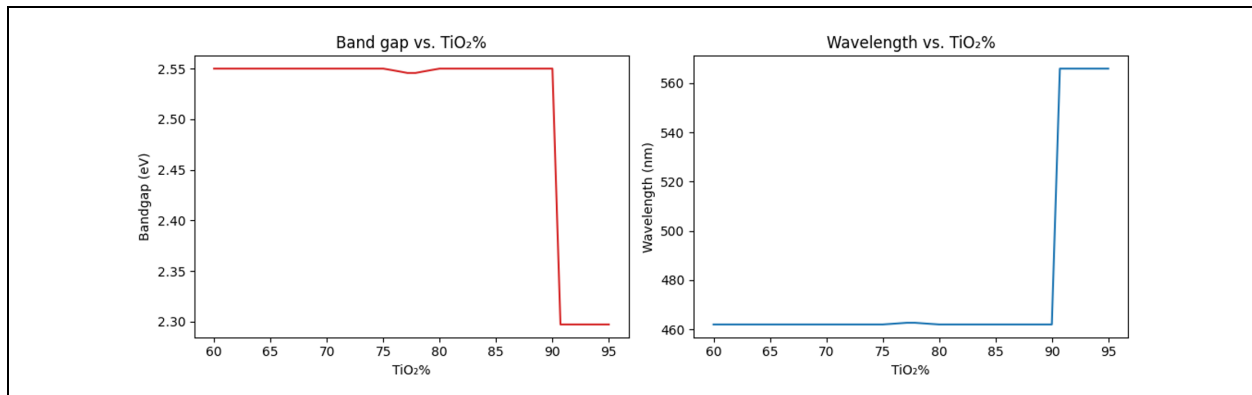


Fig. 4: Variation of (a) band gap and (b) wavelength with TiO₂ concentration

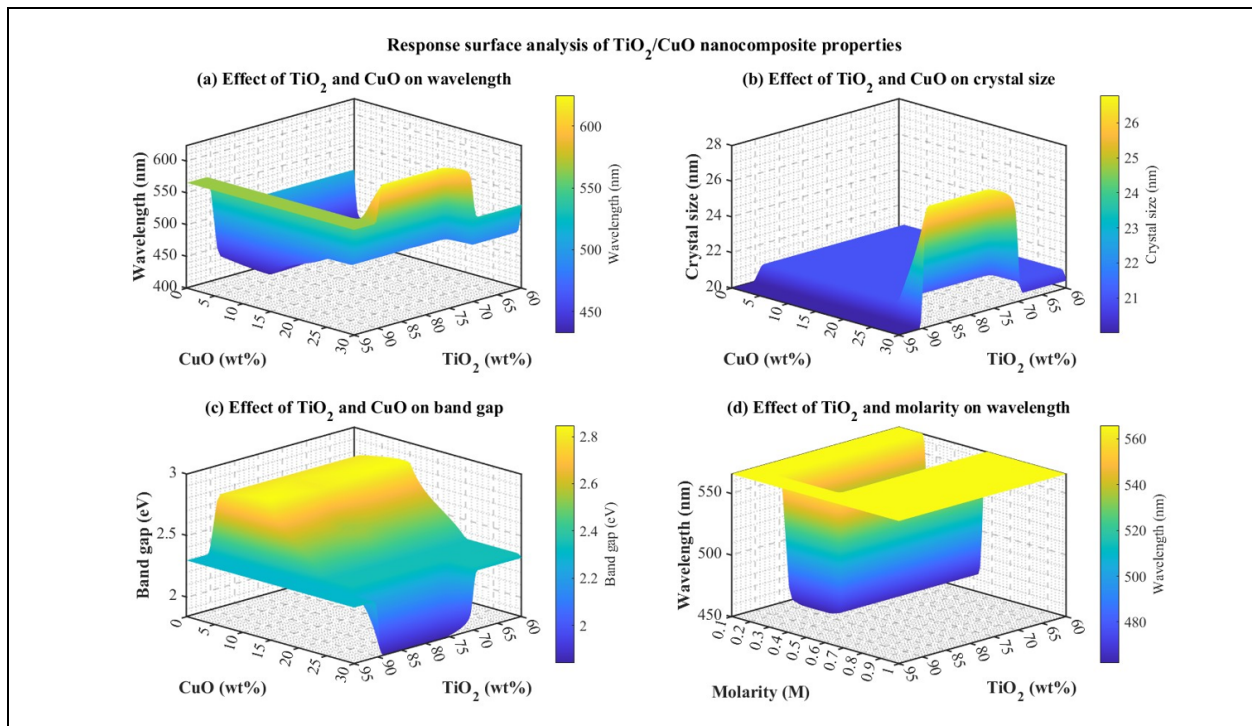


Fig. 5: 3D fuzzy logic surfaces for TiO₂ /CuO properties

The relationships between TiO₂ concentration, CuO content, molarity, and the optical and structural properties of the TiO₂/CuO nanocomposite were analyzed using three-dimensional fuzzy logic surface plots (Fig. 5 a-d). The results demonstrate a clear nonlinear dependence of wavelength, crystallite size, and band gap on compositional and synthesis parameters. The wavelength shows a gradual increase with CuO concentration, followed by a sharp transition at higher TiO₂ levels, indicating strong compositional influence on photoluminescence behavior. Similarly, the crystallite size remains relatively stable at lower CuO

concentrations but increases significantly at higher doping levels, suggesting enhanced particle growth due to interaction effects. The band gap exhibits a noticeable decrease with increasing CuO content, particularly at higher TiO₂ percentages, reflecting modifications in the electronic band structure. Additionally, molarity plays a critical role in influencing wavelength, where higher molarity leads to a substantial increase in optical response, highlighting the importance of synthesis conditions. These observations confirm that both compositional and processing parameters govern the material behavior in a highly nonlinear manner. The

fuzzy logic model, implemented using a Mamdani inference system with triangular membership functions, effectively captures these interactions through fuzzification, rule evaluation, aggregation, and defuzzification processes. The close agreement between simulated and experimental results demonstrates the reliability of the proposed model for predicting the behavior of TiO₂/CuO nanocomposites.

Table 1. Comparison of simulated and measured values

Property	Simulated Value	Measured Value	Error (%)
Band gap value (eV)	2.55	2.51	1.593625
Wavelength at maximum intensity (nm)	462	458	0.873362
Crystal size (nm)	21	20.74	1.253616

3.1 Machine Learning-based Method

This study employed machine learning approaches to forecast essential structural, electrochemical and optical features of TiO₂/CuO for energy storage. Utilizing experimentally obtained data, including crystallite size (nm), optical band energy (eV), energy-related parameters and PL wavelength at peak intensity (nm), like energy density (Wh/kg), charge transfer resistance (Ω), power density (W/kg) and specific capacitance (F/g), various models, comprising hybrid models, Multilayer Perceptron, Support Vector Regression (SVR), and Artificial Neural Networks, were trained and developed.

The approaches play a crucial role in augmenting conventional machine learning models. In this study, the models act as benchmarks for assessing the efficacy of hybrid fuzzy model. The robust correlation were noted among experimental and estimated values, signifying elevated model correctness. Overall predictive performance of the hybrid model surpassed that of other models employed in this investigation. To evaluate accuracy of utilized models, various metrics, including R² score and Mean Absolute Error were applied. These factors demonstrated remarkable concordance between the expected and experimental outcomes. The datasets were partitioned in 80:20 ratio for testing and training, utilizing 1000 experimental data points for prediction. Multiple data pretreatment methods, including scaling, cleaning and transformation, were employed to guarantee model stability. Grid search technique was utilized to tune hyperparameters such as learning rate, hidden layers, regularization and kernel type, to improve model accuracy.

Figure 6 illustrates relative importance of different synthetic and structural parameters influencing electrical properties of TiO₂/CuO nanocomposite. The analysis clearly indicates that CuO percentage is the most dominant factor, exhibiting a significantly higher contribution compared to all other features. Electrical conductivity shows a moderate influence, while thermal stability contributes only marginally. In contrast, parameters such as wavelength, chemical stability, molarity, diffusion density, formation temperature, capacity retention, crystallite size, and TiO₂ percentage exhibit negligible impact on the predicted electrical behavior. These results suggest that the electrical performance of the nanocomposite is primarily governed by CuO content, with limited contribution from other structural and synthesis-related parameters. Therefore, optimizing CuO concentration is critical for enhancing electrical efficiency in energy storage applications.

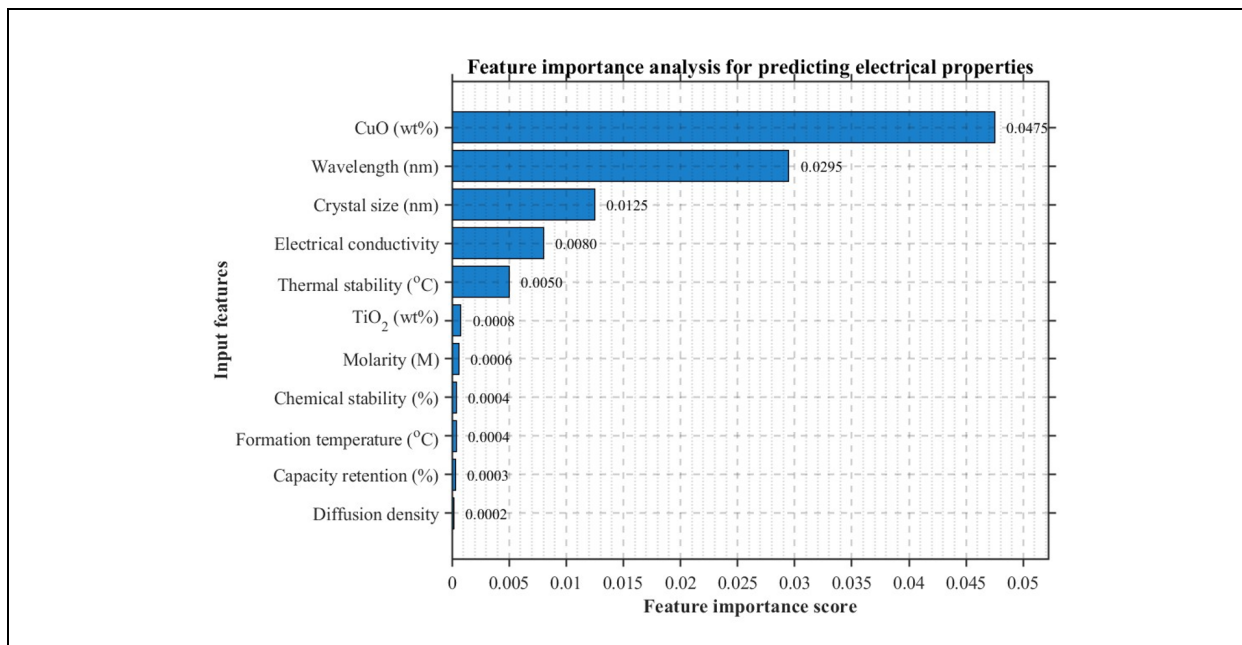


Fig. 6: Feature importance for electrical property prediction

Figure 7 illustrates the variation in band gap of TiO₂/CuO nanocomposites as a function of CuO concentration. A clear and nearly linear decreasing trend is observed, where the band gap reduces from approximately 3.0 eV at 0% CuO to about 2.1 eV at 30% CuO. This reduction indicates improved electrical conductivity with increasing CuO content, which is advantageous for energy storage applications. The decline in band gap can be attributed to the introduction of CuO-induced defect and enhanced interfacial charge transfer within the composite system. Strong agreement among experimental data points, smooth trend, and linear fit further confirms the reliability and predictive capability of the applied ML-based modeling approach. In another study, Sn doping decreased crystallite size, while the optical band gap of CuGaS₂ thin films was 2.33 eV (1 wt% Sn), optimal for solar cell applications (Krishna and Vasu, 2024).

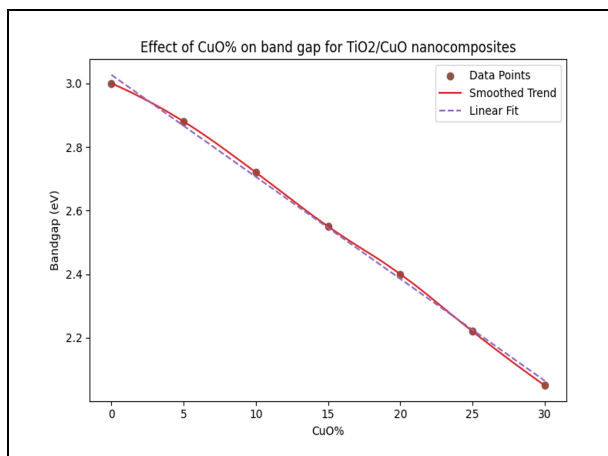


Fig. 7: Effect of CuO content on bandgap

Figure 8 illustrates the effect of CuO concentration on the charge transfer resistance (Ω) of TiO₂/CuO nanocomposites. A pronounced non-linear trend is observed, where the resistance initially decreases significantly from approximately 16.8 Ω at 0% CuO to a minimum of about 5.8 Ω at 15% CuO, indicating enhanced charge transport due to improved conductivity and interfacial charge transfer. Beyond this optimum concentration, the resistance gradually increases, reaching nearly 9.5 Ω at 30% CuO. This rise at higher CuO loadings can be attributed to particle agglomeration and the obstruction of effective electron transport pathways. The consistency between the experimental data points, smoothed curve, and linear fit highlights the capability of the ML and fuzzy logic models to accurately capture the non-linear relationship between CuO concentration and electrochemical performance, thereby supporting their applicability in optimizing nanocomposite design for energy storage applications.

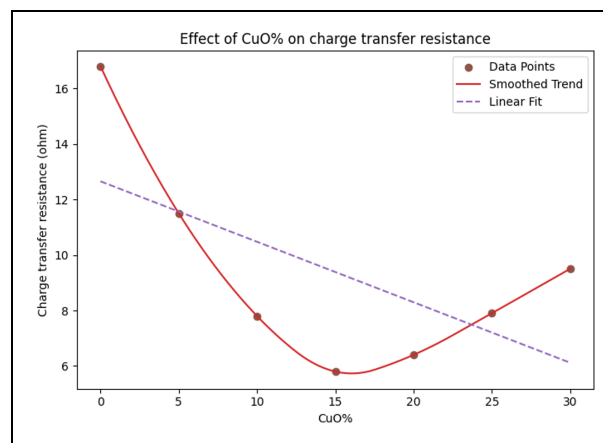


Fig. 8: CuO effect on charge resistance

Figure 9 illustrates the influence of thermal stability on the band gap of TiO_2/CuO . A strong linear decreasing trend is observed, where the band gap reduces from approximately 2.95 eV at 300 °C to about 2.12 eV at 600 °C. This reduction indicates that increasing thermal stability (or heat treatment temperature) enhances the electronic properties of the nanocomposite. The observed decrease in band gap can be attributed to improved crystallinity, reduced defect density, and enhanced interfacial interaction between TiO_2 and CuO at higher temperatures, which facilitate better charge transport. The close alignment of experimental data points with the smooth trend and linear fit confirms a clear linear correlation between thermal stability and band gap. This agreement further demonstrates the effectiveness of machine learning and fuzzy logic models in accurately predicting material behavior, while also indicating that linear regression is sufficient to describe this relationship without requiring more complex modeling approaches.

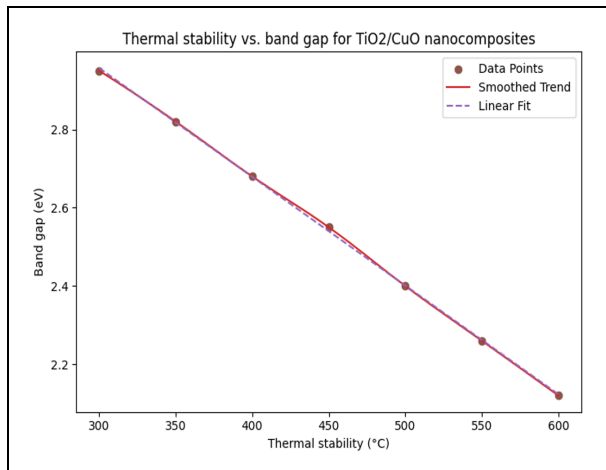


Fig. 9: Thermal stability versus band gap

Figure 10 presents a comparative analysis of experimental and predicted band gap for TiO_2/CuO nanocomposites with different ML models, namely MLP, ANN, hybrid and SVR model. Among these, SVR model exhibits the closest agreement between predicted and experimental values across all samples, indicating superior predictive accuracy and consistency. The ANN model also demonstrates good correlation, with only minor deviations. In contrast, the MLP and hybrid models show comparatively larger discrepancies, particularly at certain sample indices, suggesting reduced prediction reliability. Overall, the results confirm that ML-based approaches are effective in capturing the band gap behavior of TiO_2/CuO nanocomposites, with SVR emerging as the most robust model. The strong alignment between predicted and experimental values highlights the potential of these techniques to accelerate material characterization, reduce experimental effort, and enable efficient optimization of nanocomposites for energy storage applications.

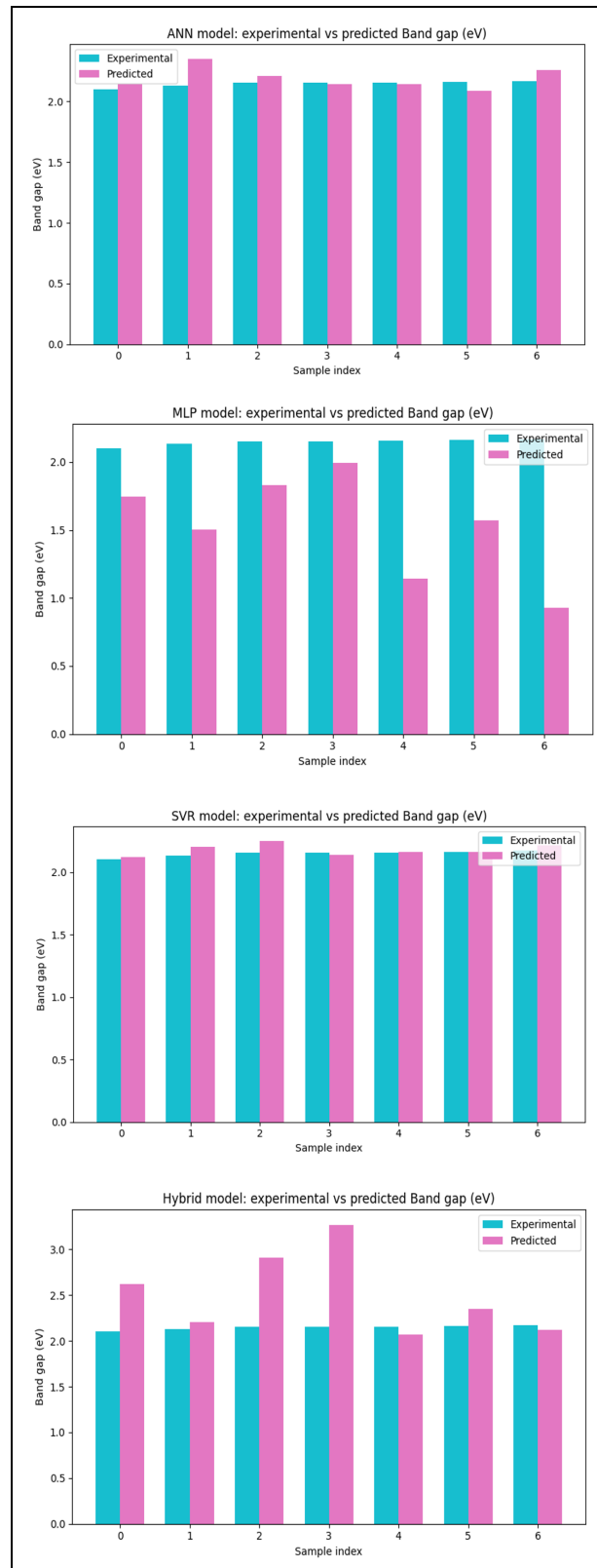


Fig. 10: Predicted bandgap of TiO_2/CuO using ANN, MLP, SVR, and hybrid models

Figure 11 presents the comparison between experimental and predicted charge transfer resistance values of TiO_2/CuO nanocomposites using MLP, ANN,

hybrid and SVR model. The experimental values remain consistently high ($\sim 10\text{--}11\ \Omega$) across all samples, whereas the predicted values vary significantly depending on the model. The SVR model demonstrates the closest agreement with experimental data, accurately capturing both the magnitude and trend of resistance. In contrast, the ANN, MLP, and hybrid models significantly underestimate the charge transfer resistance, with predicted values largely confined to a much lower range ($\sim 0.5\text{--}4\ \Omega$), indicating poor predictive performance. Among these, the hybrid model shows relatively better consistency than ANN and MLP but still exhibits substantial deviation from experimental observations. The results highlight that SVR is the most reliable model for predicting charge transfer resistance in TiO_2/CuO nanocomposites, emphasizing the importance of model selection for accurate electrochemical property prediction in energy storage applications.

Figure 12 presents a comparison between experimental and predicted values of key properties of TiO_2/CuO nanocomposites using MLP, ANN, hybrid, and SVR models. The results indicate that SVR model consistently demonstrates the highest predictive accuracy across all properties, including band gap, charge storage capacity, power density and transfer resistance, with predictions closely aligning with experimental trends. In contrast, the ANN and MLP models exhibit significant deviations and underestimation, particularly for charge storage capacity, resistance, and power density, where predictions are largely confined to lower values. The hybrid model shows inconsistent performance, with noticeable fluctuations in band gap prediction and poor agreement in other properties. The strong correlation between SVR predictions and experimental data highlights its robustness and suitability for modeling complex nonlinear relationships in TiO_2/CuO nanocomposites, thereby offering an effective approach for accurate property prediction and accelerated optimization in energy storage applications. In prior study, the material $\text{NiMn}_2\text{O}_4/\text{TiO}_2$ -Chitosan ternary composite demonstrated remarkable electrochemical performance, with a specific capacitance of $1089.41\ \text{F g}^{-1}$ and an energy density of $45.77\ \text{Wh/kg}$, highlighting its potential for advanced energy storage applications (Shandhiya *et al.* 2026).

Notwithstanding the discrepancies in trends arising from varying CuO concentrations, which can be attributed to differences in their learning methodologies, SVR, MLP, ANN, and hybrid models effectively predicted the characteristics of TiO_2/CuO nanocomposite materials. All models had distinct advantages, hybrid model showed enhanced generality and dependability, rendering it more efficacious for forecasting characteristics of smart energy materials. The superior performance of the hybrid model highlights its appropriateness for predicting energy materials with more precision and consistency.

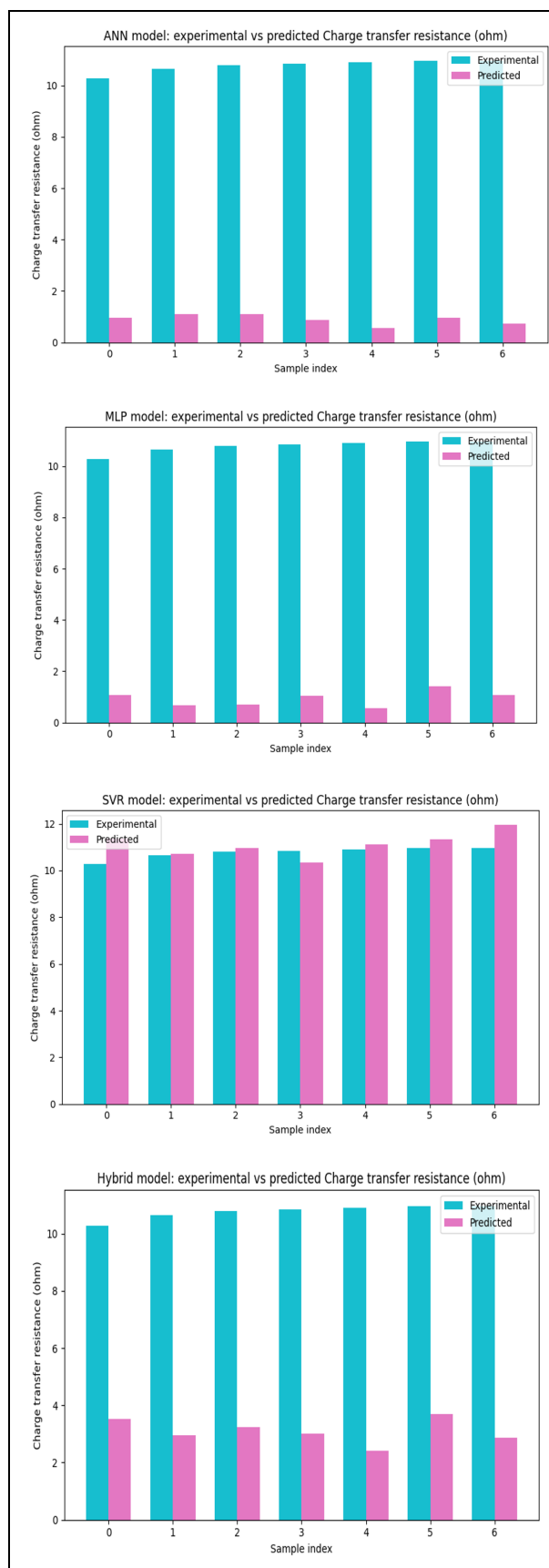


Fig. 11: Charge resistance prediction of ANN, MLP, SVR and hybrid models

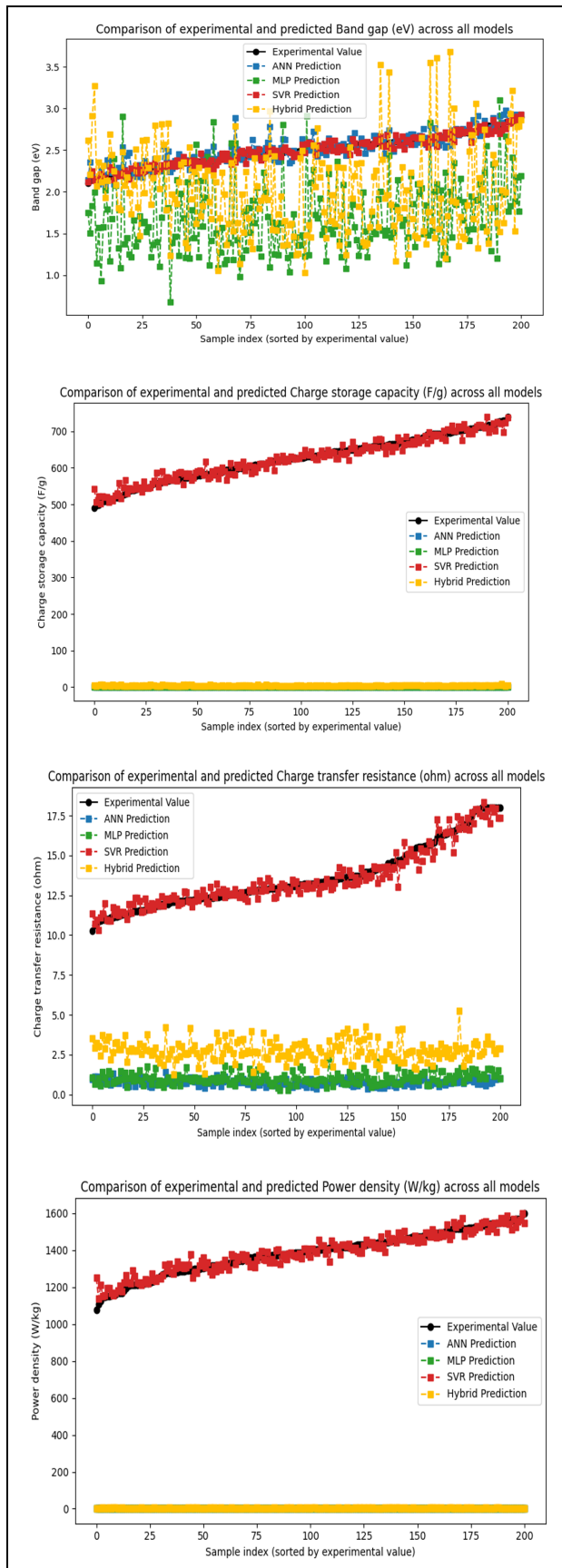


Fig. 12: Experimental vs ML plots for band gap, energy storage, charge resistance, energy density

An Artificial Neural Network model was built to predict physicochemical and electrochemical characteristics of TiO₂/CuO nanocomposites, as shown in Fig. 13. The input layer has eleven neurons, denoting essential variables like wavelength, molarity, crystallite size, TiO₂ percentage, formation temperature, and CuO %. This model has four hidden layers, viz., Dense1, Residual Block1, Residual Block2, and Dense2, featuring 64 to 32 neurons with activation functions such as Switch, ReLU, and GELU to represent nonlinear interactions. The output layer including five neurons, forecasts values of power density, energy density, charge transfer resistance, and band gap. The ANN model was trained with backpropagation with Adam optimizer and mean squared error loss. The correlation between material performance and input synthesis was effectively established, improving prediction accuracy and convergence within the multilayered structure.

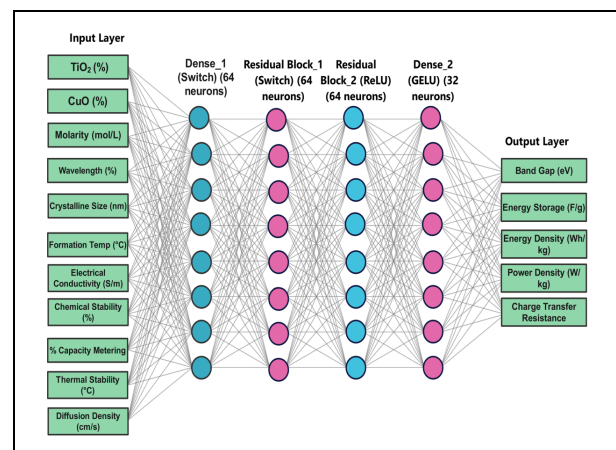


Fig. 13: ANN architecture for nanocomposite prediction

Diverse machine learning models, such as SVR, MLP, hybrid and ANN models were utilized to evaluate their efficiency. Support Vector Regression uses Radial Basis Kernel to manage nonlinear relationships with their parameters refined by grid search to reduce prediction error. The MLP model intended to identify intricate patterns in input data had two hidden layers by ReLU activation functions. Combining FL with ML enhances data interpretation, wherein hybrid fuzzy integrates input fuzzy with learned SVR and ANN.

Figure 14 presents the R^2 comparison for five predicted properties, band gap, charge storage capacity, charge transfer, power density, and energy density, across MLP, hybrid, ANN and SVR models for TiO₂/CuO nanocomposites. The results reveal that SVR consistently exhibits R^2 values closest to unity (near 1) for all properties, indicating superior predictive performance and strong agreement with experimental data. In contrast, the ANN, MLP, and hybrid models show significantly negative R^2 values, particularly for charge storage capacity and power density, reflecting poor model fit and limited reliability. Although slight variations exist among

ANN, MLP, and hybrid predictions, none approach the accuracy demonstrated by SVR. Overall, the analysis confirms that SVR is the most robust and reliable model for predicting the electrochemical and energy storage properties of TiO₂/CuO nanocomposites, emphasizing its effectiveness in capturing complex material behavior.

Table 2: Comparison of different models for MAE

Target	Model	MAE	R ²
Band gap (eV)	ANN	0.055691	0.712684
Band gap (eV)	MLP	0.609466	-22.7242
Band gap (eV)	SVR	0.012249	0.975626
Band gap (eV)	Hybrid	0.581489	-21.9629
Charge storage capacity (F/g)	ANN	688.3208	-1081.23
Charge storage capacity (F/g)	MLP	687.9155	-1079.98
Charge storage capacity (F/g)	SVR	7.135553	0.808861
Charge storage capacity (F/g)	Hybrid	685.1806	-1071.41
Charge transfer resistance (ohm)	ANN	23.52988	-22.9589
Charge transfer resistance (ohm)	MLP	23.25104	-22.3726

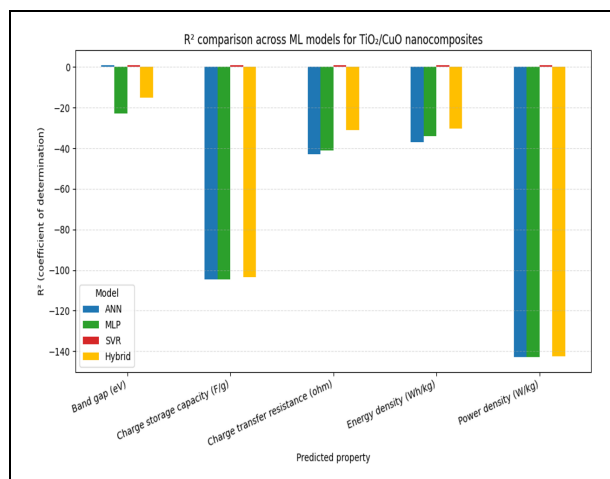


Fig. 14: R² comparison across ML models

Table 3 shows the forecasts for diverse characteristics of TiO₂/CuO nanocomposites utilizing four models: SVR, MLP, ANN and a hybrid model. The hybrid model excels in forecasting the band gap but has inconsistency with other parameters, underscoring the complexity inherent in ensemble approaches. This model comparison demonstrates that ensemble and hybrid

techniques are useful in the creation of smart nanocomposites for energy storage applications.

Table 3. Model-wise R² scores for TiO₂/CuO nanocomposite

Model	ANN	Hybrid	MLP	SVR
Band gap (eV)	0.737	-15.228	-22.965	0.927
Charge storage capacity (F/g)	-	-	-	0.956
Charge transfer resistance (ohm)	-43.081	-30.940	-41.289	0.948
Energy density (Wh/kg)	-36.877	-30.193	-34.110	0.950
Power density (W/kg)	-	-	-	0.930

In several instances, SVR demonstrates superior performance with fewer datasets and non-linear patterns under particular conditions. Every model possesses distinct advantages and disadvantages; nonetheless, the hybrid model provides the optimal equilibrium of dependability and accuracy. Methods to mitigate overfitting, including Bayesian approach and halting were implemented. Inaccuracies mostly come from system non-linearity, experimental uncertainties, and limited dataset sizes. Significant limitations include potential overfitting in artificial neural networks/multi-layer perceptrons, sensitivity to support vector regression hyperparameters, and the complexity of the hybrid model. These criteria demonstrate how the characteristics of the dataset and the particular attribute predicted affect the model's efficacy.

3.2 XRD Analysis

Figure 15 presents the XRD pattern of CuO-doped TiO₂ nanocomposites (90 wt.% TiO₂ and 10 wt.% CuO), confirming the crystalline nature and phase composition of the material. The diffraction pattern exhibits two prominent peaks at approximately 39.5° and 42.0°, along with additional reflections at 51.5°, 56.8°, 60.5°, 63.5°, 66.8°, 68.5°, 72.0°, and 75.5°, indicating well-defined crystallinity. The major peaks correspond to characteristic TiO₂ planes, while the secondary peaks confirm the successful incorporation of CuO within the TiO₂ matrix. The absence of impurity peaks suggests high phase purity, and slight peak broadening indicates nanoscale crystallite size and lattice strain induced by CuO doping, enhancing interfacial interaction and electrochemical performance.

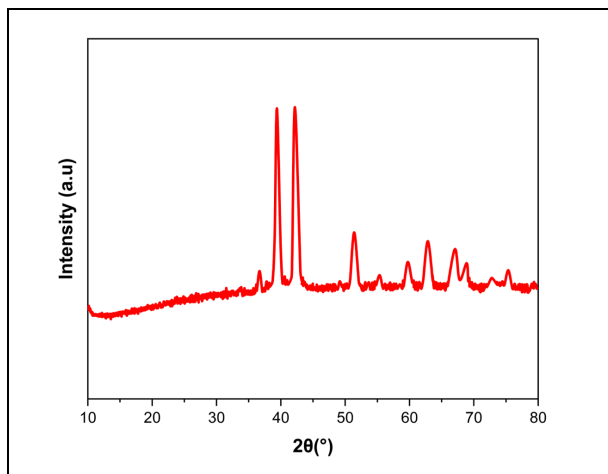


Fig. 15: XRD pattern of TiO₂/CuO

The peak width and intensity observed in the XRD pattern provide significant insight into the crystalline nature of the synthesized TiO₂/CuO nanocomposite. The relatively sharp and intense peaks indicate a well-defined crystalline structure, while slight peak broadening suggests a nanoscale crystallite size. The crystallite size was estimated using the Debye–Scherrer equation based on the prominent diffraction peak corresponding to the TiO₂ phase. From the analysis, the average crystallite size of the TiO₂/CuO nanocomposite was determined to be approximately 12.22 nm, indicating fine nanocrystalline formation. The observed peak at $2\theta \approx 32.22^\circ$ with a full width at half maximum (FWHM) of 0.22° supports this estimation. The reduction in crystallite size compared to pure TiO₂ can be attributed to the incorporation of CuO, which introduces lattice strain and inhibits crystal growth. Furthermore, the optical band gap obtained from PL analysis (2.22 eV), confirming enhanced electronic interaction between TiO₂ and CuO. These results indicate that CuO doping modifies the structural and optical properties of TiO₂, making the composite more suitable for energy storage and electrochemical applications.

Table 4. Structural parameters and optical band gap values

Sample	FWHM (Degree)	2θ of (101) Peak (Degree)	Optical Band Gap (eV) by PL	Crystallite Size (nm)
TiO ₂ /CuO	0.28	39.5	2.15	11.8

$$\frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2} \quad \dots (1)$$

The mean crystallite size (D) of the CuO-doped TiO₂ nanocomposite was calculated utilizing the Debye–Scherrer equation (Eq. 2).

$$D = \frac{K\lambda}{\beta \cos \theta} \quad \dots (2),$$

where K is a dimensionless constant, referred to as the shape factor; θ is Bragg angle; λ denotes wavelength of the X-ray beam; and β indicates line broadening. Table 4 presents computed values for band gap and crystallite size (eV).

3.3 SEM and EDS Analyses

Figure 16(a) presents high-resolution SEM image of TiO₂/CuO nanocomposite, revealing a well-defined morphology with TiO₂ nanoparticles uniformly distributed over the CuO sheet surface. The close contact between TiO₂ and CuO suggests strong interfacial interactions, which are expected to enhance surface area and facilitate charge transfer, making the composite suitable for energy storage and photocatalytic applications. The CuO sheets appear relatively thin, with some regions showing denser stacking due to particle agglomeration. Figure 16(b) displays the corresponding EDS spectrum, confirming the elemental composition of the nanocomposite as Ti ~12.0 wt.%, O ~62.0 wt.%, and Cu ~26.0 wt.%, indicating homogeneous dispersion of TiO₂ across the CuO matrix. Figure 16(c) shows the particle size distribution derived from ImageJ analysis, indicating grain diameters ranging from 0.5 to 5 μm , with particle size of 2.49 μm . Microscale aggregation reflects the clustering of nanoscale crystallites (XRD crystallite size ~12.22 nm), which is typical for polycrystalline nanocomposites because of van der Waals forces and surface energy effects. Overall, the SEM, EDS, and particle size analyses confirm the successful synthesis of a uniform TiO₂/CuO nanocomposite with structural features conducive to enhanced electrochemical performance.

3.4 FTIR Analysis

The FTIR spectrum of the TiO₂/CuO nanocomposite, shown in Figure 17, confirms the presence of characteristic functional groups and metal–oxygen bonds in the synthesized material. A broad peak centered at 3601.9 cm^{-1} is attributed to O–H stretching vibration, indicating surface hydroxyl groups or adsorbed moisture. The weak peak at 2100.6 cm^{-1} may be associated with adsorbed molecular species. The peak at 1792.8 cm^{-1} is assigned to C=O stretching, which may arise from residual precursor-related species. The strong peaks at 613.4 cm^{-1} and 422.9 cm^{-1} correspond to metal–oxygen vibrations, confirming the formation of Ti–O, Cu–O, and Ti–O–Ti lattice bonds in the nanocomposite. These peaks confirm the successful formation of the TiO₂/CuO composite structure.

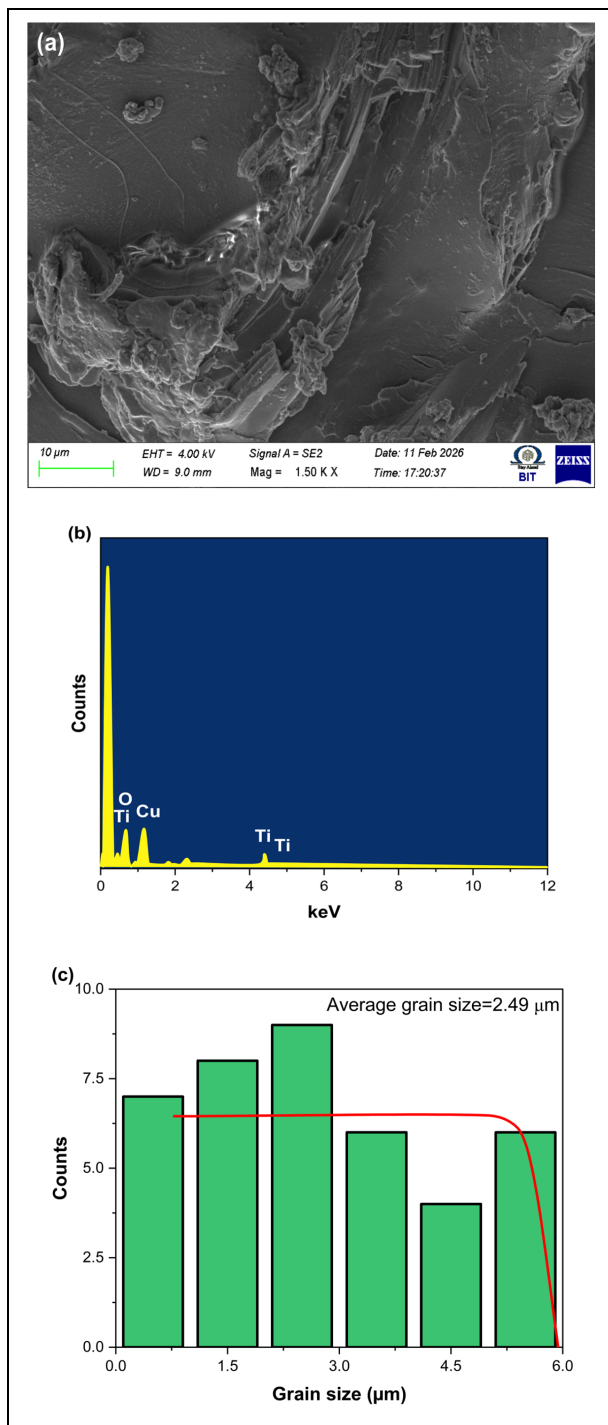


Fig. 16: (a) SEM microstructure of nanocomposite, (b) EDS elemental analysis spectra and (c) Particle size distribution plot

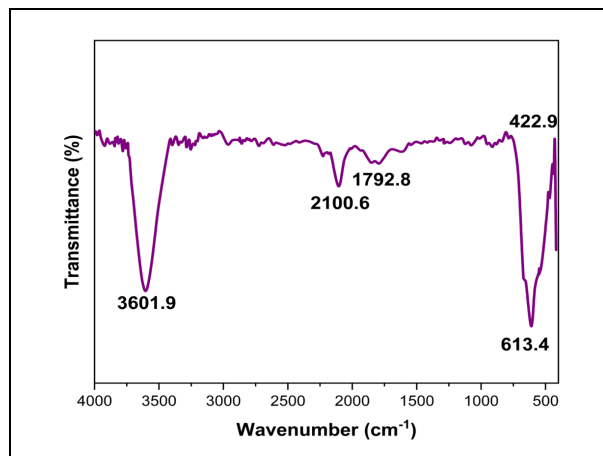


Fig. 17: FTIR analysis of TiO_2/CuO

3.5 Photoluminescence Spectroscopy

Photoluminescence spectroscopy was utilized to analyse the defect states and optical characteristics of the TiO_2/CuO nanocomposite. The PL emission band moved to 392 nm for TiO_2/CuO nanocomposite, indicating robust interfacial interactions between CuO and TiO_2 . The observed redshift in emission indicates enhanced charge transfer at the CuO- TiO_2 interface, achieved by diminishing exciton recombination and augmenting electron mobility (Ganvir *et al.* 2024). The noted reduction in emission intensity, linked to defects, further substantiates the passivation of trap states resulting from the inclusion of CuO, which were essential for improving efficiency of nanocomposite at energy applications (Figure 18(a)). Photoluminescence was employed to ascertain band gap energy of TiO_2/CuO nanocomposite. The anticipated band gap of 3.07 eV illustrated impact of CuO on electrical configuration of TiO_2 . The band gap in TiO_2/CuO nanocomposite diminishes relative to pure TiO_2 , attributable to improved charge transfer, rendering it a favorable characteristic for energy devices. The interaction among titanium dioxide and copper oxide nanocomposites diminishes optical band gap by enhancing defect passivation and charge mobility, facilitated by inclusion of oxygen-containing functional groups. The incorporation of copper oxide into titanium dioxide boosts visible light absorption, alters electronic structure of nanocomposites and affects density of states. Fluctuation in band gap values is a critical factor for energy storage, especially in modern smart energy storage system.

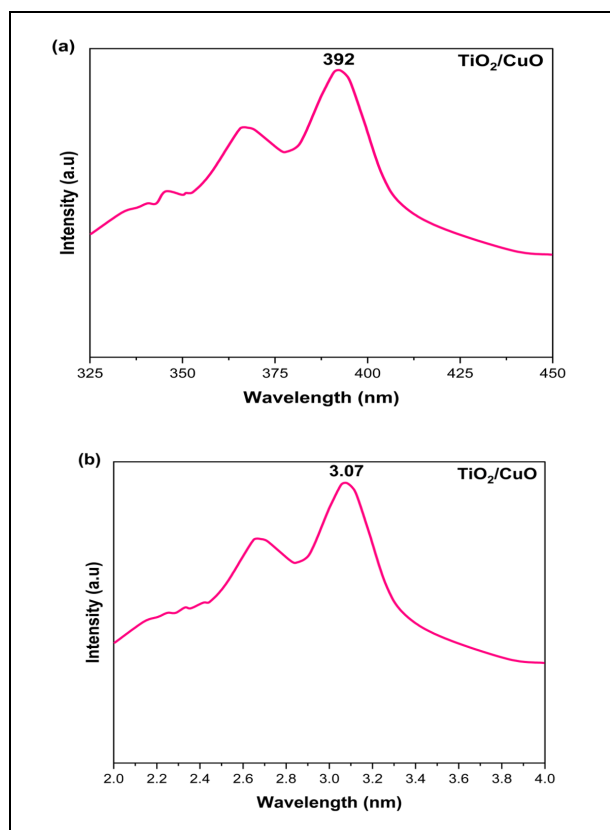


Fig. 18: (a) PL and (b) Optical band gap spectra

The efficacy of CuO-doped TiO₂ nanocomposites in charge and discharge processes may be markedly improved by the incorporation of CuO with TiO₂, enhancing electrochemical stability and diminishing electron-hole recombination. This interaction guarantees prolonged cycle stability, rendering these nanocomposites optimal for rapid and efficient energy storage devices with superior supercapacitive characteristics. This combination, in contrast to traditional CuO dopants, improves structural stability and yields an outstanding band gap, facilitating accelerated ion transport and effective energy conversion. CuO-doped TiO₂ serves as an exceptional nanocomposite, demonstrating significant potential for sustainable energy applications. This work distinctly combines machine learning, fuzzy logic, and experimental evaluation to create smart nanocomposite for energy storage applications. The integration of various approaches yields critical metrics, including crystallite size, band gap, charge transfer, wavelength, charge storage, power density and energy storage. Prior research predominantly concentrated on discrete simulations or experimental assessments. The experimental results in this work confirm the resilience and accuracy of generated models, showing high concordance with both machine learning and fuzzy logic predictions.

Materials exhibiting prolonged cycle stability and high energy density were optimal for energy storage applications. Carbonaceous materials, like activated copper oxide and carbon were frequently employed in supercapacitors because of their extensive surface area, which improves rapid charge-discharge rates and electrode-electrolyte interface interaction. These materials can also be employed in innovative energy devices, sensors, and applications including chemical or electrochemical sensors (Khawale *et al.* 2024). The preceding discussion indicates that the copper oxide-doped TiO₂ nanocomposite is suitable for energy applications, such as piezoelectric devices, nanoenergy materials, wearable and stretchable smart devices, electrochemical sensors, and nanostructures, especially as electrode materials. Machine-learning models were trained to predict sensor response, demonstrating high accuracy, and the optimized structure offers a cost-effective, stable platform for non-invasive glucose sensing (Shanmugam *et al.* 2026).

4. CONCLUSION

TiO₂/CuO nanocomposites were successfully fabricated using controlled hydrolysis and precipitation methods, resulting in nanoparticles with uniform morphology and crystallite sizes around 20.74 nm. The integration of CuO into the TiO₂ matrix enabled precise tuning of the band gap, which decreased from 3.0 eV at 0% CuO to 2.1 eV at 30% CuO, while charge transfer resistance reached a minimum of ~5.8 Ω at 15% CuO. Structural characterization using XRD confirmed the formation of well-defined crystalline phases, and scanning electron microscopy revealed uniform particle distribution without significant agglomeration. Photoluminescence studies indicated strong correlations between composition, crystallite size, and optical response, validating the effectiveness of compositional engineering.

Machine learning models, particularly SVR provided accurate predictions for band gap, charge storage capacity, power density, and charge transfer, with R² ranging from 0.927 to 0.956. The integration of hybrid fuzzy logic and ANN further enhanced the interpretability of nonlinear relationships between synthesis parameters and material performance. These results demonstrate that optimized CuO incorporation significantly improves electrical conductivity, energy density, and charge transfer efficiency. Thus, the study confirms that the TiO₂/CuO nanocomposite exhibits excellent potential for high-performance supercapacitors, batteries, and flexible electronic devices. The combined approach of experimental synthesis and predictive ML modeling establishes a robust framework for rapid design, optimization, and deployment of next-generation energy storage materials with tunable structural, optical, and electrochemical properties.

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CONFLICTS OF INTEREST

The authors declare that there is no conflict of interest.

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