Predictive Modeling of Thermal Stability in Zn-MOF Using Multilayer Perceptron

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Abstract - *Indonesia's heavy reliance on fossil fuels, which account for approximately 80% of its national energy supply, poses a significant obstacle to achieving Net Zero Emissions (NZE) by 2060. Metal-Organic Frameworks (MOF) have emerged as promising innovative materials for sustainable energy applications; however, their limited thermal stability at elevated temperatures remains a major challenge. This study aims to develop a Multilayer Perceptron (MLP -based predictive model for the thermal stability of zinc-based MOF (Zn-MOF) using four structural descriptors nZn, nN, Lig, and Het derived from a dataset of 151 Zn-MOF compounds. Three hidden-layer configurations with 3, 6, and 9 neurons were evaluated using 10-fold cross-validation and three regression metrics: Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2). The 9-neuron configuration achieved the highest predictive accuracy, with MAE = 0.0020, RMSE = 0.0022, and R^2 = 0.9991. SHAP analysis identified nN and Het as the most influential descriptors for thermal stability prediction. These results demonstrate that the MLP architecture effectively captures nonlinear structure–property relationships in Zn-MOFs, offering a computationally efficient tool to accelerate the design of thermally stable materials for sustainable energy applications.*

Keywords*: Metal-Organic Frameworks (MOF); Multilayer Perceptron (MLP); Thermal stability (TS).*

INTRODUCTION

The global energy crisis is deepening with heavy reliance on fossil fuels, which by 2023 accounted for approximately 82% of the world's total primary energy supply. In Indonesia, approximately 80% of the national energy system still relies on fossil fuels. This dependence not only drives increased carbon emissions but also hinders the accelerated transition to energy storage and sustainable systems. In response, the Indonesian government has committed to achieving Net Zero Emissions (NZE) by 2060 and increasing the renewable energy mix to 23% by 2025 (Zahira & Fadillah, 2022). To reach this objective, breakthroughs are needed in renewable energy technologies and advanced materials capable of operating effectively in extreme environments, including high temperatures.

Metal-Organic Frameworks (MOF) have emerged as innovative, highly porous materials with potential for hydrogen storage, clean energy catalysts, and carbon capture. However, MOF implementation still faces challenges due to their low thermal stability at extreme temperatures (Escobar-Hernandez et al., 2022). Thermal stability is an important factor in energy storage applications because it affects the material's ability to maintain its structure under high operational conditions, such as in hydrogen storage or clean energy catalytic reactors (Valdebenito et al., 2022). Low thermal stability reduces the efficiency of MOF in energy storage and conversion, rendering them unsuitable for industrial-scale applications.

To date, many studies still rely on conventional experimental testing methods,

such as thermogravimetry. This method to be less efficient because it requires significant resources and a significant amount of time. So that computational approaches such as machine learning (ML) are increasingly being considered to accelerate material discovery through predictive modeling (Shahzad et al., 2024; Ariyanto et al., 2024; Azies, Ariyanto, et al., 2024; Rahman et al., 2025).

Numerous studies have demonstrated the effectiveness of machine learning (ML) in accelerating the discovery of metal-organic framework (MOF)-based materials. Moharramnejad et al. (2022) developed a Quantitative Structure–Property Relationship (QSPR) model based on Multiple Linear Regression (MLR) to predict the thermal stability of zinc-based MOF using four structural descriptors (Moharramnejad et al., 2022). In addition, Azies et al. (2024) proposed a robust regression (RR) based QSPR model to improve prediction reliability, particularly in handling outlier data that were identified across all descriptors through exploratory data analysis. The RR model outperformed the traditional Multiple Linear Regression (MLR) approach and was further validated by successfully predicting the thermal stability of a novel Zn-MOF, $Zn_3(DDB)(DPE)\cdot H_2O$, confirming the model's reliability in real-world applications (Azies, Akrom, et al., 2024). This data-driven approach not only increases efficiency in materials research, but also reduces the need for time consuming and costly experimental testing.

Although machine learning has been increasingly applied to predict properties of metal-organic frameworks, several limitations remain in previous studies. Models such as the QSPR model by Moharramnejad et al. (2022) and the robust regression model by Azies et al. (2024) are based on linear approaches, which have difficulty capturing complex, nonlinear relationships between structural descriptors. In MOF systems, the interactions between atoms are often nonlinear, therefore linear-based models are not always capable of adequately representing these relationships. In addition, no previous study on Zn-MOF thermal stability has specifically examined how the number of neurons in the hidden layer affects prediction accuracy and model stability.

To address these limitations, this study uses the Multilayer Perceptron (MLP) neural network. MLP consists of an input layer, one or more hidden layers, and an output layer, where each neuron uses a nonlinear activation function. This allows MLP to learn complex patterns in data that cannot be captured by linear models. MLP also employs a backpropagation algorithm that iteratively updates model weights during training to minimize prediction error. (Saputra et al., 2025; Arifuddin et al., 2025). In this study, MLP is employed to predict the thermal stability of Zn-MOF compounds based on four structural descriptors (nZn, nN, Lig, and Het), with systematic evaluation of the effect of different neuron configurations on model performance. This model is built based on the Quantitative Structure Property Relationship (QSPR) paradigm, which utilizes structural descriptors to capture the intrinsic relationship between molecular architecture and its thermal behavior (Pratama et al., 2025).

This approach is expected to accelerate material design efficiently and encourage the development of clean and sustainable energy technologies. By using MLP neural networks, this study aims to develop a predictive model designed to analyze the thermal stability of Zn-based metal-organic frameworks (Zn-MOFs),

which demonstrates significant potential for renewable energy storage applications. In addition, this study also aims to determine the configuration of the number of neurons that provide the best performance and identify structural features that have the greatest influence on TS prediction.

RESEARCH METHODS

Research Stages

The research process involves various stages as shown in Figure 1.

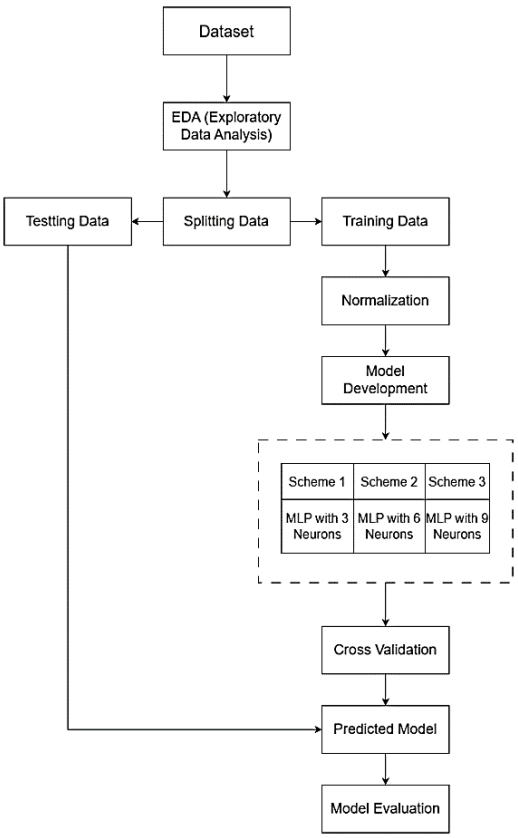

Figure 1. Research Flow

Dataset Collection

In this study, the data used was taken from the publication by Moharramnejad et al. (2022), which recorded information on 151 zinc-based metal-organic frameworks (Zn-MOFs) in the context of thermal stability (Moharramnejad et al., 2022). The thermal stability values in this study represent the temperature of the Zn-MOF material expressed in degrees Celsius (°C), which was then transformed using a logarithmic function (log TS). The dataset contains a number of structural descriptors that describe the chemical composition and atomic interactions of each compound, which are then used as the basis for constructing a ANN model to predict thermal stability values.

The predictive model was constructed based on four main descriptors selected according to their relevance to the thermal stability of MOF, namely nN, which represents the number of nitrogen atoms, and nZn, which indicates the number of zinc atoms in the MOF structure. The Het. parameter represents the contribution of interactions between hetero atoms in the linker and metal center, while Lig. describes the molecular fragments present in the linker. These four descriptors play an important role in determining the thermal stability of Zn-MOF and contribute to the accuracy of the resulting prediction model.

Exploratory Data Analysis (EDA)

Exploratory Data Analysis is a crucial step in data analysis to comprehensively understand the structure and characteristics of a dataset. Through statistical and visualization techniques, EDA helps identify patterns, relationships between variables, and non normal data distributions such as outliers, which can impact the performance of machine learning models (Akrom et al., 2025; Budi et al., 2024). Therefore, normalization is often applied to balance data distribution (Willa Dhany & Izhari, 2023). In addition, EDA is also used to evaluate the correlation between features and the target variable, remove irrelevant or redundant features, and simplify the model. Thus, EDA plays a crucial role in improving data quality and overall model performance (Diallo et al., 2025).

Splitting Data

Splitting a dataset into two parts is a standard step in developing machine learning models to prevent overfitting, which is a condition where the model only memorizes training data without being able to recognize new data (Sivakumar et al., 2024). In this study, 80% of the data was used as a training set to train the model to recognize patcoterns, while the remaining 20% was used as a test set to test the model's generalization ability to data that had never been seen before.

Data Normalization

Data normalization is carried out to standardize the scale and distribution of data to suit the needs of analysis or modeling (Nabila & Pamungkas 2025). The presence of outliers can disrupt data stability and reduce model performance (Nuraeni et al., 2024). To overcome this, Robust Scaler is used, which utilizes the median and interquartile range (IQR) to minimize the influence of outliers and maintain data stability (Garlits et al., 2023).

Multi-Layer Perceptron

In this study, the MLP Regressor algorithm is used to predict the Thermal Stability value of MOF materials. MLP (Multi-Layer Perceptron) is a type of feedforward artificial neural network (ANN) consisting of three main components (Adelia et al., 2025; Fikriah et al., 2024; Maheswari & Gunawan, 2025): an input layer, a hidden layer, and an output layer. In a feedforward architecture, data flows in one direction from the input to the output. After generating a prediction, the backpropagation algorithm is used to calculate the error and determine how the weights need to be adjusted to make the next output more accurate. The input layer is responsible for receiving input data which is then forwarded to the hidden layer for processing, and the results are sent to the output layer to produce the final prediction (Saputra et al., 2025; Arifuddin et al., 2025). This architecture allows MLP to capture complex nonlinear patterns in data. However, increasing the number of neurons in the hidden layer makes the model more complex and requires longer processing time. Mathematically, the structure of an MLP is described in Equations 1 and 2.

$$Z_j = f\left(\sum_{i=1}^{n} w_{ij}X_i + b_j\right) \quad (1)$$

And the output is calculated as:

$$Y_k = f\left(\sum_{j=1}^{n} v_{jk}\,Z_j + b_k\right) \quad (2)$$

In an artificial neural network, each input entering the network is denoted by X_i and then multiplied by the connection weights w_{ij} between the input layer and the hidden layer. This multiplication result is added to the bias b_j in the hidden layer and passed to the activation function $f(x)$ to produce the output in the hidden layer called Z_j. Next, the output from the hidden layer is passed to the output layer through the connection weights v_{jk}, which connect the hidden layer with the output layer. A bias b_k is also added to the output layer before being processed again through the activation function to produce the final output of the network, namely Y_k.

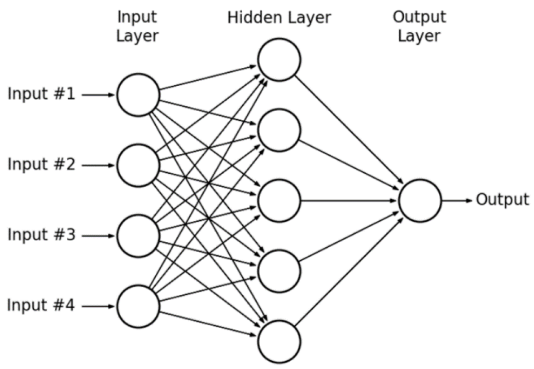

Figure 2. MLP architecture

The activation function used in this network can be sigmoid, ReLU, tanh, or other types that function to provide non linear properties to the model (Arifuddin et al., 2025). The MLP architecture can be seen in Figure 2. This model was built using the Python scikit-learn library.

The number of neurons in the hidden layer was determined through a systematic trial and error process. Three configurations were tested, namely 3, 6, and 9 neurons, to observe how increasing model complexity affects prediction accuracy and generalization ability. The value of 3 neurons represents the simplest configuration, 6-neurons represent a moderate configuration, and 9-neurons represents a more complex configuration. Each layer uses a ReLU (Rectified Linear Unit) activation function to introduce non-linearity into the model. The output layer has only one neuron because this model is used for regression. The training process was performed using the lbfgs optimization algorithm, which is known to be efficient for small to medium sized datasets. Furthermore, the random_state = 42 parameter was used to ensure consistent model training results.

Model Evaluation

After the Multi-Layer Perceptron Regressor model was built and trained, the next step was to evaluate its performance in predicting TS values. The evaluation was conducted using three main regression metrics: Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2). These three metrics were used to assess the model's accuracy on the test data. Mean Absolute Error (MAE) measures the average absolute error between the predicted TS value and the actual TS value. This metric does not consider the direction of the error, only its magnitude. The smaller the MAE, the better the model's performance (Chicco et al., 2021;Prayuda & Pratama, 2024). The MAE formula is shown in Equation 3.

$$\text{MAE} = \frac{\sum_{i=1}^{n} |y_i - \hat{y}_i|}{n} \qquad (3)$$

Root Mean Squared Error (RMSE) is more sensitive to large errors because it imposes a larger penalty on predictions that are far from the true value (Hodson, 2022). The RMSE formula is shown in Equation 4:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n}} \qquad (4)$$

The coefficient of determination (R^2) indicates how much of the variation in TS values can be explained by the MLP model (Sukmananda et al., 2026). A value close to 1 indicates that the model is able to explain most of the variation in the data The R^2 formula can be shown in Equation 5.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \qquad (5)$$

In Equation (5), n denotes the total number of observations in the test dataset. The term y_i represents the actual Thermal Stability value of the i-th observation, while $\hat{y}_i$ refers to the corresponding value predicted by the Multilayer Perceptron model. The symbol $\bar{y}$ indicates the mean of all observed Thermal Stability values. The summation operator expresses the accumulation of squared differences across all observations, where the numerator reflects the residual variation between predicted and actual values, and the denominator represents the total variation of the observed data around their mean.

RESULTS AND DISCUSSION

Exploratory Analysis of Feature Distributions and Outliers

Before starting the modeling process, a crucial initial step is a thorough data exploration through statistical analysis and visualization. At this stage, boxplots are used to examine the data distribution and detect the presence of extreme values (outliers) in each feature. Based on the visualization in Figure 3, all features, including nN, nZn, Het, Lig, and TS, show the presence of outliers, although the number and level of distribution vary. The nN and Het features have the most outliers, with extreme points spread quite far from the interquartile range, reflecting high value variation in both descriptors. The nZn feature has the fewest outliers, as seen from its narrow distribution and only a few extreme values appearing. The Lig feature also contains outliers, but their number and distance from the center of distribution are not as many as in nN and Het.

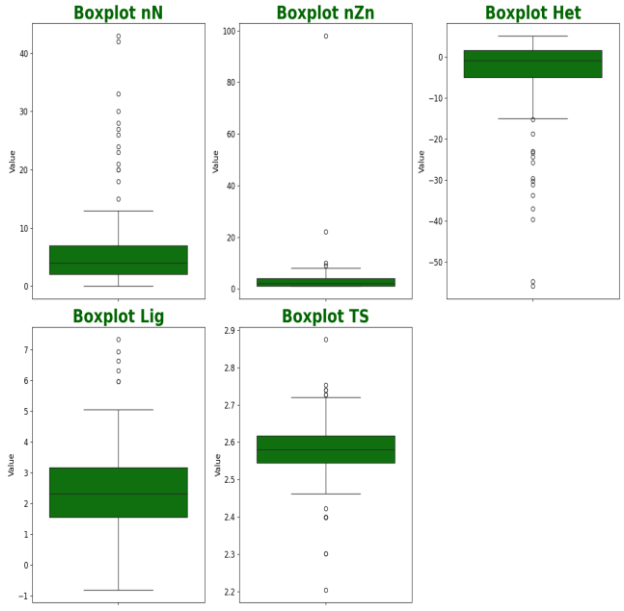

Figure 3. Outlier Visualization with Boxplot

The existence of these outliers can affect model training, so the Robust Scaler normalization method is used to reduce the impact of extreme values without deleting data, preserving information from outliers but minimizing their influence on the model. In addition to boxplots, correlations between features were also visualized using heatmaps to understand the relationship between input and target variables. This is a crucial step in determining the appropriate model for the data used.

Correlation analysis using a heatmap in Figure 4 shows a linear relationship between features and between features and the Thermal Stability target. The results show a very strong and negative correlation between the nN and Het features with a correlation value close to -1, indicating that increasing the value of one feature will significantly decrease the value of the other feature linearly. However, the correlation between the other features and the TS target is very low, ranging from close to zero, indicating a weak or even no significant linear relationship between the features and the target.

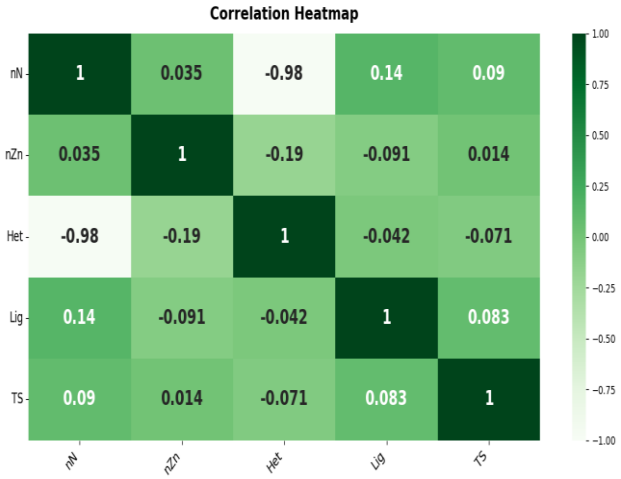

Figure 4. Correlation Visualization

This condition indicates that predictive models that assume a linear relationship, such as simple linear regression, are likely to be unable to provide good results. Therefore, a nonlinear model such as the MLP was chosen to capture complex and nonlinear patterns in the data. This analysis is important to ensure that the model used is appropriate to the characteristics of the data.

Model Performance Evaluation

This section discusses the development of a regression model to predict thermal stability values by evaluating three MLP model architectures with 9 neurons, 6 neurons, and 3 neurons to determine the most suitable model and provide optimal predictive performance. Based on Table 1, which displays the results of model evaluation using the 10-fold cross-validation technique, all three MLP configurations demonstrated excellent predictive performance across most folds. The 3 neuron model produced generally high R^2 values close to 1, but negative R^2 values were observed in the 7th, 8th, and 10th folds.

Table 1. Results of MLP Model Performance Evaluation with Cross Validation

Fold	R^2		
	3 Neurons	**6 Neurons**	**9 Neurons**
1	0.9997	0.9952	0.9996
2	0.9990	0.9991	0.9991
3	0.9990	0.9822	0.9985
4	0.9985	0.9785	0.9983
5	0.9993	0.9992	0.9992
6	0.9982	0.9981	0.9923
7	-0.2294	0.9981	0.9982
8	-0.4247	0.9992	0.9989
9	0.9994	0.9994	0.9987
10	-0.0014	0.9996	0.9995

This indicates that the model failed to generalize well in these folds, although overall performance remained strong. The 6-neuron model demonstrated more stable results with an R^2 range between 0.9785 and 0.9996, indicating improved consistency compared to the previous configuration. Meanwhile, the 9-neuron model performed best, with high and stable R^2 values across almost all folds, with no negative values. The 9-neuron configuration in the hidden layer provided the most stable and accurate results in predicting thermal stability values.

While cross-validation results indicate differences in predictive performance and stability across neuron configurations, a descriptive evaluation alone is insufficient to determine whether these differences are statistically meaningful. Therefore, a nonparametric statistical test was employed. To compare model performance, the Wilcoxon signed-rank test was conducted using paired R^2 values obtained from 10-fold cross-validation (CHEN, 2025). Each fold was treated as a repeated evaluation unit, allowing direct comparison of model performance under consistent data partitions. This approach is more appropriate than parametric methods because it does not assume normality and is robust to small sample sizes and outliers. The results of the pairwise comparisons are presented in Table 2.

Table 2. Wilcoxon Signed-Rank Test Results for Model Performance

Comparison	p-value
3 vs 6 Neurons	0.0195*
3 vs 9 Neurons	0.0137*
6 vs 9 Neurons	0.3125

Note: *) Statistical significance was evaluated at $\alpha = 0.05$.

The results indicate that the 3-neuron model tends to perform worse than both the 6 neuron and 9 neuron models. However, after applying Bonferroni correction for multiple comparisons ($\alpha = 0.0167$), only the difference between the 3 neuron and 9 neuron models remains statistically significant. No statistically significant difference is observed between the 6 neuron and 9 neuron configurations. These findings suggest that increasing the number of neurons from 3 to 6 improves model performance, but further increasing to 9 neurons does not yield a statistically significant improvement. Nevertheless, the 9-neuron model demonstrates more stable performance across folds, as indicated by the absence of negative R^2 values. In contrast, the 3 neuron model exhibits instability, with several folds producing negative R^2 values, indicating poor generalization in specific

cases. In addition, descriptive statistics were calculated further to examine the distribution of model performance across folds. The results show that the 3-neuron model achieves a mean R^2 of 0.634 ± 0.60, indicating substantial variability. In contrast, the 6 neuron and 9 neuron models achieve mean R^2 values of 0.995 ± 0.007 and 0.998 ± 0.002, respectively, demonstrating consistently high and stable performance. The variability of the 3-neuron model is also reflected in its wider performance dispersion across folds.

Table 3. MLP Model Performance Evaluation Results

Neuron	MAE	RMSE	R^2
3	0.0029	0.0055	0.9947
6	0.0020	0.0023	0.9991
9	0.0020	0.0022	0.9991

In Table 3 presents the performance evaluation results of the MLP model in predicting the Thermal Stability of Metal-Organic Framework based on variations in the number of Neurons. Based on the results in the table, an increase in the number of Neurons shows a trend of improving model performance. In an architecture with 3 Neurons, the model produces an MAE value of 0.0029, RMSE of 0.0055, and R^2 of 0.9947. When the number of Neurons is increased to 6, the MAE and RMSE values decrease to 0.0020 and 0.0023, while the R^2 value increases to 0.9991. Meanwhile, configuration with 9 Neurons providesThe best results with MAE of 0.0020, RMSE of 0.0022, and R^2 of 0.9991. The R^2 values obtained in this study are very high, reaching 0.9991 for the 9-neuron configuration. While this indicates excellent predictive performance, such high values may raise concerns abo9-neurontial overfitting, where the model memorizes the training data rather than learning generalizable patterns. However, several pieces of evidence suggest that overfitting is unlikely in this case. First, the model was evaluated using 10-fold cross-validation, which tests the model on data it has never seen during training. The consistently high R^2 values across almost all folds for the 6 neuron and 9 neuron configurations indicate that the model generalizes well to new data. Second, the dataset used is relatively small (151 samples), and the model architecture is kept simple (one hidden layer), which reduces the risk of overfitting compared to deeper networks. Thus, it can be concluded that increasing the number of Neurons contributes to increasing the accuracy of the MLP model in predicting the thermal stability of MOF, with optimal performance obtained at 9 Neurons.

Table 4. Performance Comparison Between Proposed MLP Model and Benchmark Model

Model	MAE	RMSE	R^2
MLP (Proposed)	0.0020	0.0022	0.9991
RR (Azies et al., 2024)	0.0010	0.0010	0.9989

Table 4 compares the proposed MLP model developed in this study with the Robust Regression (RR) model reported by Azies et al. (2024), both based on the same dataset of 151 Zn-MOF compounds. The RR model results are adopted from the original study and used as a benchmark for comparison. The results indicate that both models achieve comparable predictive performance. The RR model records slightly lower MAE (0.0010) and RMSE (0.0010). In contrast, the proposed MLP model achieves a marginally higher R^2 of 0.9991 compared to 0.9989 for the RR model. These findings suggest that the MLP model achieves competitive performance while capturing nonlinear relationships in the data.

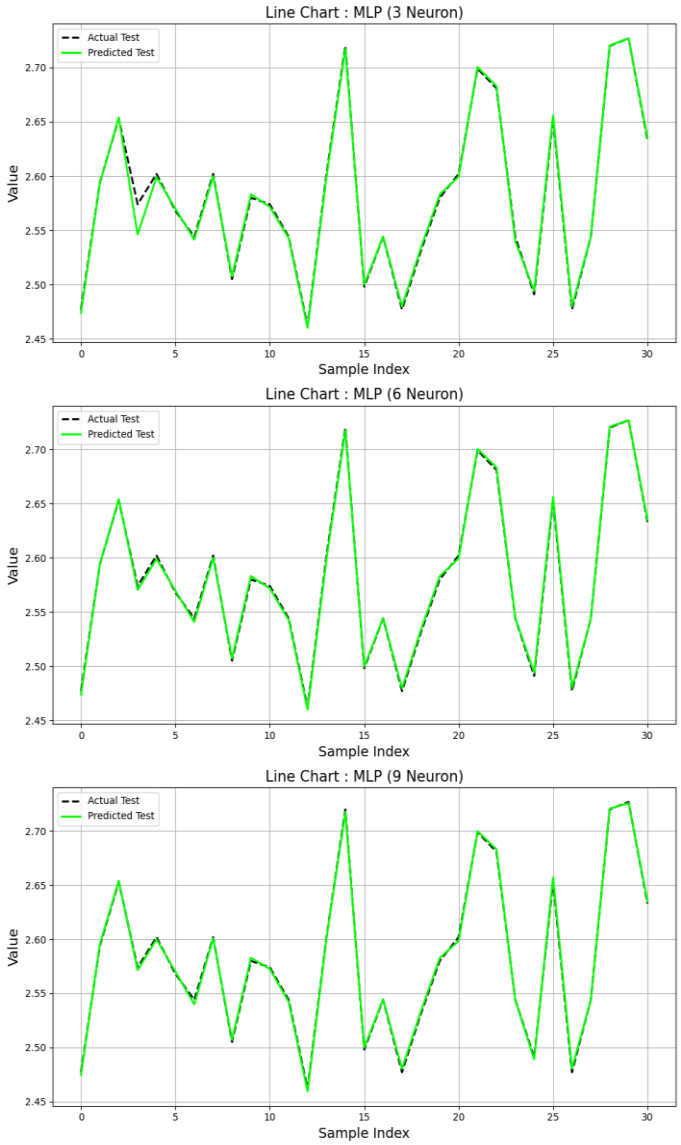

Figure 5. Comparison of actual and predicted values of MLP models with 3, 6, and 9 Neurons

Figure 5 shows a comparison between the actual and predicted Thermal Stability values on the test data for each MLP model configuration with 3, 6, and 9 neurons. Visually, all models are able to follow the fluctuation pattern of the actual data well, indicated by the green (predicted) line that almost entirely overlaps with the black (actual) line. In the model with 3 neurons, the prediction is quite accurate, although there are several points that do not completely follow the actual value. In the 6 neuron configuration, the predicted line appears to align more closely with the actual value, indicating an increase in accuracy and the model's ability to capture data patterns. Meanwhile, the model with 9 neurons shows the best performance, with the predicted line almost entirely following the actual line without deviation. This consistency strengthens the finding that the 9 neuron configuration provides the most stable and accurate prediction performance.

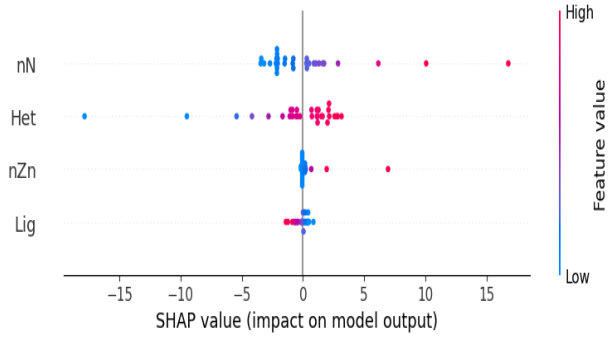

Figure 6. SHAP summary plot of feature contributions to TS prediction.

Based on Figure 6, the nN and Het features have the greatest influence on TS predictions, as indicated by the wider distribution of SHAP values compared to other features. High nN values tend to increase TS predictions, while high Het values also contribute positively to predictions. On the other hand, the nZn and Lig features show a smaller influence, as seen from the SHAP value distribution centered near zero, so their contribution to the model prediction is relatively low.

This study contributes to the field of materials informatics by demonstrating that a neural network based approach can be used to predict the thermal stability of Zn-MOF compounds accurately using only four simple structural descriptors. In materials informatics, one of the main goals is to reduce the time and cost needed to discover new materials by replacing or complementing experimental testing with computational prediction. The MLP model developed in this study can serve as a fast screening tool, allowing researchers to estimate the thermal stability of a candidate

Zn-MOF compound before it is synthesized in the laboratory. This is useful because experimental methods such as thermogravimetric analysis (TGA) require physical samples, equipment, and significant time, while a trained MLP model can produce predictions almost instantly.

From the perspective of energy materials research, thermal stability is one of the most important properties for MOF intended for applications such as hydrogen storage, carbon capture, and catalysis at high temperatures. A MOF that breaks down at low temperatures cannot function reliably in these applications. By providing an accurate and efficient method to predict thermal stability, this study supports the broader effort to accelerate the development of MOF materials suitable for energy applications. This is especially relevant for Indonesia, which is targeting Net Zero Emissions by 2060 and needs reliable advanced materials to support the transition to renewable energy.

CONCLUSION

This study successfully developed a MLP-based predictive model to predict the Thermal Stability value of Zn-MOF materials by utilizing four main structural descriptors, namely nZn, nN, Lig, and Het. The model with 9 neurons produced the most optimal performance with an MAE of 0.0020, RMSE of 0.0022, and R^2 of 0.9991. SHAP analysis also showed that the nN and Het features had the greatest contribution to the prediction of TS values. These findings confirm that MLP is able to provide very high prediction accuracy and can be utilized to accelerate the design process of thermally stable Zn-MOF materials, thus potentially supporting the development of sustainable clean energy technologies. However, this study has limitations, including a small dataset of only 151 compounds and the use of only four descriptors, which may limit the model's generalizability to other MOF types. Future research is therefore encouraged to expand the dataset and add more structural descriptors to further improve prediction accuracy.

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