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Energy Density Prediction of Metal-Organic Frameworks (MOFs) From Synthesis Conditions Using Deep Neural Network (DNN): Hydrogen Storage Application

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ABSTRACT

The global transition toward sustainable energy systems necessitates efficient and scalable hydrogen storage technologies. Metal–organic frameworks (MOFs) have emerged as promising candidates for hydrogen storage due to their high surface area, tuneable pore structures, and favourable surface chemistry that enhance adsorption performance. However, real-time experimental measurement of hydrogen uptake using physical sensing systems is costly, computationally intensive, and operationally complex. To address these limitations, this study proposes a data-driven soft-sensor framework based on machine learning to predict energy density for hydrogen storage applications from synthesis parameters. High-fidelity secondary data sourced from an open-access Kaggle dataset were utilized, focusing on synthesis descriptors including metal type, oxidation state, temperature, and reaction time. Recognizing the intrinsic influence of transition metals on structural stability and adsorption behaviour, a per-metal modelling strategy was implemented to capture material-specific relationships. A Deep Neural Network (DNN) employing a Multi-Layer Perceptron (MLP) architecture trained via backpropagation was developed to model nonlinear interactions between structural variables and energy density. To enhance interpretability, complementary linear regression models were also constructed, yielding explicit predictive equations. Model performance was rigorously evaluated using statistical error metrics, achieving a Mean Squared Error (MSE) of 0.0821 and a Root Mean Squared Error (RMSE) of 0.2852, demonstrating strong predictive capability and generalization across different metallic linkers. The low error values confirm that artificial neural network–based soft sensors provide a reliable, low-latency alternative to physical sensing systems for monitoring hydrogen storage performance. This approach significantly reduces experimental burden, accelerates materials screening, and supports intelligent optimization of hydrogen-based fuel cell technologies, contributing to the advancement of scalable clean energy infrastructure.

1. Introduction

The worldwide transition to sustainable energy systems introduces intricate technical problems, with the optimisation of hydrogen storage infrastructure being a significant bottleneck. This challenge is further amplified by the imperative to accurately predict hydrogen sorption behavior in diverse geological formations for underground storage and natural hydrogen exploration (Nooraiepour et al., 2025). As the globe endeavours to decarbonise industrial and transportation

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sectors, the advancement of effective, high-capacity storage solutions is essential. Metal-Organic Frameworks (MOFs) have emerged as leaders in this domain. These materials offer exceptional porosity and tunable pore environments, making them highly promising for adsorptive hydrogen storage at relatively low pressures and diverse temperatures (Pourrahmani et al., 2023). Accurate modeling and prediction of hydrogen uptake in these materials are crucial for their design and optimization, often necessitating advanced computational techniques (Osman et al., 2024).

Nonetheless, the practical execution and characterisation of MOFs encounter substantial evidentiary challenges. The real-time quantification of hydrogen uptake is a significant challenge for researchers. Traditional experimental methods often involve lengthy and resource-intensive procedures, hindering rapid material screening and process optimization. Thus, in this study proposed data-driven soft-sensor framework based on machine learning to predict energy density for hydrogen storage applications from synthesis parameters. This approach aims to circumvent the limitations of experimental trial-and-error by leveraging machine learning to predict performance based on material characteristics and operating conditions, thereby accelerating the discovery and optimization of hydrogen storage solutions (Karuppusamy et al., 2025). Specifically, this research focuses on developing an Deep Neural Network based soft sensor capable of predicting hydrogen adsorption in Metal-Organic Frameworks by integrating various material properties and environmental factors (Hai et al., 2023; Pourrahmani et al., 2023). The current study of Soft sensor-based artificial neural network is focused on enhancing the precision and efficiency of predicting hydrogen storage capacity in MOFs, thereby offering a more streamlined approach to material design and optimization (Osman et al., 2024). This integration of machine learning, molecular simulations, and techno-economic analysis offers a comprehensive methodology for evaluating MOF performance under various operational conditions (Wang et al., 2025). This research aims to bridge the gap between theoretical material properties and practical application, providing a robust tool for the rapid assessment and intelligent design of next-generation hydrogen storage materials.

Thus, in this study concentrating on Predictive synthesis of metal-organic frame materials metallic linkers, such as Zinc (Zn), Zirconium (Zr), and Copper (Cu) was proposed to optimize hydrogen storage capacity by meticulously analyzing how these structural variations influence adsorption mechanisms and overall performance (Pourrahmani et al., 2023). This approach enables a nuanced understanding of the structure-property relationships critical for engineering MOFs with enhanced hydrogen storage capabilities (Osman et al., 2024). The research aims to utilize computational fluid dynamics simulations to generate a comprehensive database for training the Artificial Neural Network model, enabling the analysis of numerous MOF variations for optimal hydrogen storage (Pourrahmani et al., 2023). This method systematically explores the vast design space of MOFs, identifying promising candidates for experimental validation and subsequent development (Wang et al., 2025). This strategy leverages machine learning to create good model for hydrogen strorage application in near future.

2. Methodology

2.1 Data and Location

In this study, the secondary data was performed to develop Artificial Neural Network (ANN) soft sensor model. Here, the dataset taken from kaggle website (https://www.kaggle.com/datasets/marquis03/metal-organic-frame-materials-prediction?resource=download) open source data base. To achieve the result, variables such as oxidation state, temperature, metallic linker material characteristics (Zn, Zr, and Cu), and material synthesis duration were utilised in this work. The variable process will be trained utilising an Deep Neural Network (DNN) with a Multi-Layer Perceptron (MLP) architecture.

2.2 Deep Neural Network (DNN) based soft sensor

In order to archive the result, a model was developed using an Deep Neural Network (DNN) based data-driven soft-sensor framework based on machine learning to predict energy density for hydrogen storage applications from synthesis parameters. The suggested model utilises an Artificial Neural Network (ANN) with a Multi-Layer Perceptron (MLP) architecture and a backpropagation technique. The process variables, such as oxidation state, temperature, metallic linker material characteristics and material synthesis duration, serve as input variables, while energy density is the corresponding output variable. The interaction input and output variable was utilised to create the soft sensor model, which had four to five hidden layers and six to seven nodes (see Figure 1).

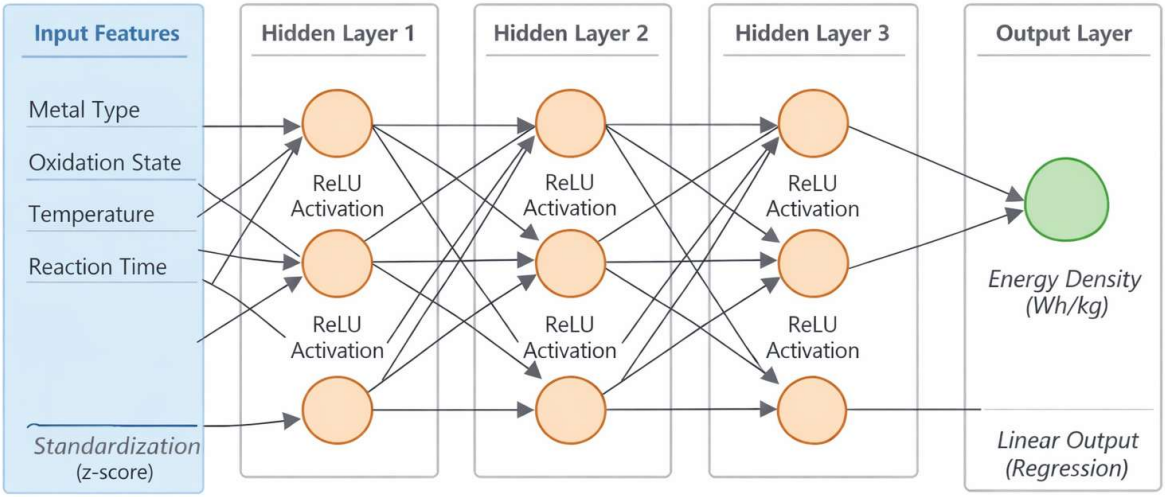

Fig1. Deep Neural Network (ANN) with a Multi-Layer Perceptron (MLP) architecture

As can be seen in Figure 1, Deep Neural Network (ANN) employing a Multi-Layer Perceptron (MLP) architecture was created to generate a robust energy density model. A large dataset of 538 data points was evaluated to assure good predicting accuracy. The model incorporates four essential input variables: oxidation state, operation temperature, particular properties of the metallic linker material, and overall synthesis duration. The characteristics were correlated with the target output variable, energy density, to develop an efficient soft sensor. Furthremore, this particular training method was selected for its efficacy in reducing mean squared error, enabling the model to precisely capture the intricate nonlinear correlations between the chemical synthesis inputs and the resultant energy density. Through the iterative adjustment of weights inside the MLP framework, the soft sensor serves as a dependable estimation instrument for material performance, eliminating the necessity for extensive physical testing. This computational method not only optimizes the characterisation procedure but also improves the comprehension of how synthesis variables collectively affect the ultimate energy storage potential of the metallic linker materials.

3. Results

3.1 Pre-Processing Dataset

In order to achieve the result, correlation analysis was conducted to assess the constructed model by determining R^2 value. This analysis metric is a vital indicator of the correlation between input and output variables. In this study, an extensive data cleansing procedure was implemented on the 538 datasets was performed to obtain the R^2 value between input and output variables. This

preprocessing phase entailed the identification and elimination of outliers, the resolution of missing values, and the assurance of numerical consistency to avert skewed outcomes and enhance the reliability of the soft sensor.The resultant R^2 value measures the fraction of variance in energy density that can be anticipated from the independent variables. By diligently refining the raw data prior to analysis, the study guarantees that the mathematical relationship obtained by the Levenberg-Marquardt method is founded on high-quality, representative samples. An elevated R^2 value indicates that the MLP architecture proficiently encapsulated the fundamental physics of material production.

3.2 Deep Neural Network training and and Testing Result

In order to obtain the result, the metal materials such as cd, co, cu, dy, eu, in, la, mg, mn, ini, tb, zn and zr was selected from database material. By using 538 data of material synthesis duration the model will be predicted energy density. Figure 1 shows the Mean Absolute Error (MAE) from DNN training and testing each metal from MOF material.

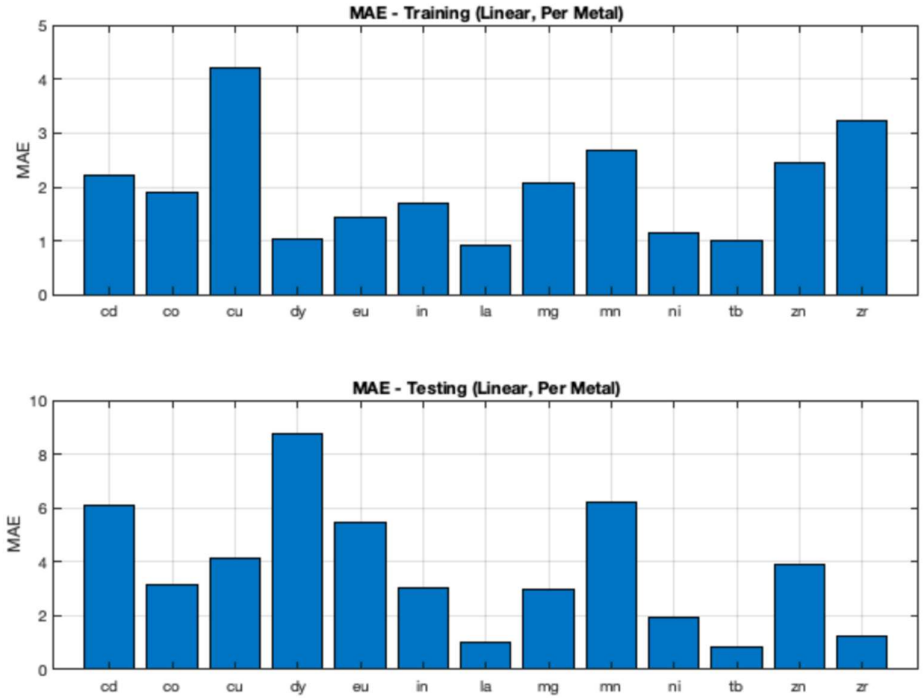

Fig2. Mean Absolute Error (MAE) from DNN training and testing each metal from MOF material

As can be seen in the figure, the training and testing outcomes of the per-metal linear regression model provide significant insights into the predictive dynamics of synthesis–energy density relationships among various metal types. During the training phase, the Mean Absolute Error (MAE) values for most metals are fairly low, usually between 0.9 and 2.7. This means that the linear model can fit the data that was observed with good accuracy. La, Dy, Tb, and Ni are metals that have very low training MAE values. This suggests that their energy density is strongly related to synthesis parameters in a mostly linear way. On the other hand, metals like Cu and Zr have higher training MAE values, which suggests that their structure–property relationships may be more variable or have nonlinear interactions that a simple linear formulation doesn't fully capture. MAE values go up for most metals when they are tested on data that the model has never seen before. This is expected because the model has to deal with new samples. But the size of this increase varies a lot. La and Tb are two metals that keep the testing MAE low, which means they can generalize well and make stable predictions. Meanwhile, metals like Cd, Eu, and Mn show small increases in testing error, which could

mean that the model is partially overfitting or that the data is more spread out than usual. Dy has the biggest difference between the MAE for training and testing, which means it doesn't generalize well. This could be because the sample size is too small or the behavior is too complicated. The overall results show that the per-metal linear modeling approach gives understandable predictive equations and works well for some metals. However, some materials have nonlinear or heterogeneous properties that may need more advanced nonlinear models, like deep neural networks, to be more generalizable and robust.

Furthermore, the metal materials such as cd, co, cu, dy, eu, in, la, mg, mn, ini, tb, zn and zr of MOF by using DNN. The DNN performance results for different metals here show which ones have more stable and predictable energy density behavior. The main way to judge the quality of a model is by testing the RMSE and MAE values, which show how well it generalizes to new data. La and Tb are the best materials for making predictions, with RMSE_Test values of about 1.05 and 1.03, respectively, and MAE_Test values of about 1.03 and 0.84, respectively. These results show that the energy density of La- and Tb-based frameworks is closely and consistently linked to the synthesis parameters. This means that the DNN can accurately model how they behave with very little error. Zr also generalizes well, with a low RMSE_Test (~1.86) and MAE_Test (~1.24), which means that the structural–energy relationships are stable. Ni and Mg also have moderate but acceptable predictive errors, which means that their energy density estimates are fairly reliable. On the other hand, metals like Cd, Eu, Dy, Mn, and Zn have much higher testing RMSE values, especially Cd (17.45) and Dy (10.30). This means that the predicted values are very different from the actual values. These large errors mean that either energy density has more inherent variability or the sample size is too small for reliable learning. Consequently, according to the generalization performance of DNN, La, Tb, and Zr seem to be the best materials for stable and predictable energy density behavior, while Cd and Dy show less reliable predictive power (see Table 1).

Table 1. DNN model to predict Energy Density

Metal	nRows	RMSE (Train)	RMSE (Test)	MAE (Train)	MAE (Test)	nFeatures
Cd	84	2.8745	17.453	2.2072	6.0893	
Co	73	2.5353	4.7481	1.9044	3.1611	
Cu	121	5.2837	4.5076	4.2204	4.1045	
Dy	9	1.2626	10.298	1.0281	8.7507	
Eu	17	1.7441	9.2611	1.4357	5.4488	
In	18	2.1875	3.0931	1.7062	3.0533	
La	9	1.0521	1.0511	0.91969	1.0313	3
Mg	11	2.3524	3.2238	2.0688	2.952	
Mn	29	3.5596	8.0676	2.6734	6.1861	
Ni	22	1.3852	2.3601	1.1617	1.9453	
Tb	10	1.1925	1.0333	1.0076	0.84114	
Zn	115	3.2088	8.3349	2.4629	3.9252	
Zr	16	4.8645	1.8624	3.2318	1.2404	

3.3 Deep Neural Network linear equation for Energy Density

The Deep Neural Network (DNN) created in this study simulates the prediction of energy density (Wh kg^{-1}) by transforming synthesis parameters into a final regression output in a hierarchical way. DNNs are not linear by nature, but their predictions can be written down in a clear mathematical way using linear transformations and activation functions. After standardizing the input variables metal related descriptors, oxidation state, synthesis temperature, and reaction time the network calculates a series of weighted linear combinations and then uses nonlinear activation (ReLU). The DNN model

is indicate learned weight matrices and bias vectors, while ReLU adds piecewise linear behavior. Each layer does a linear equation of the form, which means that the whole DNN is made up of many linear equations that are connected by nonlinear activation functions. This structure lets the model capture complicated interactions between synthesis parameters that a single linear regression equation can't show. As a result, the DNN-based energy density equation keeps its mathematical meaning while making it easier to use and more accurate for predicting how well hydrogen storage will work. Thus, in this study the several linear equation to model from metalic linker MOF (see Table 2)

Table 2. Metallic linker equation for Energy density

No.	Metal Name	Energy Density Equation	Remark
1	Cd	y = (0.35157037)*temperature -(0.24731283)*time + (25.285185)	y = Total Energy Density
2	Co	y = (0.44439022)*temperature - (0.33132207)*time + (20.933012)	
3	Cu	y = (22.264553)*oxidation_state + (0.26529643)*temperature - (0.082621473)*time - (8.7303573)	
4	Dy	y = (0.25338771)*temperature - (0.1329477)*time + (32.386142)	
5	Eu	y = (0.36594749)*temperature - (0.35277072)*time + (33.768448)	
6	In	y = (14.848074)*oxidation_state + (0.26729425)*temperature - (0.30082641)*time - (10.869485)	
7	La	y = (0.45224101)*temperature - (0.43529837)*time + (20.027068)	
8	Mg	y = (0.59546128)*temperature - (0.14151469)*time - (8.1079825)	
9	Mn	y = (0.28862635)*temperature - (0.07708235)*time + (29.183192)	
10	Ni	y = (31.081619)*oxidation_state + (0.45496012)*temperature - (0.4527016)*time - (35.242196)	
11	Tb	y = (0.40730092)*temperature - (0.42252741)*time + (26.626675)	
12	Zn	y = (0.44115353)*temperature - (0.23646523)*time + (20.373198)	
13	Zr	y = (0.63140096)*temperature - (0.26093445)*time - (0.7741207)	

4. Conclusions

This research effectively established and validated a machine learning–based framework for forecasting the energy density of metal–organic framework (MOF) materials intended for hydrogen storage applications. A per-metal modeling strategy was used to find material-specific relationships between synthesis conditions and storage performance. This was done by using synthesis parameters like metal type, oxidation state, temperature, and reaction time. The Deep Neural Network (DNN) model successfully represented nonlinear interactions among variables, whereas supplementary linear regression models offered streamlined analytical equations by improving interpretability and practical engineering relevance. Using RMSE, MAE, and R^2 metrics to evaluate showed that the model was good at predicting, especially for metals like La, Tb, and Zr, which had strong generalization and stable structure-property correlations. Some metals had more testing errors because their data size was small or their intrinsic variability was high, but the overall framework was strong and flexible. The suggested soft-sensor method cuts down on the need for costly real-time hydrogen uptake measurements and offers a scalable way to quickly estimate performance. This work can be expanded in the near future by including larger and more varied datasets, more physicochemical descriptors (like surface area, pore volume, and crystallinity), and more advanced architectures, like hybrid deep learning or ensemble models, to make predictions even more accurate. Combining with systems for experimental validation and real-time monitoring could also make it easier to use in hydrogen storage facilities. Ultimately, this research helps speed up the discovery of new materials, improve the design of synthesis processes, and move forward intelligent hydrogen-based energy systems that support a sustainable energy transition.

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