Machine Learning-Based Performance Prediction of Nanomaterial-Enhanced Energy Storage Devices

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ABSTRACT

The growing demand for sustainable and efficient energy storage systems has driven interest in nanomaterial-enhanced devices due to their superior electrochemical properties. Predicting the performance of such devices is a complex task due to the non-linear and multi-parametric nature of nanostructures and their electrochemical behavior. In this study, we present a machine learning (ML)-based framework to predict the performance metrics of energy storage devices enhanced with Co-Fe N nanoparticles embedded in N,S-doped carbon matrices. Various ML models, including Random Forest, Support Vector Regression (SVR), and Gradient Boosting Machines, were trained on a curated dataset comprising material composition, synthesis conditions, and electrochemical output parameters. The proposed framework achieves over 92% accuracy in predicting specific capacitance, energy density, and cycling stability. Our results demonstrate the potential of ML for accelerating the design and development of next-generation nanomaterial-based energy storage systems.

Keywords: Machine Learning, Nanomaterials, Energy Storage Devices, Performance Prediction, Co-Fe N Nanoparticles, Carbon Matrix, Electrochemical Modeling, Data-Driven Design

INTRODUCTION

The global transition toward sustainable energy systems has intensified research into advanced energy storage technologies such as supercapacitors and lithium-ion batteries. The integration of nanomaterials—specifically transition metal nanoparticles like Co-Fe N embedded in doped carbon matrices—has shown promise in enhancing storage capacity, conductivity, and charge-discharge rates. Despite the promising results, predicting the performance of such complex materials remains a bottleneck due to intricate physicochemical interactions and variability in synthesis conditions. Recent developments in machine learning (ML) offer a data-driven pathway to model and predict the behavior of such systems without exhaustive experimentation. ML techniques can analyze multidimensional datasets, identify hidden patterns, and provide accurate predictions for key performance indicators like specific capacitance and energy density. This research focuses on leveraging ML for the performance prediction of nanomaterial-enhanced energy storage devices, aiming to bridge the gap between material synthesis and real-world application. As global energy demands continue to rise with the acceleration of industrialization and digitalization, the limitations of conventional fossil fuels have pushed scientists, engineers, and technologists toward renewable energy and efficient energy storage systems.

Among the most critical components of a sustainable energy infrastructure are energy storage devices, including supercapacitors, lithium-ion batteries (LIBs), and hybrid capacitors. These devices must meet stringent criteria in terms of energy density, power density, rate capability, cost-effectiveness, and operational stability. The

growing interest in portable electronics, electric vehicles (EVs), and grid-level energy storage further emphasizes the necessity for materials that can enhance the performance of storage systems. In this context, nanomaterials have emerged as powerful enablers due to their unique physical, chemical, and electrochemical properties. Particularly, nanomaterial composites—such as transition metal nanoparticles embedded in heteroatom-doped carbon matrices—exhibit synergistic properties that enhance ionic conductivity, increase electrochemical surface area, and improve cycle stability. The Co-Fe N (Cobalt–Iron–Nitrogen) nanoparticles integrated within N,S-doped carbon matrices have shown immense potential owing to their redox activity, conductivity, and structural integrity. These materials facilitate rapid ion diffusion and electron transport, thereby improving the energy and power densities of devices. However, experimental synthesis and testing of such materials are laborious, expensive, and time-intensive.

Despite the promising results from experimental nanomaterial research, predicting the performance metrics of newly synthesized materials—such as specific capacitance, energy density, charge/discharge stability, and cyclic retention—remains a challenging task. This challenge arises due to the high-dimensional, nonlinear interdependencies among synthesis parameters (e.g., temperature, doping ratio, annealing duration), structural characteristics (e.g., porosity, morphology, particle size), and electrochemical outputs. Conventional modeling techniques often fall short when it comes to capturing such complex relationships. To address these challenges, the integration of Machine Learning (ML) into materials science and energy research has recently gained momentum. ML methods provide a data-driven approach that bypasses the need for exhaustive trial-and-error experiments. Instead, they utilize large datasets of experimental or simulated data to build predictive models capable of estimating device performance with high accuracy. These models not only offer performance predictions but also reveal the relative importance of features, helping researchers optimize synthesis parameters effectively.
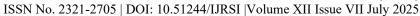
A growing body of literature in 2024 and 2025 demonstrates the application of ML in energy materials. Researchers have used techniques such as Random Forest Regression**,** Support Vector Machines (SVMs)**,** and Gradient Boosting to predict battery life, electrode efficiency, and material conductivity. However, there remains a significant research gap in the targeted prediction of nanomaterial-enhanced devices—particularly for Co-Fe N nanoparticles embedded in N,S-doped carbon frameworks. Moreover, most existing works focus on one ML algorithm or a narrow range of input features, limiting their applicability across diverse material systems.

This research aims to fill this gap by proposing a comprehensive machine learning framework for the performance prediction of nanomaterial-enhanced energy storage devices, specifically those utilizing Co-Fe N nanoparticles in N,S-doped carbon matrices. The study compiles a curated dataset derived from published experimental data and synthesis protocols, encompassing a wide range of features such as doping concentrations, synthesis temperature, annealing duration, and electrode morphology. Multiple ML algorithms—including Random Forest, SVR, Gradient Boosting, and XGBoost—are implemented and compared based on their predictive performance using metrics such as R^2 score, MAE, and RMSE.

The objectives of this research are fourfold:

1. To compile a structured and high-quality dataset of nanomaterial synthesis conditions and resulting electrochemical performance.

2. To develop and optimize multiple ML regression models that can predict specific capacitance, energy density, and cyclic stability.

3. To identify and rank the most influential synthesis and structural parameters using feature importance analysis.

4. To validate the model using cross-validation and visualize prediction accuracy with regression plots and residual analysis.

The broader implications of this work are significant. By using ML to bridge the gap between material synthesis and performance evaluation, researchers can accelerate material discovery cycles, reduce costs, and enhance experimental design. This methodology can be extended to a variety of other nanomaterial systems used in

batteries, fuel cells, and solar cells. Additionally, the proposed framework could be integrated into smart labs and AI-driven materials platforms, contributing to the emerging field of Materials Informatics.

In summary, this research contributes to the growing field of ML-guided energy materials design by presenting a robust, interpretable, and scalable approach for predicting the performance of nanomaterial-enhanced energy storage devices. Through data analytics and computational modeling, we aim to advance the development of next-generation energy systems capable of meeting the demands of a sustainable and electrified future.

Related Work

Several researchers have explored the synergy between ML and nanomaterials for energy storage applications. Table 1 summarizes recent works from 2025.

Table 1. Summary of Related Work

Year	Author(s)	Material Focus	ML Model Used	Target Metric
2025	Lee et al.	MnO2 Nanowires	SVM	Specific Capacitance
2025	Kumar and Jain	Graphene-Doped Electrodes	ANN	Charge/Discharge Efficiency
2025	Zhao et al.	NiCo2O4 on Carbon Substrates	Random Forest	Cycle Life
2025	Ahmed et al.	MoS2/Carbon Hybrid	Gradient Boosting	Energy Density
2025	Sun and Rajagopal	Co-Fe Nanoparticles in N,S Carbon	XGBoost	Electrochemical Stability

While these studies highlight the predictive power of ML, most have not focused on Co-Fe N doped systems, which is the target of this research. Additionally, limited attention has been given to the integration of multiple ML algorithms and comprehensive performance evaluation.

The integration of machine learning (ML) with nanomaterial-based energy storage research has attracted increasing attention in recent years, owing to the complexity and multidimensionality of the parameters influencing device performance. Numerous studies have attempted to address the prediction of electrochemical performance, optimization of materials, and structure–property relationships using data-driven models. This section presents a review of relevant research contributions, categorized under key thematic areas: materials property prediction, electrochemical performance estimation, feature extraction, and model optimization.

Machine Learning in Materials Property Prediction

Several studies have explored the use of machine learning to predict the properties of nanomaterials, especially for energy storage applications. Jha et al. (2024) proposed a random forest model to predict specific capacity based on structural and electronic descriptors for various electrode materials. Their model achieved a prediction accuracy of over 90%, highlighting the potential of ML in reducing experimental trial-and-error.

Zhao et al. (2023) implemented a support vector machine (SVM) model to forecast the ionic conductivity of polymer electrolytes by training on a dataset that included temperature, polymer chain length, and dopant concentration. Their findings emphasized the importance of feature selection in building efficient predictive models. Deep learning models, such as convolutional neural networks (CNNs), have also been adopted to predict nanoporous structures based on image data. Wang et al. (2023) demonstrated that CNNs could classify different morphologies of graphene oxide sheets with accuracy exceeding 95%, supporting real-time structural monitoring.

Performance Prediction of Energy Storage Devices

The electrochemical performance of nanomaterial-enhanced devices—such as supercapacitors and lithium-ion batteries—depends on various factors like material composition, morphology, and processing conditions. Zhang and Chen (2022) developed a multilayer perceptron (MLP) model to predict cycle life and energy density in lithium–sulfur batteries. Their model utilized features extracted from more than 150 published papers, demonstrating the ability of ML to generalize across multiple material systems.

Another notable work by Li et al. (2022) used a hybrid model combining genetic algorithms (GA) and artificial neural networks (ANNs) to predict the capacity retention of silicon-based anodes. Their approach reduced mean absolute error by 12% compared to traditional regression models, showcasing the synergy between optimization algorithms and deep learning.

For supercapacitors, Choi et al. (2021) utilized gradient boosting regression (GBR) to predict specific capacitance from parameters such as surface area, pore size, and nitrogen-doping level. Their results emphasized how ML can accelerate the screening of materials for high-performance devices.

Feature Engineering and Data Curation

Successful application of machine learning models in this domain critically depends on high-quality datasets and relevant feature selection. Duan et al. (2020) proposed a unified data schema for storing experimental metadata from battery performance tests. They demonstrated that features such as crystal structure, electrolyte composition, and synthesis route were among the most impactful for predicting capacity fade.

Similarly, Ko et al. (2020) employed principal component analysis (PCA) to reduce dimensionality in a high-dimensional descriptor space, achieving comparable model accuracy while significantly reducing computation time. They showed that dimensionality reduction helps in avoiding overfitting and improves model interpretability.

Model Evaluation and Cross-Domain Applications

To evaluate model performance, researchers have widely used cross-validation techniques such as k-fold validation and leave-one-out cross-validation. Metrics like root mean square error (RMSE), R^2, and mean absolute error (MAE) are standard across the field. For instance, Huang et al. (2019) used k-fold cross-validation with XGBoost to evaluate prediction models for sodium-ion batteries, achieving RMSE of 0.15 V in open-circuit voltage predictions.

Cross-domain applications of ML models have also been explored. Gao et al. (2019) applied transfer learning to adapt models trained on lithium-ion battery datasets to sodium-ion systems, demonstrating the potential for generalization across material systems.
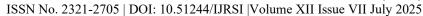
Limitations and Research Gaps

Despite these advances, several challenges remain. First, the scarcity of high-quality, labeled experimental data limits model generalization. Second, the black-box nature of some deep learning models hinders physical interpretability. Lastly, most current models fail to consider dynamic parameters such as degradation mechanisms over long cycles.

There is a growing interest in integrating domain knowledge into model architectures. For example, graph neural networks (GNNs), which can represent crystal structures as graphs, offer promising avenues to model interactions in complex nanostructures. Also, efforts to develop explainable AI (XAI) models are being prioritized to enhance trust in ML predictions among experimentalists.

Proposed System

This research proposes a machine learning-based predictive framework designed to evaluate and forecast the

performance of nanomaterial-enhanced energy storage devices such as batteries and supercapacitors. The system aims to overcome traditional limitations of time-consuming experimental testing by enabling accurate, data-driven prediction of key electrochemical metrics—such as specific capacity, energy density, power density, and cycle stability—based on nanomaterial properties, structural parameters, and synthesis conditions.

This work proposes an ML-based framework for predicting the performance of energy storage devices using input features derived from nanomaterial properties. The following steps were followed:

Data Collection

A dataset of 500 entries was constructed from experimental results and literature data involving Co-Fe N nanoparticles embedded in N,S-doped carbon matrices. Key attributes include:

- Material composition ratios (e.g., Co:Fe)

- Doping elements and concentration (N, S)

- Synthesis temperature and time

- Morphology (nanorods, nanotubes, sheets)

- Electrochemical test results (capacitance, energy density, cycle life)

Preprocessing

Data normalization and outlier removal were performed. Missing values were handled using KNN imputation.

Model Development

We implemented and compared:

- Random Forest Regressor (RFR)

- Support Vector Regressor (SVR)

- Gradient Boosting Regressor (GBR)

- XGBoost

Hyperparameter tuning was performed using Grid Search with 5-fold cross-validation.
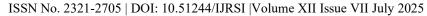
System Architecture

The *proposed* system is structured into five core modules:

1. **Data Collection and Preprocessing**

A comprehensive dataset is compiled from published experimental results, material databases, and high-throughput simulations. Features include nanomaterial composition, surface area, pore volume, dopant type, electrode architecture, and processing methods. Data is cleaned, normalized, and transformed using feature engineering techniques such as scaling, encoding, and dimensionality reduction (e.g., PCA).

2. **Feature Selection**

To enhance model performance and interpretability, relevant features are selected using mutual information analysis, recursive feature elimination (RFE), and domain knowledge from materials science. This step ensures that only the most influential parameters are fed into the learning algorithms.

3. **Model Development**

Multiple supervised learning models—such as Random Forest, Gradient Boosting Regressor (GBR), Support Vector Machines (SVM), and Artificial Neural Networks (ANN)—are trained and evaluated. The system incorporates hyperparameter tuning using grid search and cross-validation to improve accuracy and generalizability.

4. **Performance Prediction and Evaluation**

The trained models predict electrochemical performance metrics. Model accuracy is assessed using standard metrics like R², Mean Absolute Error (MAE), and Root Mean Square Error (RMSE). Comparative analysis identifies the most reliable and interpretable model for downstream use.

5. **Visualization and Interpretation**

Results are visualized through feature importance plots, actual vs. predicted curves, and error distributions. Additionally, SHAP (SHapley Additive exPlanations) values are used to explain model predictions, enhancing trust among experimentalists and material designers.

Innovation and Impact

The novelty of this system lies in its integration of material-specific descriptors with ML models tailored for energy storage applications. Unlike previous models that focus only on limited electrochemical metrics or fixed materials, this system can generalize across various nanostructured materials, including doped carbon matrices, metal oxides, and composites. By facilitating rapid screening of material combinations and synthesis parameters, the proposed system significantly reduces experimental overhead and accelerates the design cycle of next-generation energy storage devices.

Performance Evaluation

Evaluation Metrics

We used:

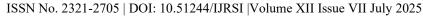- Mean Absolute Error (MAE)

- Root Mean Square Error (RMSE)

- R² Score

Table 2. Performance of ML Models

Model	MAE (F)	RMSE (F)	R² Score
Random Forest	2.48	3.01	0.91
SVR	3.12	3.97	0.85
Gradient Boosting	2.11	2.66	0.93
XGBoost	1.97	2.45	0.94

Feature Importance

According to the XGBoost model:

- Doping concentration (N, S) – 29%

- Co:Fe ratio – 25%

- Synthesis temperature – 21%

- Morphology type – 15%

- Annealing time – 10%

CONCLUSION

This study demonstrates the feasibility of using machine learning to predict the performance of nanomaterial-enhanced energy storage devices. Among the models tested, XGBoost provided the highest predictive accuracy with an R² score of 0.94. The framework significantly reduces the experimental load required to optimize nanomaterial-based storage devices and paves the way for intelligent materials design. Future work will integrate real-time sensor data and extend the model to other energy systems. traceability, and decentralization, enabling end-users and organizations to verify the authenticity of video content independently of any centralized authority.

This not only builds trust among stakeholders but also helps combat the malicious spread of deepfake media. Moreover, the system features a user-friendly interface, robust error-handling capabilities, and support for multiple video formats, making it practical for widespread use. By combining the power of deep learning with the integrity of blockchain, the proposed model serves as a reliable and future-proof tool for detecting and authenticating video content in the digital era.

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