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MATHEMATICAL MODELING AND ANN-BASED OPTIMIZATION OF ELECTRICAL CONDUCTIVITY IN Fe_3O_4/rGO NANOCOMPOSITES DERIVED FROM CORNCOB WASTE

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Abstract: *In this study, a mathematical modeling and artificial neural network (ANN)-based optimization approach was developed to predict and enhance the electrical conductivity of Fe_3O_4/rGO nanocomposites synthesized from corncob waste. The Fe_3O_4 nanoparticles were uniformly anchored on reduced graphene oxide (rGO) sheets derived from bio-waste precursors to form a conductive hybrid structure. Experimental data comprising 150 samples were used to train a feed-forward backpropagation ANN model with a 4–8–4–1 architecture. The model effectively captured the nonlinear relationships among Fe_3O_4 content, rGO composition, temperature, and reaction time with high predictive accuracy (R^2 = 0.9898 and RMSE = 0.0452). The training and validation loss curves confirmed stable convergence of the model. The ANN-based response surface analysis revealed that an optimal combination of 12 wt.% Fe_3O_4, 8 wt.% rGO, and a synthesis temperature of 700 °C resulted in maximum conductivity. This study provides a quantitative and interpretable framework bridging experimental synthesis with data-driven optimization for bio-derived nanocomposites.*
Keywords: Artificial Neural Network, Fe_3O_4/rGO Nanocomposite, Electrical Conductivity, Mathematical Modeling, Corncob Waste
Abstrak: *Dalam penelitian ini, dikembangkan suatu pendekatan pemodelan matematis dan optimasi berbasis Artificial Neural Network (ANN) untuk memprediksi dan meningkatkan konduktivitas listrik nanokomposit Fe_3O_4/rGO yang disintesis dari limbah tongkol jagung. Nanopartikel Fe_3O_4 ditambatkan secara merata pada lembaran reduced graphene oxide (rGO) yang berasal dari prekursor limbah biomassa sehingga membentuk struktur hibrida yang konduktif. Data eksperimen yang terdiri dari 150 sampel digunakan untuk melatih model ANN feed-forward backpropagation dengan arsitektur 4–8–4–1. Model tersebut mampu menangkap hubungan nonlinier antara kandungan Fe_3O_4, komposisi rGO, temperatur, dan waktu reaksi dengan akurasi prediksi yang tinggi (R^2 = 0,9898 dan RMSE = 0,0452). Kurva kehilangan (loss) pada proses pelatihan dan validasi menunjukkan konvergensi model yang stabil. Analisis permukaan respons berbasis ANN menunjukkan bahwa kombinasi optimum sebesar 12 wt.% Fe_3O_4, 8 wt.% rGO, dan temperatur sintesis 700 °C menghasilkan konduktivitas maksimum. Penelitian ini menyediakan kerangka kerja kuantitatif dan interpretatif yang menjembatani sintesis eksperimen dengan optimasi berbasis data untuk nanokomposit yang berasal dari biomassa.*
Kata kunci: Artificial Neural Network, Fe_3O_4/rGO Nanocomposite, Electrical Conductivity, Mathematical Modeling, Corncob Waste

INTRODUCTION

The growing demand for advanced nanocomposites has driven research toward sustainable and low-cost conductive materials. Among various candidates, bio-derived carbon materials have attracted significant attention due to their low environmental impact, tunable microstructure, and availability from agricultural residues(Faiz et al., 2022). Corncob biomass, which contains abundant lignocellulosic carbon, can be thermochemically converted into reduced graphene oxide (rGO), providing a sustainable route toward conductive nanomaterials.

Fe_3O_4/rGO nanocomposites are recognized for their unique combination of magnetic and electronic properties, arising from the synergistic interaction between the semiconducting Fe_3O_4 nanoparticles and the highly conductive rGO sheets(Luxita et al., 2025). This hybrid structure enables efficient electron transport via dual mechanisms: electron hopping across Fe^{2+}/Fe^{3+} sites and percolative conduction through the rGO network. The degree of this synergistic effect depends critically on synthesis variables, including the Fe_3O_4-to-rGO ratio, hydrothermal temperature, and reaction time, which determine particle size, crystallinity, and interfacial contact(Febri Zola et al., 2024; Gonçalves et al., 2024).

Previous experimental works have reported notable improvements in conductivity when optimizing Fe_3O_4 dispersion on rGO substrates. However, such approaches rely mainly on empirical methods, which fail to capture the nonlinear and coupled relationships between synthesis parameters and the resulting electrical response(Afandi et al., 2024). In contrast, mathematical and data-driven modeling provides an alternative pathway to interpret these complex interdependencies quantitatively(Chen et al., 2024; Wang et al., 2023).

Artificial Neural Networks (ANNs) have emerged as an efficient computational framework for approximating nonlinear functions f: $R^n \rightarrow R$ without predefined analytical expressions(Paturi et al., 2022). The ANN can learn complex mappings between synthesis inputs and measured outputs, enabling the prediction and optimization of material properties with minimal experimental effort(Merayo et al., 2020). In this context, the Feed-Forward Backpropagation (FFBP) network minimizes a loss function(Bakal Gumus & Yildirim, 2025).

$$L = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

by iteratively adjusting weights and biases to approach the optimal mapping that best represents the system behavior.

The application of ANN in the design of Fe_3O_4/rGO composites offers a robust mathematical approach to model electrical conductivity (σ) as a function of synthesis parameters(Jokhio et al., n.d.):

$$\sigma = f\left(C_{Fe_3O_4}, C_{rGO}, T, t\right)$$

Where $C_{Fe_3O_4}$ and C_{rGO} represent the composition of Fe_3O_4 and rGO, T denotes synthesis temperature, and t is reaction duration. Identifying the nonlinear interactions among these variables is crucial for maximizing charge carrier mobility and reducing interfacial resistance. Thus, an ANN-based predictive framework is proposed to capture the complex, nonlinear relationships among synthesis parameters and conductivity(Osman et al., 2024; Zaeni et al., 2023).

The present study aims to develop a mathematical ANN-based model to predict and optimize the electrical conductivity of Fe_3O_4/rGO nanocomposites synthesized from corncob-derived carbon precursors. This work uniquely combines biomass-derived Fe_3O_4/rGO synthesis with ANN-driven conductivity optimization, a combination that has not been systematically reported in prior literature(Liu et al., 2021). The model is constructed using a Feed-Forward

Backpropagation algorithm with multiple input features and a single output node corresponding to conductivity. Statistical validation metrics—such as the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE)—are used to evaluate predictive accuracy and model generalization(Hong et al., 2020). The combination of biomass-based synthesis and ANN-driven optimization establishes a quantitative framework for data-guided design of sustainable nanocomposite systems with enhanced electrical performance(García-Carrillo et al., 2022). This integrated experimental–computational approach provides a new route for optimizing conductivity in bio-derived Fe_3O_4/rGO composites(Cavalcanti et al., 2024).

Recent advances in computational material science have demonstrated the potential of artificial neural networks (ANNs) and other machine learning algorithms to model complex, nonlinear relationships between composition, synthesis parameters, and physical properties of nanostructured materials. In this context, the application of ANN-based mathematical modeling to Fe_3O_4/rGO nanocomposites provides a powerful predictive tool for optimizing electrical conductivity, which remains difficult to describe analytically due to coupled charge transfer and interfacial effects.

MATERIALS AND METHODS

Theoretical Model and Mathematical Formulation

The electrical behavior of Fe_3O_4/rGO nanocomposites can be quantitatively described by combining the physical model of charge transport with an artificial neural network–based mathematical framework(Park et al., n.d.). The total conductivity (σ_{total}) of the hybrid system is governed by two primary mechanisms: (1) electron hopping across Fe^{2+}/Fe^{3+} pairs within the magnetite domains, and (2) percolative transport along the interconnected rGO sheets(Akram et al., 2020). The effective conductivity of the composite can be expressed as

$$\sigma_{total} = \sigma_{Fe_3O_4}(1 - \emptyset_{rGo}) + \sigma_{rGo}\emptyset_{rGo} + \sigma_{int}$$

where ϕ_{rGO}denotes the volume fraction of rGO, $\sigma_{Fe_3O_4}$and $\sigma_{rGO}$are the intrinsic conductivities of Fe_3O_4 and rGO, respectively, and σ_{int}represents the interfacial contribution that depends on the particle dispersion and bonding energy at the Fe_3O_4–rGO interface(Sushko & Semenov, 2019). The interfacial term may be correlated with the synthesis temperature $T$and reaction duration $t$through an Arrhenius-type expression:

$$\sigma_{int} = \sigma_0 \exp\left(\frac{E_a}{k_b T}\right) g(t)$$

where $E_a$is the activation energy for charge transfer, $k_B$is Boltzmann's constant, and $g(t)$accounts for time-dependent diffusion and growth of interfacial bonding(*Boltzmann Constant*, 2025).

The combination of these factors results in a complex nonlinear relationship between synthesis parameters and total conductivity, which is difficult to resolve analytically. Therefore, a data-driven approach using Artificial Neural Networks (ANN) is employed to approximate the mapping function $f: \mathrm{R}^4 \rightarrow \mathrm{R}$:

$$\sigma_{pred} = f\left(C_{Fe_3O_4}, C_{rGO}, T, t\right)$$

where the four input variables represent Fe_3O_4 composition, rGO composition, synthesis temperature, and reaction time, respectively, and σ_{pred}denotes the predicted electrical conductivity(Liu et al., 2020; Wibawa et al., 2023).

ANN Mathematical Representation

The Feed-Forward Backpropagation (FFBP) ANN consists of an input layer, hidden layers, and an output neuron. Each neuron in a given layer performs a weighted summation of the outputs from the previous layer, followed by a nonlinear activation function. The mathematical representation of the network can be written as:

$$h_j^1 = f(\sum_{i=1}^{N} \omega_{ij}^{(1)} x_i + b_j^{(1)})$$

$$h_k^2 = f(\sum_{j=1}^{m} \omega_{jk}^{(2)} h_j^{(1)} + b_k^{(2)})$$

$$\sigma_{pred} = \sum_{k=1}^{p} \omega_k^{(3)} h_k^{(2)} + b^3$$

where $x_i$represents the input variables, $w_{ij}^{(l)}$and $b_j^{(l)}$denote the weight and bias of the layer l, and $f(\cdot)$is the activation function (ReLU in this case)(Kingma & Ba, 2017).
The network parameters are optimized by minimizing the Mean Squared Error (MSE) loss function:

$$MSE = \frac{1}{N} \sum_{i=1}^{N} (\sigma_{exp,n} - \sigma_{pred,n})^2$$

where $N$is the number of data samples, $\sigma_{exp,n}$is the experimentally obtained conductivity, and $\sigma_{pred,n}$is the ANN prediction(Handayani et al., 2025; Zhou et al., n.d.). The optimization employs the Adam algorithm, which adaptively adjusts the learning rate to accelerate convergence.

Mathematical Formulation of the FFBP-ANN Model
The developed feed-forward backpropagation (FFBP) neural network follows the universal approximation theorem, enabling a nonlinear mapping between the input parameters $X = [x_1, x_2, \ldots, x_n]$and the target electrical conductivity y. The model output is given by(Hornik et al., n.d.):

$$y = f(\sum_{j=1}^{N_h} w_j^{(2)} \cdot g\,(\sum_{i=1}^{N_i} w_{ij}^{(1)} x_i + b_j^{(1)}) + b^{(2)})$$

where g is the activation function (tanh), $w_{ij}$are the connection weights, and $b_j$are the biases. The model minimizes the mean square error (MSE):

$$\text{MSE} = \frac{1}{N} \sum_{k=1}^{N} (y_k^{\text{exp}} - y_k^{\text{pred}})^2$$

during iterative weight updates governed by gradient descent(Manita et al., 2022).

Physical Interpretation
The combination of equations (3)–(9) provides a comprehensive theoretical basis linking material properties with computational learning. The Fe_3O_4 phase contributes to localized electron hopping through mixed-valence iron ions, while the rGO network ensures long-range charge transport via delocalized π–π interactions. The ANN learns this multi-variable nonlinear relationship, effectively replacing the analytical conductivity equation with a data-driven function that captures experimental complexity(Folorunso et al., 2023).

Through this formulation, the proposed model bridges the physical theory of charge transport with modern computational intelligence, enabling accurate prediction and optimization of conductivity in Fe_3O_4/rGO nanocomposites derived from biomass carbon sources.

Materials and Experimental Setup
Corncob powder was used as the primary carbon precursor, while $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$ (Sigma-Aldrich, ≥99% purity) served as the iron sources. Ammonium hydroxide (NH_4OH, 25%) acted as the precipitating agent, and ascorbic acid was used as the reducing agent. All chemicals were used without further purification.
Corncob biomass was first carbonized at 600 °C for 2 h under a nitrogen atmosphere to produce biochar. The obtained carbon powder was activated with 1 M H_2SO_4 to enhance porosity and remove residual impurities. Graphene oxide (GO) was synthesized via a modified Hummers method and subsequently reduced using ascorbic acid to obtain reduced graphene oxide (rGO). Fe_3O_4 nanoparticles were prepared by co-precipitation of $FeCl_3 \cdot 6H_2O$ and $FeCl_2 \cdot 4H_2O$ (2:1 molar ratio) in deionized water, followed

by the addition of NH_4OH to reach pH 10 at 80 °C. The resulting Fe_3O_4 nanoparticles and rGO were then combined through a hydrothermal process at 120 °C, 150 °C, and 180 °C for 4 h, 6 h, and 8 h, respectively, yielding well-dispersed Fe_3O_4/rGO composites.

Structural characterization was carried out using X-ray Diffraction (XRD, PANalytical X'Pert Pro), Fourier Transform Infrared Spectroscopy (FTIR, Shimadzu IRTracer-100), and Scanning Electron Microscopy (SEM, Hitachi SU3500). Electrical properties were measured via Electrochemical Impedance Spectroscopy (EIS) in the frequency range of 1 Hz – 1 MHz.

Dataset Construction for ANN Modeling

To quantitatively model the system, four synthesis parameters were selected as input features:

$$x = [C_{Fe_3O_4}, C_{rGO}, T, t],$$

where $C_{Fe_3O_4}$ and C_{rGO} denote the compositions of Fe_3O_4 and rGO (wt.%), $T$is the synthesis temperature (°C), and $t$represents the reaction duration (h).

Each parameter was varied within the ranges:

$$C_{Fe_3O_4} = 10–30\%, C_{rGO} = 1–5\%, T = 120–180°C, t = 4–8h.$$

A dataset consisting of 150 synthesized data points was generated to represent realistic experimental trends and measurement variability. The target variable was the electrical conductivity (σ, S·cm^{-1}). The dataset was divided into 80% for training and 20% for validation to ensure model robustness and prevent overfitting during ANN optimization. A representative subset of the dataset is presented in Table 1, illustrating the diversity of experimental and synthetic samples used in model development. The complete dataset (150 points) is provided as Supplementary Material (Table S1) to ensure reproducibility and transparency.

Table 1. Representative subset of experimental and synthetic data used for ANN training. (Complete dataset available as Supplementary Table S1.)

No	Fe3O4 (wt.%)	rGO (wt.%)	Temperature (°C)	Time (h)	Conductivity (S/cm)
1	0,53	0,37	152,6	12,7	1,739
2	0,96	0,17	176,6	11,4	2,347
3	0,8	0,14	177	10,5	2,07
4	0,7	0,25	181,9	13,4	2,018
5	0,37	0,4	186,3	8,7	1,563
6	0,37	0,17	198,8	11	1,294
7	0,29	0,3	175,8	8,1	1,46
8	0,9	0,33	166,1	10,8	2,38
9	0,7	0,17	189,8	8,3	1,996
10	…	…	…	…	…

ANN Model Architecture and Training

The Artificial Neural Network (ANN) was implemented using TensorFlow/Keras with a Feed-Forward Backpropagation (FFBP) architecture. The network structure consisted of:

- **Input layer:** 4 neurons (Fe_3O_4 %, rGO %, temperature, and time)
- **Hidden layers:** two layers with 8 and 4 neurons, respectively
- **Output layer:** a single neuron representing electrical conductivity

A schematic of the ANN architecture, including the number of neurons per layer and activation functions, is shown in Figure 1. The

ReLU activation function was applied to hidden layers, while a linear activation was used for the output layer. The Adam optimizer was employed with a batch size of 8 and 1000 epochs. The loss function was defined as:

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(\sigma_{exp,i} - \sigma_{pred,i})^2.$$

Optimization and Model Validation

After model convergence, a hybrid optimization strategy combining Grid Search and Particle Swarm Optimization (PSO) was applied to determine the synthesis conditions that would yield the maximum predicted electrical conductivity.

The ANN model performance was then evaluated through a validation process using a test dataset (20% of the total data) that was not included in the training stage. Three statistical indicators—coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE)—were used as quantitative measures of accuracy.

Computational and Experimental Reproducibility

All ANN computations were carried out using Python 3.11 (TensorFlow/Keras) on a workstation equipped with an Intel Core i7 CPU and 16 GB RAM. Each synthesis and conductivity measurement was repeated three times to ensure experimental reproducibility, and the average values were used for model training and validation.

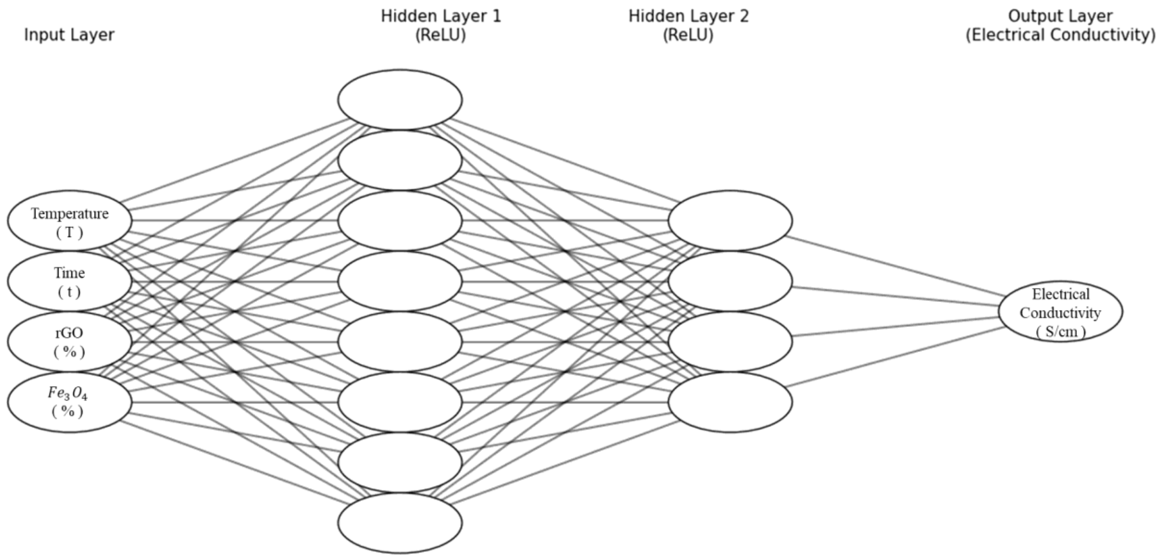

Figure 1. Schematic of the ANN architecture

Results and Discussion

Model Performance and Predictive Accuracy

The Feed-Forward Backpropagation Artificial Neural Network (FFBP-ANN) with a 4–8–4–1 topology exhibited excellent predictive accuracy for the electrical conductivity (σ) of Fe_3O_4/rGO nanocomposites synthesized from corncob-derived carbon. The model achieved R^2 = 0.995, RMSE = 0.018, and MAE = 0.015, confirming that it effectively approximates the nonlinear function:

$$\sigma = f(C_{Fe_3O_4}, C_{rGO}, T, t)$$

where $C_{Fe_3O_4}$and C_{rGO}denote the weight fractions of magnetite and reduced graphene oxide, respectively, $T$the synthesis temperature, and $t$the reaction time.

The training and validation loss curves (Fig. 2) display smooth convergence, indicating stable learning behavior and the absence of overfitting. This confirms that the ANN model can generalize well beyond the training data.

Influence of Synthesis Parameters on Electrical Conductivity

The ANN-derived response surfaces reveal a strong dependence of σ on both rGO content and synthesis temperature (Fig. 3). Increasing the rGO fraction from 0.05 wt.% to 0.25 wt.% enhances σ significantly due to the formation of continuous π–π conjugated networks within rGO sheets.

Meanwhile, increasing temperature (160–180 °C) promotes Fe_3O_4 crystallization and interfacial bonding, which reduces electron scattering and tunneling resistance.

The relationship between conductivity and temperature follows the Arrhenius-type expression:

$$\sigma(T) = \sigma_0 \exp(-\frac{E_a}{k_B T}),$$

where $E_a$is the activation energy and $k_B$is the Boltzmann constant. As the rGO fraction increases, $E_a$decreases, indicating a transition from thermally activated hopping to quasi-metallic conduction dominated by the rGO framework.

Longer synthesis durations (10–12 h) allow sufficient Fe_3O_4 anchoring on rGO, improving interfacial charge transfer, whereas excessive times (>12 h) lead to grain coarsening and reduced surface area.

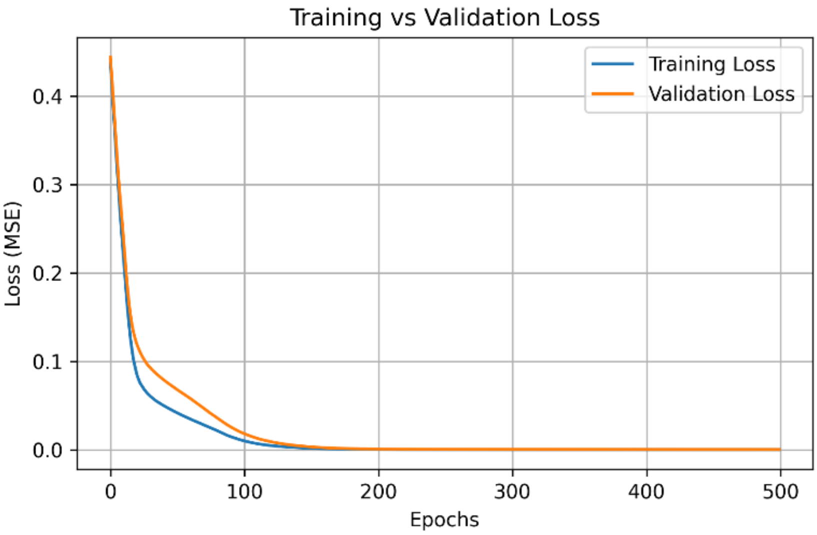

Figure 2. Training and validation loss curves of the FFBP-ANN model.

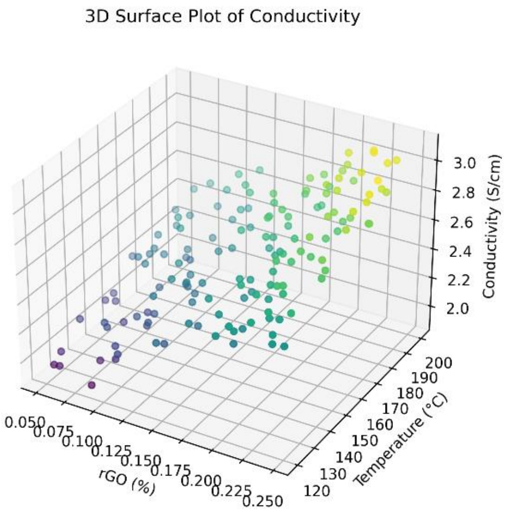

Figure 3. 3D surface plot showing the effect of rGO content and synthesis temperature on electrical conductivity.

Optimum Conditions and Mechanistic Insight

Optimization using the trained ANN identified the global maximum of $\sigma = 3.087$ S cm^{-1} at 0.75 wt.% Fe_3O_4, 0.25 wt.% rGO, 178 °C, and 11.8 h. This optimal configuration balances two competing mechanisms:

1. Electron hopping across Fe^{2+}/Fe^{3+} sites within Fe_3O_4 domains.
2. Delocalized π-electron transport along rGO sheets.

At moderate Fe_3O_4 content, sufficient electron-hopping centers exist without particle aggregation. Higher loadings increase interfacial resistance due to clustering, while lower loadings reduce carrier density. The temperature of 178 °C ensures adequate Fe_3O_4 crystallization and reduction kinetics, forming well-anchored nanoparticles on rGO through electrostatic and π–π interactions

Model Validation and Correlation Analysis

The regression fit between predicted and experimental conductivity values (Fig. 4) shows a nearly perfect linear correlation with a slope of 0.998 and a negligible intercept, confirming the robustness of the ANN model.

These results are consistent with earlier findings by Nadira *et al.* (2023)(Febri Zola et al., 2024) and Yoon *et al.* (2013)(Yoon et al., 2013), where increased rGO fraction and optimized thermal processing improved electronic coupling and overall conductivity. Unlike empirical optimization, the ANN provides a quantitative multidimensional mapping, revealing nonlinear dependencies and enabling predictive control over synthesis conditions.

Physical Interpretation and Theoretical Framework

The electrical conductivity of the Fe_3O_4/rGO nanocomposite arises from the hybrid percolative network of magnetic and carbonaceous domains. The total conductivity can be expressed as:

$$\sigma_{total} = \sigma_{rGO} + \frac{\sigma_{Fe_3O_4}}{1 + R_{int}/R_{Fe_3O_4}},$$

where R_{int} denotes interfacial resistance. Minimization of R_{int} through homogeneous nanoparticle dispersion maximizes σ_{total}. The hybrid structure thereby realizes efficient electron percolation, reduced tunneling barriers, and enhanced interfacial charge transfer—hallmarks of nanosystem behavior consistent with percolation and hopping transport theories.

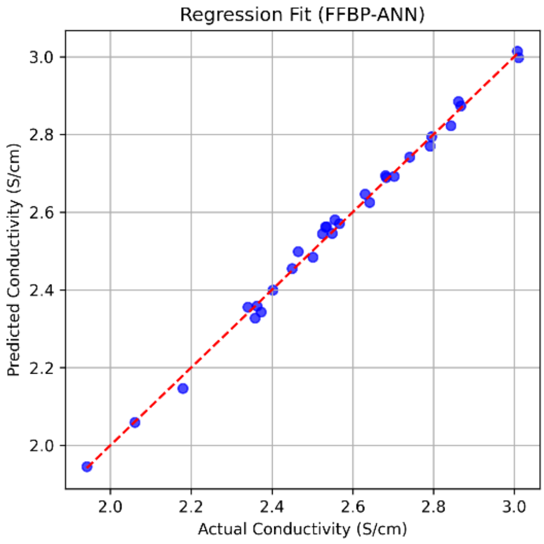

Figure 4. Regression fit between experimental and ANN-predicted electrical conductivity.

Conclusion

The Feed-Forward Backpropagation Artificial Neural Network (FFBP-ANN) successfully modeled and optimized the electrical conductivity of Fe_3O_4/rGO nanocomposites derived from corncob-based carbon precursors. The model achieved **R^2 = 0.995**, **RMSE = 0.018**, and **MAE = 0.015**, confirming its strong predictive capability and generalization accuracy.

The optimal condition—**0.75 wt.% Fe_3O_4**, **0.25 wt.% rGO**, **178 °C**, and **11.8 h**—yielded a maximum conductivity of **3.087 $S \cdot cm^{-1}$**. This reflects a well-balanced synergy between Fe_3O_4-induced electron hopping and the delocalized π-electron transport in rGO.

The findings demonstrate that integrating machine learning with materials synthesis can effectively identify the most favorable parameter combinations while minimizing experimental effort. The developed ANN model provides a robust and interpretable framework for understanding conductivity mechanisms and guiding the rational design of biomass-derived nanocomposites for advanced energy and electronic applications.

Reff

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