

Article

Black-Box and Interpretable Artificial Intelligence Models for Hydrogen Uptake Across Various Metal–Organic Frameworks

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Abstract

Hydrogen (H_2) is expected to play a critical role in modern industry, particularly in ammonia synthesis, petroleum refining, and low-carbon transportation. The safe storage of H_2 remains a major challenge due to its low volumetric density under ambient conditions. Metal–Organic Frameworks (MOFs), highly porous crystalline materials, have emerged as promising H_2 storage candidates owing to their high surface areas and tuneable pore structures. Molecular simulations such as grand canonical Monte Carlo or density functional theory are costly and limited in exploring large material spaces, motivating efficient predictive tools to accelerate discovery. Here, Machine Learning (ML) techniques are compared to an explainable artificial intelligence (XAI) approach using symbolic regression (SR), trained on 10,123 experimentally measured H_2 adsorption datapoints from real-world MOFs. The best performing model achieved a goodness of fit of 0.9986 with lower computational demand, but reduced interpretability, addressed using XAI analysis and clustering. SR achieves a lower goodness of fit of 0.914 but produces a physically meaningful equation highlighting structural features driving high gravimetric efficiencies. These results demonstrate strong ML capability for predicting how MOF properties and environmental conditions affect H_2 uptake. This offers engineers and researchers a practical means of screening potential MOFs for H_2 storage applications, with the XAI analyses providing additional confidence in the predictions. They allow researchers to understand the physical reasoning behind each output, assess the reliability of individual predictions, and make fully informed decisions, enabling predictive models to be acted upon with confidence in real-world contexts.

Keywords: AI; data-driven modelling; Gaussian process regression; high-throughput screening; ML; MOF; neural architecture search; structure property relationship; XAI

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1. Introduction

Global warming continues to be an ever-important challenge. With the United Nations Environment Programme reporting that greenhouse gas emissions had reached a record high level of 57.1 GtCO₂e in 2023 [1], it is crucial that the world shifts towards more sustainable fuel sources. Hydrogen (H_2) is a promising alternative [2], offering an increased gravimetric efficiency of 120 MJ/kg compared to gasoline at 44 MJ/kg [3]. However, the safe and efficient storage of H_2 remains a major technical challenge, primarily due to its low volumetric density under ambient conditions (liquid H_2 : 8 MJ/L, gasoline: 32 MJ/L) [3]. Maintaining the cryogenic temperatures required for liquid H_2 poses

significant logistical challenges, including the need for active cooling or venting due to heat leakage, currently prohibited in locations such as airports [4]. Storing gaseous H_2 allows for higher temperatures but requires far higher pressures, posing design and safety challenges [5]. These limitations have driven extensive research into alternative H_2 storage strategies, including dissolution in underground aquifers [6] and Liquid Organic Hydrogen Carriers (LOHCs), where H_2 is stored through hydrogenation and released through dehydrogenation. While LOHCs can achieve high volumetric efficiencies, they are often impractical for large-scale applications due to the slowness of these chemical processes [7]. Liquid hydrogen has already demonstrated to be a crucial technology for H_2 storage on board aircrafts [8,9].

Metal–Organic Frameworks (MOFs) have emerged as promising candidates for H_2 storage due to their exceptionally high surface areas and tuneable pore structures [10]. MOFs are a family of highly porous, crystalline materials consisting of a central metal ion connected by organic linkers, as shown in Figure 1a. The overall structure of the material is determined not only by the type of metal and linker used, but also by how they are connected together, and these materials are able to store gaseous H_2 with a higher volumetric efficiency for a given pressure when compared to compressed gas [11]. MOFs achieve these high volumetric efficiencies because they contain internal pores which act to increase the amount of surface area that gas molecules have to adsorb onto, as shown at different levels of magnification in Figure 1b. Factors intrinsic to the MOF such as surface area and pore volume will affect the quantity of gas stored, as will extrinsic factors such as pressure and temperature. H_2 is held at the surface via weak van der Waals forces [12], so a higher surface area creates more space for H_2 molecules. This process is called physisorption and can result in multiple layers of molecules sticking to the surface of the pores depending on the temperature [10]. Higher temperatures reduce the amount of H_2 held at the surface as the weak van der Waals forces are easily overcome by the additional thermal energy, whereas higher pressures help drive molecules onto the surface and increase the density of H_2 within the pores. A higher pore volume similarly increases the empty space available for the H_2 to occupy.

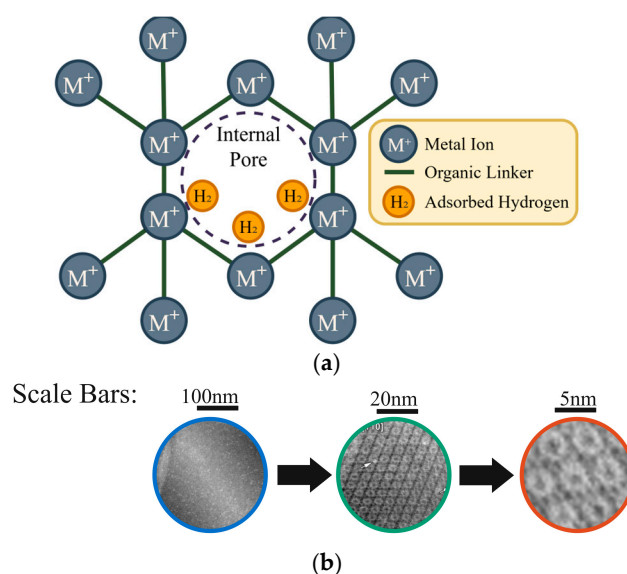


Figure 1. (a) A Structural diagram of an MOF and (b) MOFs at different levels of magnification at 100 nm [13], 20 nm [13], and 5 nm [14].

A key challenge faced by engineers when designing new MOFs is predicting their theoretical storage capacities. Measuring the uptake of H_2 requires an extensive experimental procedure, and due to the vast chemical space that MOFs exist within, it becomes

difficult to screen large quantities of potential structures quickly. Grand Canonical Monte Carlo (GCMC) simulations can provide theoretical estimates but are very computationally expensive, limiting their utility for large-scale materials discovery [15]. Data-driven approaches have therefore attracted significant interest as a faster, assumption-free alternative for generating predictions for complex phenomena [16–20], such as H₂ uptake in MOFs. These models are able to capture the complex, nonlinear behaviour of H₂ adsorption from large datasets and provide predictions far faster than conventional simulations. Additionally when trained on real-world data, they do not make the simplifying assumptions inherent to computational approaches such as GCMC. However, the widespread adoption of such black-box machine learning (ML) models is critically constrained by a fundamental limitation: they lack transparency and fail to provide any physical understanding of the mechanisms governing their predictions. For an engineer designing an H₂ storage system, this opacity makes it impossible to assess whether a given model output is physically reasonable, undermining confidence in the predictions and limiting real-world deployment.

Prior works have demonstrated the potential of AI for H₂ uptake prediction in MOFs, but several important gaps remain. Reference [21] introduced the group method of data handling to capture complex feature interactions, though their dataset contained only 35 datapoints, limiting generalisability. Reference [22] exhaustively trained 660 models across six architectures to identify an optimal topology, achieving a best R-squared of 0.9946. References [23] and [24] both incorporated more input features, six and ten respectively, with [24] notably expanding the dataset to 14,544 points by combining experimental and simulated data. Reference [23] employed a relevancy factor; however, this approach captures only linear input–output relationships and ignores the feature interactions critical to MOF behaviour. Most relevant to our paper is [25], which used the largest real-MOF database, to date, in the prior literature (2048 datapoints) and combined standard ML models with nature-inspired optimisation algorithms to improve accuracy whilst reducing computational cost.

A common limitation across these previously published papers is the use of databases that are very small and therefore not fully representative of the problem space. Black-box models require sufficient data to capture the complex behaviour of H₂ storage and generalise to new datapoints; in other words, they offer significant accuracy for interpolation but often struggle with extrapolation. Critically, none of these works fully resolve the explainability challenge: relevancy factors and post-hoc analyses do not on their own provide a transparent understanding of how input features relate to H₂ storage, as they do not reveal the model’s internal representation of the underlying physics. There are also no prior works that include databases of real-world MOFs comparable in size to the 14,544-point dataset of [24].

To address these gaps, this paper presents a comparative study on different explainable artificial intelligence (XAI) approaches to provide more human-understandable information from the AI-based techniques. To do so, this study uniquely uses data extracted from hydrogen isotherm graphs from the literature to achieve the largest database of real-world MOFs currently available in the literature. This method yields a more uniform distribution of values for pressure and gravimetric efficiency leading to better model performance in real world conditions. This database of real-world MOFs is then used to tackle two fronts: (i) benchmarking of six black-box ML models and using explainability techniques—such as Shapley Additive Explanations (SHAP) analysis and clustering—to extract the hidden pattern being identified by them; (ii) inherently explainable approaches based on Symbolic Regression (SR) that provide mathematical formulations for the prediction. Clustering specifically is a method that previously has been underutilised in other works using XAI for hydrogen storage in MOFs, but which can provide key insights that

could be missed if using SHAP alone. The key contributions of this work can be summarised below:

- Improvement of the generalisability of the findings of the study to various MOFs by collection of a large database of real-world MOFs, containing 10,123 datapoints under various temperature conditions (being five times larger in terms of the size of the database compared to the largest found reference in the literature with 2048 datapoints [25]).
- Using genetic algorithm-based symbolic AI approaches to find an interpretable closed-form equation for the estimation of gravimetric efficiency of various MOFs with high accuracy yet benefiting from easy-to-transfer equations.
- Benchmarking different families of black-box ML architectures over the large database to achieve high prediction accuracies.
- Introducing clustering-based explainability along with SHAP analysis to improve the explainability of Artificial Neural Network (ANN) predictions.

The remainder of this paper is structured as follows: Section 2.1 describes the data collection and curation process, including the selection of input features and the construction of the database. Section 2.2 details the methodology for each of the black-box models trained in this work. Section 2.3 covers the improvements to explainability through SHAP, clustering, and SR. Section 3 presents and discusses the results from each model, including a comparison against the existing literature. Finally, Section 4 draws conclusions from the findings and outlines directions for future work.

2. Methodology

2.1. Data Collection and Curation

The first step for data collection is to determine the important factors that affect H₂ uptake within MOFs. It is necessary to provide enough information for the model to be able to make accurate predictions, but too many input features could add unnecessary noise and reduce the number of MOFs for which complete data is available in the literature [26]. Based on the theory of how MOFs practically store H₂, the important input features were chosen to be Brunauer–Emmett–Teller (BET) surface area, pore volume, temperature, and pressure with gravimetric efficiency as the only output. These input features were chosen as follows: (i) surface area directly affects the amount of H₂ that can adsorb onto the surface; (ii) pore volume shows how much of the material is empty space for the H₂ to be stored within; (iii) temperature as heat is the main source of energy acting to overcome the Van der Waals attracting H₂ molecules to the surface of the pores; and (iv) pressure acts to force H₂ onto the surface [10]. Langmuir surface area has also been used in other works included in [23]; however, as it is just an alternate method for calculating surface area compared to BET, it provides little new information for a black-box ML model. Both values are very commonly measured in the literature measuring the uptake of H₂ in MOFs as they are calculated using the adsorption of nitrogen, as can be seen in Equations (1) and (2). Langmuir assumes only a single layer of molecules is adsorbed onto the surface [27], which is not true of H₂ adsorption [10].

$$\frac{P_R}{v_N(1 - P_R)} = \frac{1}{v_m c} + \frac{(c - 1)P_R}{v_m c} \quad (1)$$

$$A = v_m \sigma_0 N_{av} \quad (2)$$

where $P_R = P/P_0$ (pressure over atmospheric pressure), v_N is the volume of nitrogen adsorbed per gram of MOF, v_m is the monolayer capacity, and c is related to the isosteric

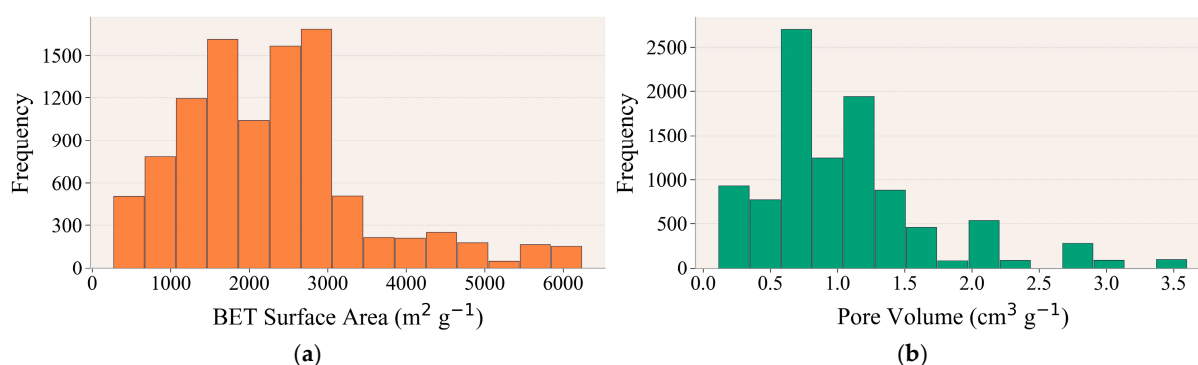
heat of adsorption. In Equation (2), σ_0 is the cross-sectional area of nitrogen at liquid density (16.2 Å), N_{av} is Avogadro's number, and A is the BET surface area [28]. By carefully considering and limiting which input features to include, this increased the number of sources which contained all the necessary information, eliminating any gaps within the database.

An extensive data collection was done from 57 different references in the literature [29–85] measuring the H₂ adsorption in MOFs for a given temperature as the pressure is increased. These references were found by combining the databases from references which also used ML to predict H₂ storage in MOFs [23,86] with other references that were found to contain sufficient information [78–85]. Typically, the H₂ adsorption is provided as a graph with a small number of important values mentioned specifically within the reference, such as the maximum adsorption achieved. In this work, the data from the graphs are extracted to achieve a far larger database. This also allows for a more continuous range of pressure values as the maximum adsorption occurs at very standard pressures such as 1 or 120 bar [81]. This also achieves a better distribution of temperature values as there were often isotherms for additional temperatures within the graphs, so a database of 10,000 datapoints could be made from 215 different temperature conditions. This still limits how many unique MOFs are included to 120, which affected the number of datapoints for surface area and pore volume.

In order to verify that the data had been extracted without error, the points were plotted back onto their respective graphs to prove they created the same plot as the original. Metadata containing information such as the name of the MOF and the reference it was taken from were also included within the database to ensure there were no duplicate samples.

From Figure 2 it can be seen that the distributions for BET surface area and pore volume are sufficiently even, with temperature and pressure both having a right skew. In order to even out this distribution the logarithm of pressure was taken, as this scales the data based off its order of magnitude. Values at 77 K are most abundant because hydrogen uptake is conventionally measured at the boiling point of liquid nitrogen and pressures up to 1 atm [87]. A correlation matrix was also plotted using both Pearson and Spearman values which is shown in Figure 3, which shows that temperature and pressure are highly independent as they are environmental conditions, but intrinsic features such as surface area and pore volume are closely linked.

The database was then divided into an 80/20% split for training and validation respectively. If a model is overfit, its predictive performance on new data will be drastically worse than its performance during training. To account for this, the accuracy of every model was measured against both sets and training was stopped before their performance diverged.



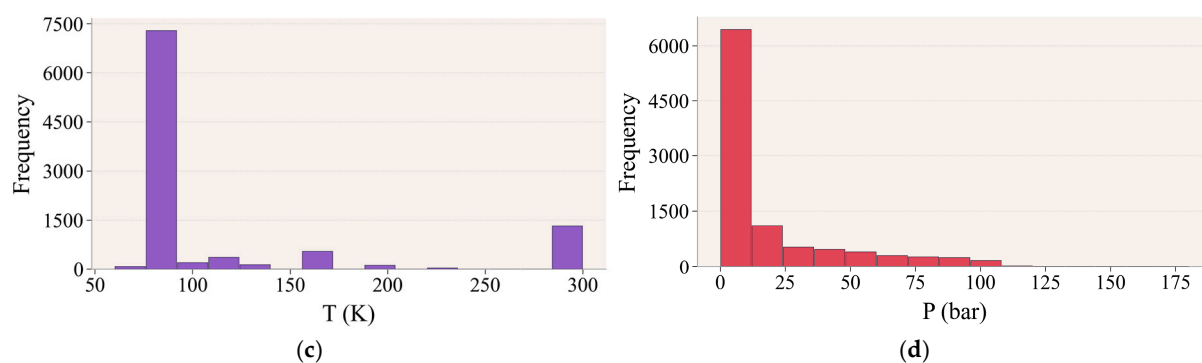


Figure 2. The distributions of (a) BET surface area, (b) pore volume, (c) temperature, and (d) pressure.

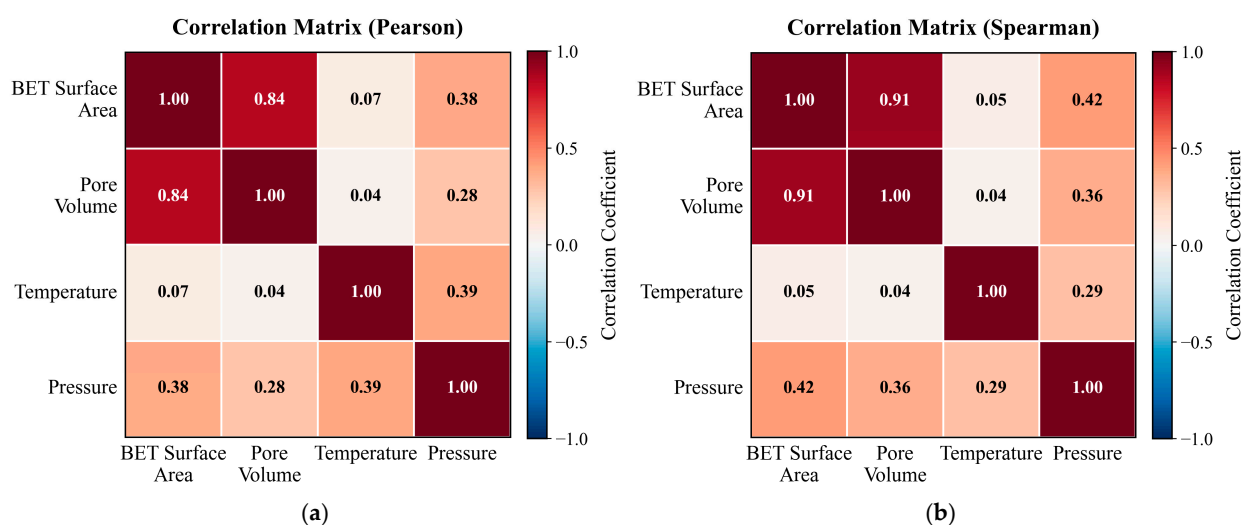


Figure 3. Pairwise relationships between BET surface area, pore volume, temperature, and pressure for this dataset, evaluated using (a) Pearson and (b) Spearman matrices.

2.2. Black-Box Models Architecture

2.2.1. Multi-Layer Perceptron

An MLP is a type of feed-forward neural network that consists of an interconnected network of nodes, shown in Figure 4 [88]. Each node is provided with a series of values from weighted connections. The node sums these values together along with its own bias term to create an output value it can pass on to other nodes down the chain.

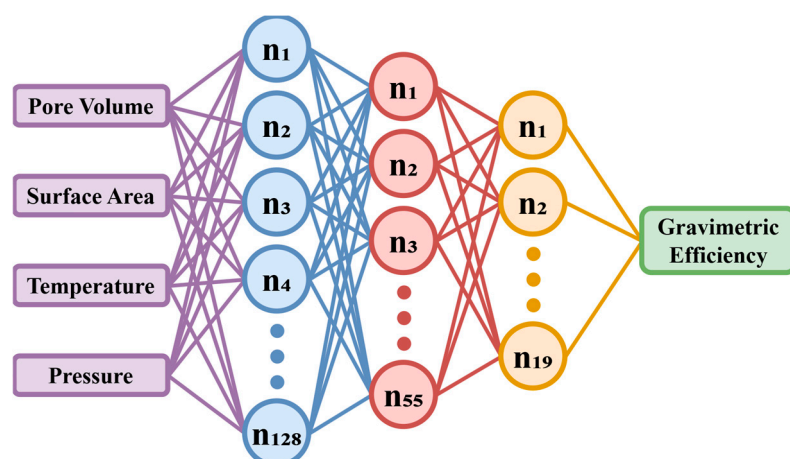


Figure 4. Diagram of the MLP model used in this work.

On its own this would not be able to capture non-linear behaviour in a dataset, so an activation function is applied to the summed value to allow for a degree of nonlinearity. Without this, the network would be unable to model more complex relationships in the data. This is applied using Equation (3) [88]:

$$o_i = \sigma \left(\sum_{j=1}^m w_{ij} x_i + b_i \right) \quad (3)$$

where x_i is an input, w_{ij} is the weight associated with each connection to a neuron with m connections, b_i is the bias term associated with that neuron, σ is the activation function, and o_i is the output. During training, the weights and biases are optimised to produce a network that is able to closely map the inputs to the outputs. A challenge when implementing an MLP is determining the architecture of the model, that is, how many nodes and layers to use. The performance of a model is heavily dependent on the architecture, but the search space of possible networks is so large that an exhaustive evaluation is impossible [89]. It is possible to suggest reasonable values for the number of nodes or layers based on the specific problem; for example, if the number of total nodes is too large for the size of the dataset, then most bias values/weightings will not be fully optimised by the time the training has concluded. In contrast, larger networks are required for more complex behaviour [90].

There are typically two methods used to find the optimal model architecture. The first used by other works is trial and error [21,22], suggesting a small number of potential structures based on the size of the dataset and complexity of the problem and then comparing their relative performances. This is quick and can lead to models which perform well; however, with so few models trialled it is very unlikely that the most optimal architecture will be found. Another method used by other works is grid search [23,86,91], which systematically tests every possible combination of hyperparameters within a pre-defined search space. This can produce better performing models than trial and error but requires the search space be sufficiently small otherwise the compute time becomes unfeasibly large [92].

In this paper, an NAS is used, which randomly tests models within the search space whilst dynamically assigning weightings to regions that have led to well-performing models previously in the search to hone in on the optimal architecture. This probabilistic approach reduces the likelihood that poorer performing models are generated whilst still allowing those regions to be periodically trialled [93]. This allows for a much larger search space than grid search whilst still minimising the compute time.

2.2.2. Generalised Regression Neural Network

A Generalised Regression Neural Network (GRNN) works by storing all training examples in memory and estimates the solution for new inputs by taking a weighted average of all stored outputs (Equation (4)). These weightings for each training example are determined by their proximity to the new inputs (Equation (5)), and a smoothing parameter sigma controls how strongly distance affects the weightings. GRNNs train very quickly but suffer from large computational requirements for very large datasets due to the need to store and take an average of every training example for each prediction [94].

$$\hat{Y}(\mathbf{x}) = \frac{\sum_{i=1}^n Y^i \exp\left(-\frac{D_i^2}{2\gamma^2}\right)}{\sum_{i=1}^n \exp\left(-\frac{D_i^2}{2\gamma^2}\right)} \quad (4)$$

$$D_i^2 = (\mathbf{X} - \mathbf{X}^i)^T (\mathbf{X} - \mathbf{X}^i) \quad (5)$$

where $\hat{Y}$ is the estimated output using the weighted mean and Y^i is a particular output from the database. D_i is the distance between the set of new inputs $\mathbf{X}$ and a particular datapoint $\mathbf{X}^i$ stored in memory.

2.2.3. Gaussian Process Regression

Gaussian Process Regression (GPR) defines a prior probability distribution that represents an infinite number of functions where the structure of this distribution is described by a mean function and a covariance function. The covariance function represents the smoothness, scale, and correlation of function values at different inputs and determines which functions are most plausible prior to training. This includes a noise term which ensures that the functions do not need to go through every data point. This accounts for the inherent inaccuracy in the measurement of any input or output [95].

During training, the gaussian process adjusts which functions are deemed plausible according to the data and when this function is provided with a new input it produces a gaussian distribution of potential solutions. The mean of this distribution corresponds to the most likely solution and is calculated using Equation (6), and the variance represents the model's uncertainty at that point using Equation (7) [96].

$$\hat{y}(\mathbf{x}) = \mathbf{k}^T(\mathbf{x})\mathbf{K}^{-1}\mathbf{t} \quad (6)$$

$$\sigma_y^2(\mathbf{x}) = \mathbf{C}(\mathbf{x}, \mathbf{x}) - \mathbf{k}^T(\mathbf{x})\mathbf{K}^{-1}\mathbf{k}(\mathbf{x}) \quad (7)$$

where $\mathbf{k}(\mathbf{x})$ is the vector of covariances between the test input $\mathbf{x}$ and each training input $\mathbf{x}^i$, $\mathbf{K}$ is the covariance matrix defined by $K_{ij} = \mathbf{C}(\mathbf{x}^i, \mathbf{x}^j)$, and $\mathbf{t}$ is the vector of observed training targets. $\mathbf{C}(\mathbf{x}, \mathbf{x})$ is the covariance of the Gaussian process evaluated at the test input $\mathbf{x}$, representing the prior variance at that point and σ_y^2 represents the predictive standard deviation.

2.2.4. XGBoost

eXtreme Gradient Boosting (XGBoost) is a tree ensemble method where predictions are calculated as the sum of many regression trees. A regression tree differs from a simple decision tree by producing a continuous score on each leaf. The model minimises a loss function $\mathcal{L}(\tau)$ defined by Equation (8) where the optimal leaf weights are computed using the first and second derivatives of the loss. These measure the prediction error and its curvature. Trees are added sequentially to correct residual errors of previous trees, and a number of methods are used to reduce overfitting such as regularisation of leaf weights and shrinkage. Shrinkage reduces the size of newly added weights to reduce their impact and allow for new trees to improve the model and column subsampling [97].

$$\mathcal{L}(\tau) = \sum_i l(\hat{y}_i, y_i) + \sum_k \Omega(\mathbf{f}_k) \quad (8)$$

where $l(\hat{y}_i, y_i)$ is the loss measuring the error between the predicted value $\hat{y}_i$ and the true target y_i , $\mathbf{f}_k$ is one of k trees in the model, Ω is the regularisation term for a single tree, and τ is the set of all parameters across all trees in the model.

2.2.5. Support Vector Regression

Support Vector Regression (SVR) uses a loss function called an ϵ -insensitive loss function, which defines an ϵ tube. For predictions which lie within this tube, the magnitude of the loss function is zero and the loss is the distance from the tube to predictions which lie outside. These points outside the tube are the only ones that are used to optimise the model and are referred to as support vectors. The model is also able to balance the trade-off between fitting the training data and generalising for unseen data by including

a term U that penalises the magnitude of the vector w . These two goals are combined to create the following function which the model aims to minimise [98]:

$$U \left(\sum_{i=1}^N \xi_i * + \sum_{i=1}^N \xi_i \right) + \frac{1}{2} (w^T w) \quad (9)$$

where N is the number of training samples, w is the weight vector defining the regression function, and ξ_i measures how far above or below the tube any datapoint is (zero if the point is inside the tube).

The advantage of using an ε tube is that the model avoids fitting to the noise of the data within the tube and only focuses on values which are poorly fit to the current function.

2.2.6. Linear Regression

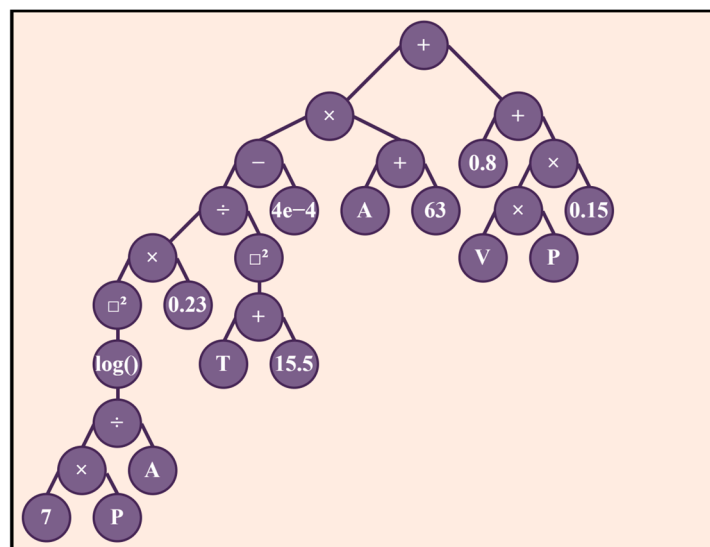
A linear regression (LR) model is a very simple form of regression where the relationship between an output variable y and a single input x is assumed to be linear. The model takes the form of a straight-line equation with an additional term θ representing the randomness or noise that would cause any individual point to deviate from this line. This can be extended for multiple inputs by summing together each value with their own regression coefficients β_i resulting in the following equation [99]:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_i x_i + \varepsilon \quad (10)$$

2.3. Interpretable AI Model

2.3.1. Symbolic Regression

SR is a method by which one can create an inherently explainable interpretation of the database through the formation of a single equation that predicts the output feature. To do this, a tree-like structure such as the one shown Figure 5 is built from a library of elementary arithmetic operations through trial and error with a loss function determining the accuracy of each equation [100]. The loss function may contain metrics such as the root mean squared error of predictions, as well as the length of any tree in order to punish overly verbose equations. This method is demonstrated in Algorithm 1 based on [101].



$$\text{Gravimetric Efficiency} = \left(\frac{0.23 \log(7P/A)^2}{(T + 15.5)^2} - 4e - 4 \right) (A + 63) + 0.15VP + 0.8$$

Figure 5. A tree diagram representation of a symbolic regression equation and the equation it represents.

Initially, SR generates a population of trees at random and evaluates their respective loss values on the dataset. The next generation of equations contain variations of the best performers from the previous generation, while also introducing new candidates continue to explore alternative methods. These variations can either have new branches added on, values of individual nodes changed or even have branches removed to avoid equations becoming unnecessarily long. This is done for a fixed number of iterations until the final best performing model can be selected.

Algorithm 1. Symbolic Regression Pseudo code

Input: Dataset $X = \{\text{BET, pore volume, } T, P\}$;

target $y = \text{H}_2 \text{ storage (\%)}$; operator set $\mathcal{O} = \{+, -, \times, \div, \sqrt{}, \exp, \log\}$

Output: Best symbolic expressions ranked by accuracy and complexity

1. Initialise n_p populations of L random expression trees; set $H \leftarrow \emptyset$
 2. for each iteration do
 3. for each population P_i (in parallel) do
 4. Select expression via tournament selection; apply genetic operator
 5. Simplify and optimise numerical constants (BFGS)
 6. Update best expressions locally (M_i) and globally (H)
 7. end for
 8. Share top expressions between populations
 9. end for
 10. return H
-

An important consideration when building a symbolic regression model is which functions to include within the library of operations. Basic functions such as additions and multiplications are always needed, but nonlinear operations such as trigonometric functions, logarithms, or powers can either be a help or a hindrance to the model.

Trigonometric functions for instance were found in testing to allow the model to very quickly adjust to the non-linear behaviour of the dataset but added an unnecessary element of periodicity that limited the accuracy for new datapoints. There are also specific combinations of operations that can be added to avoid the model needing to derive them independently, such as taking an inverse or negative of a number, but adding too many leads to worse results as it drastically increases the search space [102]. The operations which were included within the search were:

- I. Additions/Subtractions
- II. Multiplications/Divisions
- III. Taking the negative of a number
- IV. Taking the reciprocal of a number
- V. Taking the logarithm of a number

Another crucial factor when training a symbolic regression model is the length of final equation. The length is defined as being the total number of nodes within the tree and whilst longer trees do provide a higher accuracy, they cause the resulting equation to be harder to parse. Evaluating even very large equations is computationally inexpensive on modern hardware; however, in symbolic regression each candidate equation must be

evaluated for every data point, for every member of the population, and across all generations. For datasets containing 10,123 data points, this repeated evaluation can have a noticeable impact on execution time. In addition, longer expressions increase the optimisation effort, as a greater number of nodes must be adjusted during training. It is therefore important to balance model interpretability with predictive reliability. To make the decision on how long the equation used in this work should be, a series of models with varying lengths were trained to compare their relative performances.

When generating these equations there is also the decision of whether to impose unit consistency. Unit consistency means that only values of a consistent unit can be summed together, as in physics it is not possible to combine values which represent different physical properties. This can result in better equations being produced. When using this, it helps if the input features are measured in terms of their fundamental units as they are easier to combine, so in this work the units were converted to:

- Newtons per metre squared for pressure (converted from bars)
- Metres cubed per gram for pore volume (converted from centimetres cubed per gram)
- BET surface area remains in metres squared per gram

This makes each of these units easier to combine but still poses a challenge for units which only appear in a single term, such as the Newtons in pressure or Kelvin for temperature. Under the current constraints the model could only include these units in a term if it was later cancelled out, heavily restricting their use. To solve this, constants are able to have units associated with them to allow for more complex combinations of input features. The downside to this is that it becomes possible to combine any input feature regardless of if there is a physically meaningful relationship, provided there is a constant.

2.3.2. XAI Using SHAP Analysis

While black box models usually offer higher accuracy in comparison with the rest of the ML or non-AI statistical models, they lack transparency of the identified pattern of the data. To be able to explain this concealed information, techniques like SHAP can be used on the standard black-box models. The process for this has been shown in Figure 6.

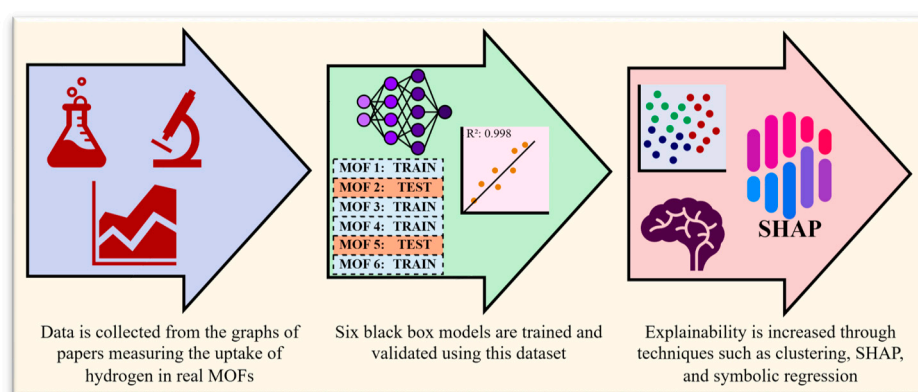


Figure 6. Conceptual figure showing the overall process of explaining the high-fidelity black-box models in this paper.

Feature importance is a useful tool for increasing the interpretability of a model. SHAP values are one such method for measuring the impact an input feature has on the accuracy of a prediction. To calculate these values, models are trained off a subset of the data with a single feature being omitted. This is compared to the accuracy of the model with that feature included, and the reduction in accuracy is therefore a measure of that

feature's importance. Features are often codependent on one another so the effect that withholding a feature has on the model's accuracy often depends on which other inputs are included. As such, this process is repeated for all possible combinations of input missing features. The weighted average is then calculated according to the following equation [103]:

$$\phi_i = \sum_{S \subseteq F \setminus \{i\}} \frac{|S|! (|F| - |S| - 1)!}{|F|!} \times [f_{S \cup \{i\}}(x_{S \cup \{i\}}) - f_S(x_S)] \quad (11)$$

where ϕ_i is the SHAP value, F is the set of all input features, and S is a subset of features that does not include feature i . $|S|$ is the number of features in subset S , and $|F|$ is the total number of features. f_S is the model trained using only features in S , and $f_{S \cup \{i\}}$ is the model trained with feature i included. x_S and $x_{S \cup \{i\}}$ denote the values of the corresponding feature subsets for the input being explained.

SHAP analysis can be presented in two different forms. A beeswarm plot displays individual SHAP values for every datapoint in the dataset, colour-coded by the magnitude of the corresponding feature value. This reveals not only the overall importance of each feature but also the direction of its effect. For example, whether high values of a feature push prediction upward or downward. A bar plot of mean absolute SHAP values provides a summary ranking of global feature importance by averaging the magnitude of contributions across all datapoints.

The magnitude of the SHAP values is determined not only by the model itself, but also by the database that it is trained on. For this reason, the size of the SHAP values themselves are not necessarily an indication of any importance or certainty, nor can the magnitude of the SHAP values be usefully compared between models. Rather, it is the relative magnitudes for each input feature that can be used to determine an order of importance.

A key advantage of SHAP over other methods such as relevancy factor is that it captures nonlinear relationships and feature interactions. Relevancy factor measures only how the output varies about its mean when a single input is varied in isolation, assuming each feature is independent [103]. SHAP evaluates contributions across all possible feature combinations, making it better suited to problems such as H₂ adsorption where intrinsic properties and extrinsic conditions interact in complex ways.

2.3.3. K-Means Clustering

Clustering is a method for understanding a model's decision making by grouping datapoints together that lead to similar model outputs. By looking at how the data has been grouped together it is possible to get a more detailed understanding of its interpretation of the dataset. This is less quantitative than SHAP values but allows for a more in-depth comparison between the clusters, and what one would expect from a physics-based perspective. For models with only a single output, it is sometimes too trivial to use a single value to determine which outputs are "similar", especially for complex phenomena such as H₂ storage. In this case, the final output layer of the model is removed, and the penultimate layer is used so that there are more values which can be compared when measuring similarity [104]. This concept is illustrated in Figure 7.

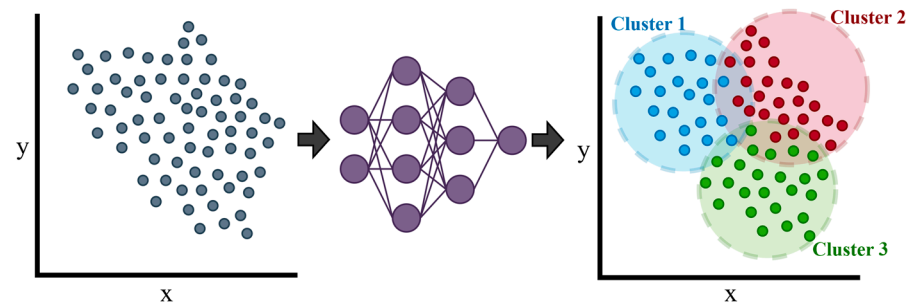


Figure 7. Conceptual figure demonstrating the result of clustering.

To group the datapoints together, a number of spheres are randomly created, and each datapoint is assigned to the nearest sphere based on its Euclidean distance to the centroid. The centroid μ_i of this cluster of datapoints is calculated using Equation (12) and the process is repeated with the datapoints being assigned to the new nearest centroid. This stops when the centroids stop moving by a significant degree. The goal is to minimise the distance of each datapoint to the centroid of its assigned cluster which is calculated with Equation (13) [105].

$$\mu_i = \frac{1}{|C_i|} \sum_{x \in C_i} x \quad (12)$$

$$J = \sum_{i=1}^k \sum_{x \in C_i} ||x - \mu_i||^2 \quad (13)$$

where J is the objective function to be minimised and C_i represents the set of points in cluster i .

When implementing clustering the number of clusters must be chosen manually at the start. The goal is to have multiple distinct groups with as little overlap as possible. To compute this, a silhouette analysis is done, which quantifies the overlap for each group and provides a silhouette score which can be used to find the best number of clusters [106]. In this work, four groups were found to yield a good mix of having enough groups to be able to draw meaningful conclusions whilst producing minimal overlap between groups.

2.3.4. Performance Evaluation Metrics

To evaluate how well a machine learning model or statistical algorithm performs on a given dataset, performance metrics are used to provide quantitative measures. Root Mean Squared Error (RMSE), R-squared, and Mean Absolute Error (MAE) are often used together to paint a complete picture of a model's predictive power. MAE measures the average absolute distance between predicted and actual values, giving a straightforward, easily interpretable baseline of average error without heavily penalising large outliers. RMSE, on the other hand, squares the errors before averaging them and taking the square root; this means it disproportionately penalises larger errors, making it highly sensitive to outliers and exceptionally useful when large mistakes are particularly undesirable. Finally, R-squared (the Coefficient of Determination) provides a relative perspective: rather than measuring the raw numerical error, it measures the proportion of variance in the dependent variable that the model successfully explains. While MAE and RMSE tell you the absolute size of the errors, R-squared tells you how well the model fits the data compared to just guessing the simple average, with a score closer to 1 indicating a perfect fit. Considering n to be the number of observations, y_i to be the actual true value, $\hat{y}_i$ to be the predicted value, and $\bar{y}$ to be the mean of the actual values, the mentioned metrics are defined as below:

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (14)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (15)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (16)$$

They provide a mathematical summary of the distance between what a model predicts and what the actual, true values are. By establishing this baseline, metrics allow researchers to objectively compare different models, tune system parameters, and determine if an algorithm is accurate and reliable enough for real-world applications.

3. Results and Discussion

The performance metrics for all six models trained in this work are summarised in Table 1, alongside results from comparable literature models. R-squared measures the goodness of fit as a percentage while RMSE and MAE measure the average error as a unitless hydrogen uptake ratio. The best performing model was GPR, achieving an R-squared of 0.9986, RMSE of 0.0995, and MAE of 0.0497, though the training time far exceeded the other models. If this was trained on a larger synthetic dataset, the computational demand may become comparable to traditional simulations. This would only be for the initial creation of the model however, as the time for predictions amongst all models is near instant. XGBoost achieved the second-best performance with an R-squared of 0.9966 whilst also having one of the fastest training times on this dataset.

Table 1. Comparison of the performance of each model.

Model	Number of Datapoints Used	R-Squared	RMSE	MAE	Inference Time [ms]	Reference
MLP	10,123	0.995	0.201	0.1259	12	This work
GRNN	10,123	0.985	0.3379	0.2203	10	This work
GPR *	10,123	0.9986	0.0995	0.0497	16	This work
XGBoost	10,123	0.997	0.1583	0.0981	28	This work
SVM	10,123	0.972	0.4661	0.2801	239	This work
LR	10,123	0.703	1.4949	1.0292	8	This work
SR-Exact	10,123	0.924	0.7193	0.5141	7	This work
SR-Rounded	10,123	0.914	0.7645	0.5352	7	This work
MLP	141	0.994	0.126	0.071	-	[22]
GRNN	141	0.998	0.197	0.104	-	[22]
MLP	35	0.9	0.26	-	-	[21]
CatBoost	717	0.991	0.032	-	-	[23]
BSLO-LightGBM	2048	0.976	0.239	0.15	-	[25]
BSLO-BPNN	2048	0.909	0.501	0.328	-	[25]
HOA-BPNN	2048	0.871	0.597	0.359	-	[25]
IGWO-BPNN	2048	0.893	0.544	0.352	-	[25]

* The best performing model from this work.

This increase in computation time for GPR became more significant when performing K-Fold cross validation to ensure the model had not been overfit. Across five folds the validation R-squared score remained consistent at 0.999 and RMSE held at 0.098 ± 0.010 .

This provides strong evidence to suggest the model has not been overfit; however, this validation would be much harder to perform on a larger database as the model must be retrained for each fold. XGBoost performed much better in this regard, also showing no drop in R-squared and an RMSE of 0.143 ± 0.012 across a 10-fold validation but computing in less than 5 s total. This method therefore would scale much better to a larger dataset of hundreds of thousands of points.

The MLP performed comparably, achieving an R-squared of 0.9950, RMSE of 0.2010, and MAE of 0.1259 following an extensive architecture search which found the optimal architecture to be three layers with 128 nodes, 55 nodes, and 19 nodes.

The worst performing model was LR with an R-squared of 0.7002, which is expected given its inability to capture the nonlinear relationships between input features and H₂ uptake. Whilst the size RMSE and MAE will vary between databases depending on the size of the datapoints, the CatBoost model by [23] did manage to get a significantly lower RMSE than all other models.

Whilst the performance of the models in this work were higher than that of others found in the literature, the relative performances of each model are the same. For instance, Reference [86] found that XGBoost achieved a higher R² score than MLP, and that MLP outperformed SVM. This even holds true for larger synthetic databases such as in Reference [24]. This provides an increased degree of confidence in the consistent predictive power of these models. It also provides evidence that the models have not been overfit, as the performance of weaker techniques, such as SVM, have not been artificially inflated to that of better models.

Even though the SR model did not achieve as high accuracies as the more sophisticated black-box models in this work, it did achieve a higher R-squared score than the BPNN models by [25]. This does support the idea that there is not necessarily an inherent trade-off between model complexity and explainability [107,108]. More work would still need to be done in this area to definitively make the assertion one way or the other.

The plots in Figure 8 highlight the relative predictive capabilities of each model. GPR has by far the most consistent predictions; however, it also shows the lack of a physics-backed understanding of H₂ adsorption due to both GPR and LR having negative predictions for H₂ uptake. There also would appear to be a run of three datapoints that both the SVM and GRNN model failed to make accurate predictions for. If these points are outliers, then their removal would potentially increase their respective accuracies; however, the fact that not every model struggled with these points suggests that they may not be anomalies.

The ability of these models to make predictions outside of the training range largely becomes a limitation of the dataset itself. By using hydrogen isotherms, this work has achieved a very continuous distribution of pressure values across a wide range. This means that interpolation is likely to be highly accurate and there is little need for extrapolation. This is because most MOFs see diminishing returns in the amount of extra hydrogen adsorbed when going beyond 100 Bar and the database already includes many points up to this limit.

Temperature remains an issue when discussing the implementation of these models for hydrogen storage predictions. The temperatures within the database are grouped together according to the boiling points of different gases. This is to keep temperatures steady and consistent when performing experiments. In practice, these MOFs are likely to be utilised under a variety of different temperatures and models trained on databases with such large gaps may prove to have large errors, even when interpolating.

The MLP was selected for improving explainability as it offers a more interpretable architecture than GPR or XGBoost whilst still achieving a competitive predictive performance. The order of feature importance from the SHAP values shown in Figure 9 are

Pressure > Temperature > Pore Volume > BET Surface Area. This aligns with what was observed when looking at graphs which illustrated the gravimetric efficiency of MOFs at different temperatures/pressures. The graphs showed that regardless of the surface area or pore volume, an increase in the pressure would always lead to a large increase in the H_2 uptake, and increasing the temperature would always lead to a large decrease.

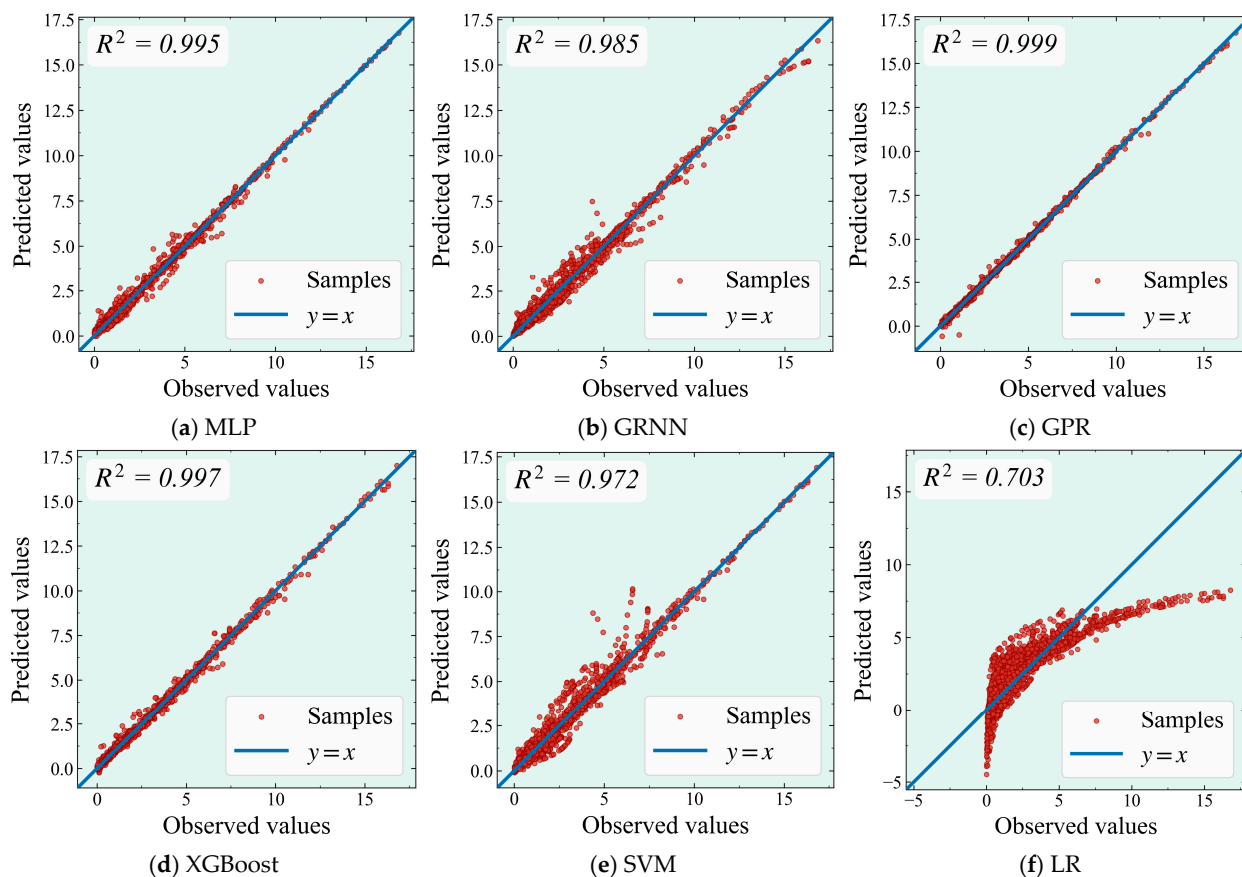
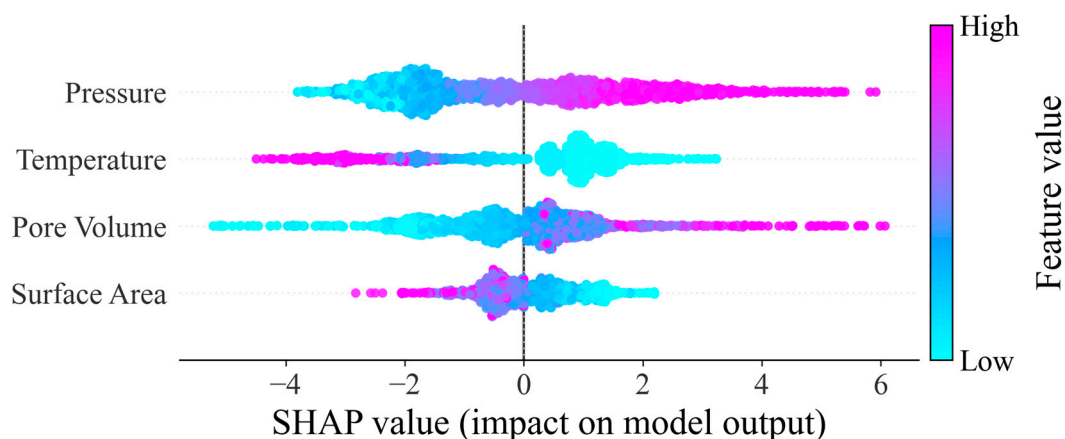


Figure 8. True values against predictions plots for the (a) MLP, (b) GRNN, (c) GPR, (d) XGBoost, (e) SVM, and (f) LR models.



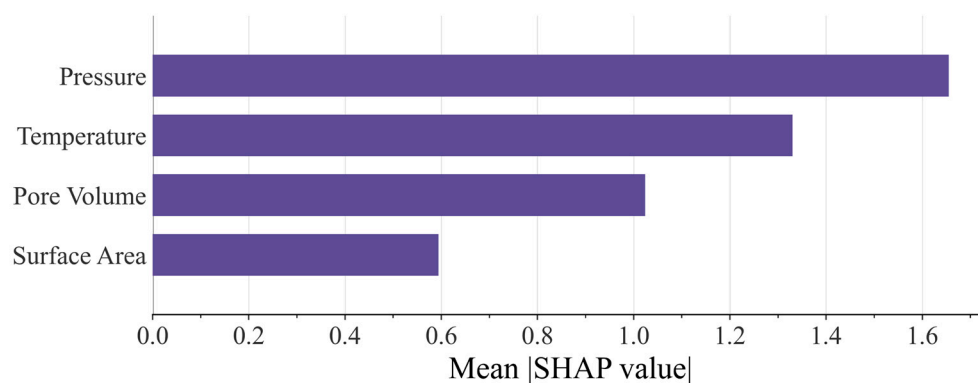


Figure 9. SHAP values for the MLP model.

The magnitude of the mean SHAP value for pore volume is $\sim 1.7\times$ bigger than that of surface area. This large difference is likely due to the high correlation between the two features that can be seen in Figure 3. If the pore volume is high, there is a high chance that the surface area will also be high, hence when this feature is removed the model's accuracy is not reduced by as significant a margin. This contrasts with the environmental conditions, where pressure was only $\sim 1.2\times$ larger. These two features are uncorrelated, so without it models are unable to infer a significant factor necessary to make their prediction.

The clustering results shown in Figure 10 were also generated using the MLP and provide several insights into the model's understanding of the data. The red cluster corresponds to low surface area and pore volume, which is associated with low adsorption rates, while the pink cluster represents higher surface area and pore volume. The light blue cluster appears to be associated primarily with high temperatures, which would also imply lower adsorption rates. However, the presence of several light blue points at lower temperatures suggests some uncertainty in the model's interpretation of adsorption behaviour within this group.

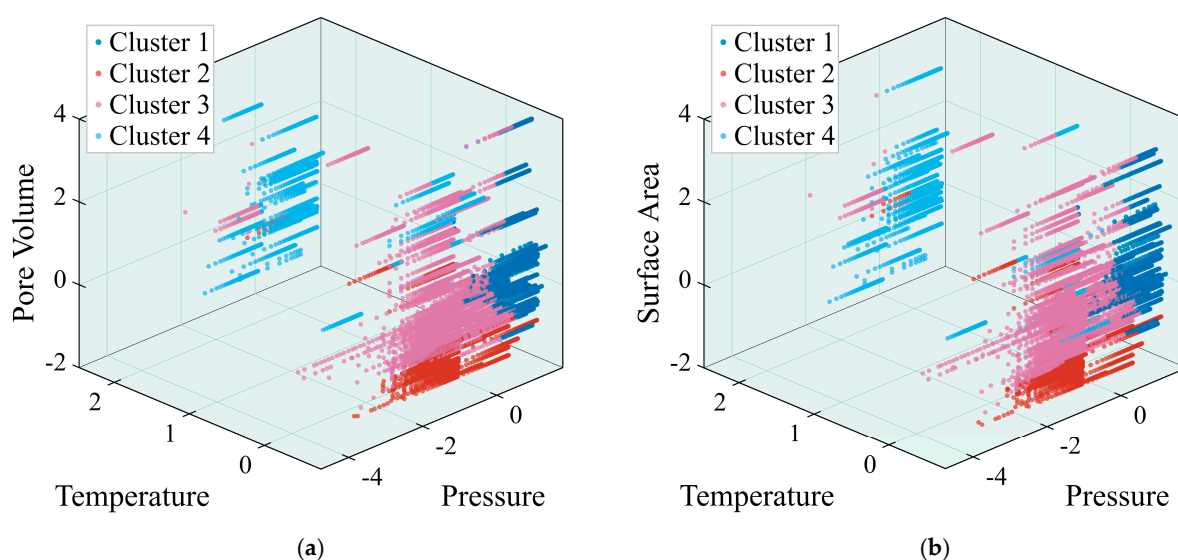


Figure 10. The clustering results for (a) temperature and pressure against pore volume, and for (b) temperature and pressure against surface area.

The dark blue cluster is the most clearly defined and is confined to conditions of low temperature and high pressure, which are consistent with high adsorption rates. This interpretation is supported by the transition of points from the dark blue cluster to the red

cluster as surface area or pore volume decreases. Notably, the influence of surface area and pore volume on this cluster appears limited, reinforcing the SHAP analysis result that temperature and pressure are more influential features than surface area or pore volume.

One limitation of these clustering results is the lack of variation at higher temperatures. Most high-temperature points are grouped into a single light blue cluster, whereas points with lower surface area or pore volume might reasonably be expected to fall into the red cluster. In addition, some overlap between clusters is observed, with points bleeding into other groups. This suggests that while the model captures key trends in H₂ adsorption, it would likely benefit from additional training data, particularly at higher temperatures and across a broader range of surface area and pore volume values.

Finally, the symbolic regression equations were generated and Figure 11 demonstrates that below a length of 30, the errors increase exponentially whilst increasing the length beyond this gives diminishing returns especially for R-squared score.

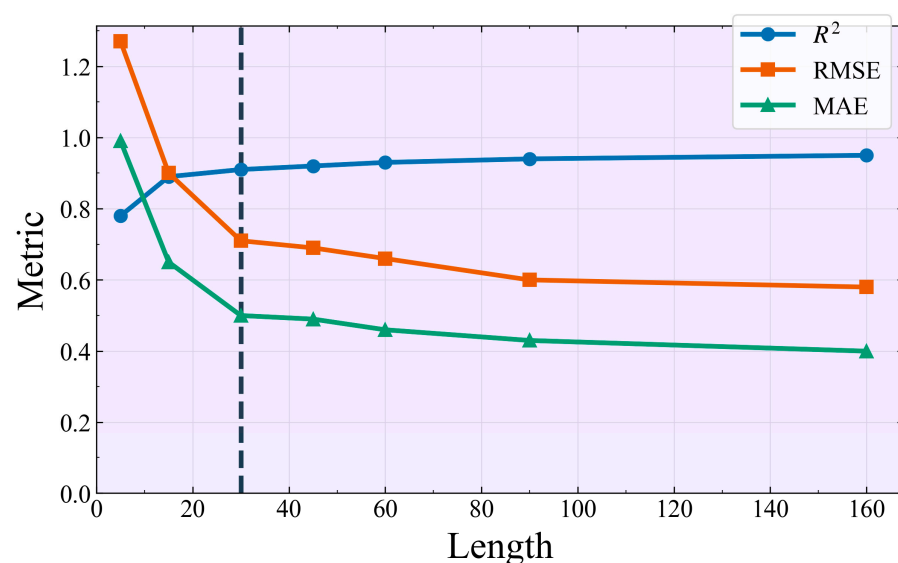


Figure 11. Graph showing how the length of an equation affects its prediction accuracy. The dashed line shows the length of the SR equation generated in this work.

Equation (17) has a length of 30 but as SR generates functions randomly without any of the steps or thought processes a mathematician would take when creating an equation, there are often additional manual steps that must be taken before any physical meaning can be derived. For example, the equation includes a near zero term that, when removed, had no measurable impact on the overall equation. The constants also have far too many significant figures that decreased the readability of the expression. Rounding these does reduce the accuracy but makes the final expression far easier to understand.

$$\text{Gravimetric Efficiency} = -P(7.608461 \times 10^{-8} - 0.15746881V) + 0.8070087 + \left(-0.00042373448 + \frac{0.22953977 \ln(6.959024P/A)^2}{(T + 15.525435)^2} \right) \times (A + 63.443703) \quad (17)$$

The final equation shown in Equation (18) contains aspects that make sense from a physics-based perspective such as dividing pressure by area to get a force and using a logarithm to generate the non-linear behaviour of the adsorption isotherms. The rationale behind many of the constants is difficult to interpret; however, this equation is a much more generally applicable representation of the database as it can be easily incorporated into any excel, MATLAB file, or similar.

$$\text{Gravimetric Efficiency} = \left(\frac{0.23 \ln(7P/A)^2}{(T + 15.5)^2} - \frac{1}{2360} \right) (A + 63.4) + 0.1574VP + 0.8 \quad (18)$$

In practice, Equation (18) smoothly interpolates between values with little noise and a strong ability to extrapolate temperature. The equation accurately maps changes in temperature to the respective change in the gradient of the adsorption isotherm, consistently providing physically meaningful predictions. Very high surface areas do pose a challenge however, since it predicts negative values of hydrogen adsorption at very low pressures (below 0.1 Bar) when the surface area exceeds 4000 m²g^{−1}. This suggests the equation is most suitable for real world predictions of hydrogen adsorption at pressures above 1 Bar.

These results show a strong ability for AI to make predictions on the uptake of H₂ in MOFs. The black-box models did achieve the highest accuracies, demonstrating their capabilities to quickly screen potential MOFs. Whilst the models show a typical drop in accuracy when extrapolating beyond the original dataset, their predictions remain sufficiently strong to be able to provide a preliminary screening of a large search space. The few frameworks which show promising performance can then be verified using slower, but more rigorous techniques.

The combination of SHAP and clustering was also able to provide insights into the model's interpretation of the dataset, improving the feasibility of using them in real-world applications. Though there will always be some degree of obscurity in how any black-box model generates its predictions, the proposed techniques demonstrate the ability to understand how features are related on a broad scale, informing engineers' design decisions when proposing potential MOFs. The inherently explainable SR model managed to achieve comparable accuracy to some of the ML models whilst providing a clearer understanding of how predictions were generated. This equation is also far easier to implement in practice, being able to generate predictions using either simple software or a calculator.

4. Conclusions

As engineers look to hydrogen (H₂) as an alternative to fossil fuels, the need for efficient storage becomes more important. Metal–Organic Frameworks (MOFs) address this need offering highly efficient volumetric efficiencies; however, the sheer number of potential frameworks and the time-consuming nature of synthesising them creates the need to be able to screen many potential structures quickly. In this work, a number of AI models were trained on the largest database of real MOFs in the literature (at the time of writing), and an in-depth analysis of the model's understanding of the database was done. The use of clustering to perform this analysis is something that has not been done by other papers predicting the uptake of H₂ in MOFs, as well as the use of Symbolic Regression (SR) to build an inherently explainable model.

The findings of this paper are as follows:

- By using the data from graphs within a paper, a database of 10,123 real MOFs can be achieved that is ~400% larger than what has been produced in other works.
- Based on the accuracies calculated from the test set, these MLs show a strong ability to model the uptake of H₂ in MOFs with an R-squared score of as high as 0.9986.
- Both SHAP and clustering can improve the explainability of an AI model and give engineers more confidence in their predictions.
- Even a small SR equation can achieve accuracies sufficient to perform a preliminary screening of potential frameworks.

This lays the foundation for future engineers and academic researchers to perform rapid, large-scale screening of potential MOFs without the need for costly synthesis or computationally expensive simulations such as GCMC. The SR equation in particular offers a lightweight tool that can be evaluated in standard software such as Excel or

MATLAB, lowering the barrier for adoption in both industrial design workflows and academic studies. The SHAP and clustering analysis also provides a framework that can be applied to future, larger datasets to further validate the physical insights identified here.

In order to improve the reliability of these techniques in such applications, important areas for future research would be: validating the performance metrics by ensuring data-points in the test set are sufficiently unique from those present in the training set; creating a database with a more continuous distribution of temperature values and including the isosteric heat of adsorption as an input feature using the corresponding graphs in the references.

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References

1. *Emissions Gap Report 2024: No More Hot Air ... Please! With a Massive Gap Between Rhetoric and Reality, Countries Draft New Climate Commitments*; United Nations Environment Programme: Nairobi, Kenya, 2024. <https://doi.org/10.59117/20.500.11822/46404>.
2. Alipour Bonab, S.; Waite, T.; Yazdani-Asrami, M. Artificially intelligent framework for multi-output performance prediction in diverse solid oxide electrolyzer cells for green hydrogen production plants. *J. Phys. Energy* **2026**, *8*, 015006. <https://doi.org/10.1088/2515-7655/ae1e2a>.
3. Hydrogen and Fuel Cell Technologies Office. Hydrogen Storage. US Department of Energy. Available online: <https://www.energy.gov/cmei/fuels/hydrogen-storage> (accessed on 29 March 2026).
4. Huete, J.; Pilidis, P. Parametric study on tank integration for hydrogen civil aviation propulsion. *Int. J. Hydrogen Energy* **2021**, *46*, 37049–37062. <https://doi.org/10.1016/j.ijhydene.2021.08.194>.
5. Anekwe, I.M.S.; Mustapha, S.I.; Akpasi, S.O.; Tetteh, E.K.; Joel, A.S.; Isa, Y.M. The hydrogen challenge: addressing storage, safety, and environmental concerns in hydrogen economy. *Int. J. Hydrogen Energy* **2025**, *167*, 150952. <https://doi.org/10.1016/j.ijhydene.2025.150952>.
6. Vo Thanh, H.; Zhang, H.; Dai, Z.; Zhang, T.; Tangparitkul, S.; Min, B. Data-driven machine learning models for the prediction of hydrogen solubility in aqueous systems of varying salinity: Implications for underground hydrogen storage. *Int. J. Hydrogen Energy* **2024**, *55*, 1422–1433. <https://doi.org/10.1016/j.ijhydene.2023.12.131>.
7. Carvalho, M.C.S.; Marques, J.; Matos, H.A.; Granjo, J.F.O. Long-distance hydrogen delivery using a toluene-based liquid organic hydrogen carrier system. In *Computer Aided Chemical Engineering*; Elsevier B.V.: Amsterdam, The Netherlands, 2021; pp. 1647–1652. <https://doi.org/10.1016/B978-0-323-88506-5.50255-2>.
8. Ford, O.; Alipour Bonab, S.; Yazdani-Asrami, M. Artificial intelligence-aided liquid hydrogen tank modelling for sustainable aviation. *Energy Rep.* **2025**, *14*, 4609–4623. <https://doi.org/10.1016/j.egyr.2025.11.054>.
9. Alipour Bonab, S.; Yazdani-Asrami, M. Investigation on the heat transfer estimation of subcooled liquid hydrogen for transportation applications using intelligent technique. *Int. J. Hydrogen Energy* **2024**, *84*, 468–479. <https://doi.org/10.1016/j.ijhydene.2024.08.257>.

10. Suh, M.P.; Park, H.J.; Prasad, T.K.; Lim, D.W. Hydrogen storage in metal-organic frameworks. *Chem. Rev.* **2012**, *112*, 782–835. <https://doi.org/10.1021/cr200274s>. PMID: 22191516.
11. Kapelewski, M.T.; Runčevski, T.; Tarver, J.D.; Jiang, H.Z.; Hurst, K.E.; Parilla, P.A.; Ayala, A.; Gennett, T.; FitzGerald, S.A.; Brown, C.M.; et al. Record High Hydrogen Storage Capacity in the Metal-Organic Framework Ni₂(m-dobdc) at Near-Ambient Temperatures. *Chem. Mater.* **2018**, *30*, 8179–8189. <https://doi.org/10.1021/acs.chemmater.8b03276>.
12. Murray, L.J.; Dincă, M.; Long, J.R. Hydrogen storage in metal-organic frameworks. *Chem. Soc. Rev.* **2009**, *38*, 1294. <https://doi.org/10.1039/b802256a>.
13. Leus, K.; Dendooven, J.; Tahir, N.; Ramachandran, R.K.; Meledina, M.; Turner, S.; Van Tendeloo, G.; Goeman, J.L.; Van der Eycken, J.; Detavernier, C.; et al. Atomic Layer Deposition of Pt Nanoparticles within the Cages of MIL-101: A Mild and Recyclable Hydrogenation Catalyst. *Nanomaterials* **2016**, *6*, 45. <https://doi.org/10.3390/nano6030045>.
14. Meledina, M.; Watson, G.; Meledin, A.; Van Der Voort, P.; Mayer, J.; Leus, K. Ru Catalyst Encapsulated into the Pores of MIL-101 MOF: Direct Visualization by TEM. *Materials* **2021**, *14*, 4531. <https://doi.org/10.3390/ma14164531>.
15. Belof, J.L.; Stern, A.C.; Eddaoudi, M.; Space, B. On the Mechanism of Hydrogen Storage in a Metal-Organic Framework Material. *J. Am. Chem. Soc.* **2007**, *129*, 15202–15210. <https://doi.org/10.1021/ja0737164>.
16. Alipour Bonab, S.; Yazdani-Asrami, M. Artificial intelligence-based model to predict the heat transfer coefficient in flow boiling of liquid hydrogen as fuel and cryogenic coolant in future hydrogen-powered cryo-electric aviation. *Fuel* **2025**, *381*, 133323. <https://doi.org/10.1016/j.fuel.2024.133323>.
17. Alipour Bonab, S.; Yazdani-Asrami, M. Machine learning-based model for the intelligent estimation of critical heat flux in nanofluids. *Nano Express* **2024**, *5*, 025012. <https://doi.org/10.1088/2632-959X/ad461d>.
18. Bonab, S.A.; Russo, G.; Morandi, A.; Yazdani-Asrami, M. A comprehensive machine learning-based investigation for the index-value prediction of 2G HTS coated conductor tapes. *Mach. Learn. Sci. Technol.* **2024**, *5*, 025040. <https://doi.org/10.1088/2632-2153/ad45b1>.
19. Alipour Bonab, S.; Waite, T.; Song, W.; Flynn, D.; Yazdani-Asrami, M. Machine learning-powered performance monitoring of proton exchange membrane water electrolyzers for enhancing green hydrogen production as a sustainable fuel for aviation industry. *Energy Rep.* **2024**, *12*, 2270–2282. <https://doi.org/10.1016/j.egy.2024.08.028>.
20. Yazdani-Asrami, M. Artificial intelligence, machine learning, deep learning, and big data techniques for the advancements of superconducting technology: a road to smarter and intelligent superconductivity. *Supercond. Sci. Technol.* **2023**, *36*, 084001. <https://doi.org/10.1088/1361-6668/ace385>.
21. Atashrouz, S.; Rahmani, M. Predicting hydrogen storage capacity of metal-organic frameworks using group method of data handling. *Neural Comput. Appl.* **2020**, *32*, 14851–14864. <https://doi.org/10.1007/s00521-020-04837-3>.
22. Cao, Y.; Dhahad, H.A.; Zare, S.G.; Farouk, N.; Anqi, A.E.; Issakhov, A.; Raise, A. Potential application of metal-organic frameworks (MOFs) for hydrogen storage: Simulation by artificial intelligent techniques. *Int. J. Hydrogen Energy* **2021**, *46*, 36336–36347. <https://doi.org/10.1016/j.ijhydene.2021.08.167>.
23. Salehi, K.; Rahmani, M.; Atashrouz, S. Hydrogen storage capacity in metal-organic frameworks: Towards elevating predictions through ensemble learning with a comprehensive preprocessed dataset. *Int. J. Hydrogen Energy* **2025**, *118*, 251–267. <https://doi.org/10.1016/j.ijhydene.2025.03.042>.
24. Sarvi, H.; Dehdari, S.; Maleki, M.; Baziari, M.; Kazemzadeh, Y. Artificial intelligence-based prediction of hydrogen uptake of metal organic frameworks with high volumetric storage density for fuel cell systems. *Clean. Eng. Technol.* **2025**, *28*, 101037. <https://doi.org/10.1016/j.clet.2025.101037>.
25. Cao, Z.H.; Bian, X.Q.; Chen, J.; Zhang, J.Y.; Fu, W. Predicting hydrogen storage in metal-organic frameworks using a novel hybrid machine learning model. *Int. J. Hydrogen Energy* **2025**, *145*, 401–411. <https://doi.org/10.1016/j.ijhydene.2025.06.112>.
26. Li, J.; Cheng, K.; Wang, S.; Morstatter, F.; Trevino, R.P.; Tang, J.; Liu, H. Feature Selection: A Data Perspective. *ACM Comput Surv.* **2018**, *50*, 1–45. <https://doi.org/10.1145/3136625>.
27. Rouquerol, J.; Llewellyn, P.; Rouquerol, F. *Is the Bet Equation Applicable to Microporous Adsorbents?*; Elsevier: Amsterdam, The Netherlands, 2007; pp. 49–56. [https://doi.org/10.1016/S0167-2991\(07\)80008-5](https://doi.org/10.1016/S0167-2991(07)80008-5).
28. Walton, K.S.; Snurr, R.Q. Applicability of the BET method for determining surface areas of microporous metal-organic frameworks. *J. Am. Chem. Soc.* **2007**, *129*, 8552–8556. <https://doi.org/10.1021/ja071174k>.
29. Zhang, X.; Lin, R.; Wang, J.; Wang, B.; Liang, B.; Yildirim, T.; Zhang, J.; Zhou, W.; Chen, B. Optimization of the Pore Structures of MOFs for Record High Hydrogen Volumetric Working Capacity. *Adv. Mater.* **2020**, *32*. <https://doi.org/10.1002/adma.201907995>.

30. Chun, H.; Dybtsev, D.N.; Kim, H.; Kim, K. Synthesis, X-ray Crystal Structures, and Gas Sorption Properties of Pillared Square Grid Nets Based on Paddle-Wheel Motifs: Implications for Hydrogen Storage in Porous Materials. *Chem. Eur. J.* **2005**, *11*, 3521–3529. <https://doi.org/10.1002/chem.200401201>.
31. Choi, S.B.; Seo, M.J.; Cho, M.; Kim, Y.; Jin, M.K.; Jung, D.-Y.; Choi, J.-S.; Ahn, W.-S.; Rowsell, J.L.C.; Kim, J. A Porous and Interpenetrated Metal–Organic Framework Comprising Tetranuclear Iron^{III}–Oxo Clusters and Tripodal Organic Carboxylates and Its Implications for (3,8)-Coordinated Networks. *Cryst. Growth Des.* **2007**, *7*, 2290–2293. <https://doi.org/10.1021/cg070640e>.
32. Yuan, D.; Zhao, D.; Sun, D.; Zhou, H. An Isorecticular Series of Metal–Organic Frameworks with Dendritic Hexacarboxylate Ligands and Exceptionally High Gas-Uptake Capacity. *Angew. Chem. Int. Ed.* **2010**, *49*, 5357–5361. <https://doi.org/10.1002/anie.201001009>.
33. Furukawa, H.; Ko, N.; Go, Y.B.; Aratani, N.; Choi, S.B.; Choi, E.; Yazaydin, A.Ö.; Snurr, R.Q.; O’Keeffe, M.; Kim, J.; et al. Ultra-high Porosity in Metal–Organic Frameworks. *Science* **2010**, *329*, 424–428. <https://doi.org/10.1126/science.1192160>.
34. Zhuang, W.; Ma, S.; Wang, X.-S.; Yuan, D.; Li, J.-R.; Zhao, D.; Zhou, H.-C. Introduction of cavities up to 4 nm into a hierarchically-assembled metal–organic framework using an angular, tetratopic ligand. *Chem. Commun.* **2010**, *46*, 5223. <https://doi.org/10.1039/c0cc00779j>.
35. Porter, W.W.; Wong-Foy, A.; Dailly, A.; Matzger, A.J. Beryllium benzene dicarboxylate: the first beryllium microporous coordination polymer. *J. Mater. Chem.* **2009**, *19*, 6489. <https://doi.org/10.1039/b912092k>.
36. Yang, W.; Lin, X.; Jia, J.; Blake, A.J.; Wilson, C.; Hubberstey, P.; Champness, N.R.; Schröder, M. A biporous coordination framework with high H₂ storage density. *Chem. Commun.* **2008**, *44*, 359–361. <https://doi.org/10.1039/B712201B>.
37. Kramer, M.; Schwarz, U.; Kaskel, S. Synthesis and properties of the metal–organic framework Mo₃(BTC)₂ (TUDMOF-1). *J. Mater. Chem.* **2006**, *16*, 2245. <https://doi.org/10.1039/b601811d>.
38. Farha, O.K.; Yazaydin, A.Ö.; Eryazici, I.; Malliakas, C.D.; Hauser, B.G.; Kanatzidis, M.G.; Nguyen, S.T.; Snurr, R.Q.; Hupp, J.T. De novo synthesis of a metal–organic framework material featuring ultrahigh surface area and gas storage capacities. *Nat. Chem.* **2010**, *2*, 944–948. <https://doi.org/10.1038/nchem.834>.
39. Zhou, W.; Wu, H.; Hartman, M.R.; Yildirim, T. Hydrogen and Methane Adsorption in Metal–Organic Frameworks: A High-Pressure Volumetric Study. *J. Phys. Chem. C* **2007**, *111*, 16131–16137. <https://doi.org/10.1021/jp074889i>.
40. Zhao, D.; Yuan, D.; Yakovenko, A.; Zhou, H.C. A NbO-type metal–organic framework derived from a polyyne-coupled diisophthalate linker formed in situ. *Chem. Commun.* **2010**, *46*, 4196. <https://doi.org/10.1039/c002767g>.
41. Nouar, F.; Eubank, J.F.; Bousquet, T.; Wojtas, L.; Zaworotko, M.J.; Eddaoudi, M. Supramolecular Building Blocks (SBBs) for the Design and Synthesis of Highly Porous Metal–Organic Frameworks. *J. Am. Chem. Soc.* **2008**, *130*, 1833–1835. <https://doi.org/10.1021/ja710123s>.
42. Wong-Foy, A.G.; Lebel, O.; Matzger, A.J. Porous Crystal Derived from a Tricarboxylate Linker with Two Distinct Binding Motifs. *J. Am. Chem. Soc.* **2007**, *129*, 15740–15741. <https://doi.org/10.1021/ja0753952>.
43. Mulfort, K.L.; Hupp, J.T. Chemical Reduction of Metal–Organic Framework Materials as a Method to Enhance Gas Uptake and Binding. *J. Am. Chem. Soc.* **2007**, *129*, 9604–9605. <https://doi.org/10.1021/ja0740364>.
44. Dincă, M.; Dailly, A.; Liu, Y.; Brown, C.M.; Neumann, D.; Long, J.R. Hydrogen Storage in a Microporous Metal–Organic Framework with Exposed Mn²⁺ Coordination Sites. *J. Am. Chem. Soc.* **2006**, *128*, 16876–16883. <https://doi.org/10.1021/ja0656853>.
45. Lin, X.; Blake, A.J.; Wilson, C.; Sun, X.Z.; Champness, N.R.; George, M.W.; Hubberstey, P.; Mokaya, R.; Schröder, M. A Porous Framework Polymer Based on a Zinc(II) 4,4′-Bipyridine-2,6,2′,6′-tetracarboxylate: Synthesis, Structure, and “Zeolite-Like” Behaviors. *J. Am. Chem. Soc.* **2006**, *128*, 10745–10753. <https://doi.org/10.1021/ja060946u>.
46. Rowsell, J.L.C.; Yaghi, O.M. Effects of Functionalization, Catenation, and Variation of the Metal Oxide and Organic Linking Units on the Low-Pressure Hydrogen Adsorption Properties of Metal–Organic Frameworks. *J. Am. Chem. Soc.* **2006**, *128*, 1304–1315. <https://doi.org/10.1021/ja056639q>.
47. Chun, H.; Jung, H.; Koo, G.; Jeong, H.; Kim, D.K. Efficient Hydrogen Sorption in 8-Connected MOFs Based on Trinuclear Pinwheel Motifs. *Inorg. Chem.* **2008**, *47*, 5355–5359. <https://doi.org/10.1021/ic800274w>.
48. Yuan, D.; Zhao, D.; Zhou, H.C. Pressure-Responsive Curvature Change of a “Rigid” Geodesic Ligand in a (3,24)-Connected Mesoporous Metal–Organic Framework. *Inorg. Chem.* **2011**, *50*, 10528–10530. <https://doi.org/10.1021/ic201744n>.
49. Sun, D.; Ma, S.; Simmons, J.M.; Li, J.R.; Yuan, D.; Zhou, H.C. An unusual case of symmetry-preserving isomerism. *Chem. Commun.* **2010**, *46*, 1329. <https://doi.org/10.1039/b920995f>.
50. Hulvey, Z.; Sava, D.A.; Eckert, J.; Cheetham, A.K. Hydrogen Storage in a Highly Interpenetrated and Partially Fluorinated Metal–Organic Framework. *Inorg. Chem.* **2011**, *50*, 403–405. <https://doi.org/10.1021/ic101153c>.

51. Wang, Y.; Cheng, P.; Chen, J.; Liao, D.Z.; Yan, S.P. A Heterometallic Porous Material for Hydrogen Adsorption. *Inorg. Chem.* **2007**, *46*, 4530–4534. <https://doi.org/10.1021/ic070097r>.
52. Wang, X.-S.; Ma, S.; Rauch, K.; Simmons, J.M.; Yuan, D.; Wang, X.; Yildirim, T.; Cole, W.C.; López, J.J.; de Meijere, A.; et al. Metal–Organic Frameworks Based on Double-Bond-Coupled Di-Isophthalate Linkers with High Hydrogen and Methane Uptakes. *Chem. Mater.* **2008**, *20*, 3145–3152. <https://doi.org/10.1021/cm800403d>.
53. Perles, J.; Iglesias, M.; Martín-Luengo, M.Á.; Monge, M.Á.; Ruiz-Valero, C.; Snejko, N. Metal–Organic Scandium Framework: Useful Material for Hydrogen Storage and Catalysis. *Chem. Mater.* **2005**, *17*, 5837–5842. <https://doi.org/10.1021/cm051362e>.
54. Liu, X.; Oh, M.; Lah, M.S. Adsorbate Selectivity of Isorecticular Microporous Metal–Organic Frameworks with Similar Static Pore Dimensions. *Cryst. Growth Des.* **2011**, *11*, 5064–5071. <https://doi.org/10.1021/cg200983y>.
55. Liu, X.; Oh, M.; Lah, M.S. Size- and Shape-Selective Isostructural Microporous Metal–Organic Frameworks with Different Effective Aperture Sizes. *Inorg. Chem.* **2011**, *50*, 5044–5053. <https://doi.org/10.1021/ic200328q>.
56. García-Holley, P.; Schweitzer, B.; Islamoglu, T.; Liu, Y.; Lin, L.; Rodriguez, S.; Weston, M.H.; Hupp, J.T.; Gómez-Gualdrón, D.A.; Yildirim, T.; et al. Benchmark Study of Hydrogen Storage in Metal–Organic Frameworks under Temperature and Pressure Swing Conditions. *ACS Energy Lett.* **2018**, *3*, 748–754. <https://doi.org/10.1021/acsenerylett.8b00154>.
57. Ramirez-Vidal, P.; Canevesi, R.L.S.; Celzard, A.; Fierro, V. Modeling High-Pressure Hydrogen Uptake by Nanoporous Metal–Organic Frameworks: Implications for Hydrogen Storage and Delivery. *ACS Appl. Nano Mater.* **2022**, *5*, 759–773. <https://doi.org/10.1021/acsanm.1c03493>.
58. Takei, T.; Kawashima, J.; Ii, T.; Maeda, A.; Hasegawa, M.; Kitagawa, T.; Ohmura, T.; Ichikawa, M.; Hosoe, M.; Kanoya, I.; et al. Hydrogen Adsorption Properties of Lantern-Type Dinuclear M(BDC)(DABCO)_{1/2}. *Bull. Chem. Soc. Jpn.* **2008**, *81*, 847–856. <https://doi.org/10.1246/bcsj.81.847>.
59. Li, M.; Wang, Z.; An, Y.; Wang, X.; Li, P.; Yao, W.; Chen, K.; Song, J.; Feng, X.; Liu, N. Cryogenic gas chromatographic separation of hydrogen isotopes using pillared-layer MOFs composites as stationary phase. *Int. J. Hydrogen Energy* **2022**, *47*, 339–347. <https://doi.org/10.1016/j.ijhydene.2021.10.039>.
60. Garg, A.; Almáši, M.; Saini, R.; Paul, D.R.; Sharma, A.; Jain, A.; Jain, I.P. A highly stable terbium(III) metal-organic framework MOF-76(Tb) for hydrogen storage and humidity sensing. *Environ. Sci. Pollut. Res.* **2022**, *30*, 98548–98562. <https://doi.org/10.1007/s11356-022-21290-y>.
61. Yan, Y.; Blake, A.J.; Lewis, W.; Barnett, S.A.; Dailly, A.; Champness, N.R.; Schröder, M. Modifying Cage Structures in Metal–Organic Polyhedral Frameworks for H₂ Storage. *Chem. Eur. J.* **2011**, *17*, 11162–11170. <https://doi.org/10.1002/chem.201101341>.
62. Lin, X.; Telepeni, I.; Blake, A.J.; Dailly, A.; Brown, C.M.; Simmons, J.M.; Zoppi, M.; Walker, G.S.; Thomas, K.M.; Mays, T.J.; et al. High Capacity Hydrogen Adsorption in Cu(II) Tetracarboxylate Framework Materials: The Role of Pore Size, Ligand Functionalization, and Exposed Metal Sites. *J. Am. Chem. Soc.* **2009**, *131*, 2159–2171. <https://doi.org/10.1021/ja806624j>.
63. Park, H.J.; Lim, D.; Yang, W.S.; Oh, T.; Suh, M.P. A Highly Porous Metal–Organic Framework: Structural Transformations of a Guest-Free MOF Depending on Activation Method and Temperature. *Chem. Eur. J.* **2011**, *17*, 7251–7260. <https://doi.org/10.1002/chem.201003376>.
64. Sumida, K.; Hill, M.R.; Horike, S.; Dailly, A.; Long, J.R. Synthesis and Hydrogen Storage Properties of Be₁₂(OH)₁₂(1,3,5-benzenetribenzoate)₄. *J. Am. Chem. Soc.* **2009**, *131*, 15120–15121. <https://doi.org/10.1021/ja9072707>.
65. Prasad, T.K.; Hong, D.H.; Suh, M.P. High Gas Sorption and Metal-Ion Exchange of Microporous Metal–Organic Frameworks with Incorporated Imide Groups. *Chem. Eur. J.* **2010**, *16*, 14043–14050. <https://doi.org/10.1002/chem.201002135>.
66. Denysenko, D.; Grzywa, M.; Tonigold, M.; Streppel, B.; Krkljus, I.; Hirscher, M.; Mugnaioli, E.; Kolb, U.; Hanss, J.; Volkmer, D. Elucidating Gating Effects for Hydrogen Sorption in MFU-4-Type Triazolate-Based Metal–Organic Frameworks Featuring Different Pore Sizes. *Chem. Eur. J.* **2011**, *17*, 1837–1848. <https://doi.org/10.1002/chem.201001872>.
67. Yang, S.; Lin, X.; Dailly, A.; Blake, A.J.; Hubberstey, P.; Champness, N.R.; Schröder, M. Enhancement of H₂ Adsorption in Coordination Framework Materials by Use of Ligand Curvature. *Chem. Eur. J.* **2009**, *15*, 4829–4835. <https://doi.org/10.1002/chem.200802292>.
68. Park, H.J.; Suh, M.P. Mixed-Ligand Metal–Organic Frameworks with Large Pores: Gas Sorption Properties and Single-Crystal-to-Single-Crystal Transformation on Guest Exchange. *Chem. Eur. J.* **2008**, *14*, 8812–8821. <https://doi.org/10.1002/chem.200801064>.
69. Tan, C.; Yang, S.; Champness, N.R.; Lin, X.; Blake, A.J.; Lewis, W.; Schröder, M. High capacity gas storage by a 4,8-connected metal–organic polyhedral framework. *Chem. Commun.* **2011**, *47*, 4487. <https://doi.org/10.1039/c1cc10378d>.
70. Wang, X.; Ma, S.; Forster, P.M.; Yuan, D.; Eckert, J.; López, J.J.; Murphy, B.J.; Parise, J.B.; Zhou, H. Enhancing H₂ Uptake by “Close-Packing” Alignment of Open Copper Sites in Metal–Organic Frameworks. *Angew. Chem. Int. Ed.* **2008**, *47*, 7263–7266. <https://doi.org/10.1002/anie.200802087>.

71. Ma, S.; Wang, X.; Yuan, D.; Zhou, H. A Coordinatively Linked Yb Metal–Organic Framework Demonstrates High Thermal Stability and Uncommon Gas-Adsorption Selectivity. *Angew. Chem. Int. Ed.* **2008**, *47*, 4130–4133. <https://doi.org/10.1002/anie.200800312>.
72. Yan, Y.; Yang, S.; Blake, A.J.; Lewis, W.; Poirier, E.; Barnett, S.A.; Champness, N.R.; Schröder, M. A mesoporous metal–organic framework constructed from a nanosized C₃-symmetric linker and [Cu₂(isophthalate)₂₄] cuboctahedra. *Chem. Commun.* **2011**, *47*, 9995. <https://doi.org/10.1039/c1cc13170b>.
73. Lin, X.; Jia, J.; Zhao, X.; Thomas, K.M.; Blake, A.J.; Walker, G.S.; Champness, N.R.; Hubberstey, P.; Schröder, M. High H₂ Adsorption by Coordination-Framework Materials. *Angew. Chem. Int. Ed.* **2006**, *45*, 7358–7364. <https://doi.org/10.1002/anie.200601991>.
74. Kesanli, B.; Cui, Y.; Smith, M.R.; Bittner, E.W.; Bockrath, B.C.; Lin, W. Highly Interpenetrated Metal–Organic Frameworks for Hydrogen Storage. *Angew. Chem. Int. Ed.* **2005**, *44*, 72–75. <https://doi.org/10.1002/anie.200461214>.
75. Lee, J.Y.; Pan, L.; Kelly, S.P.; Jagiello, J.; Emge, T.J.; Li, J. Achieving High Density of Adsorbed Hydrogen in Microporous Metal Organic Frameworks. *Adv. Mater.* **2005**, *17*, 2703–2706. <https://doi.org/10.1002/adma.200500867>.
76. Krawiec, P.; Kramer, M.; Sabo, M.; Kunschke, R.; Fröde, H.; Kaskel, S. Improved Hydrogen Storage in the Metal–Organic Framework Cu₃(BTC)₂. *Adv. Eng. Mater.* **2006**, *8*, 293–296. <https://doi.org/10.1002/adem.200500223>.
77. Zheng, S.; Bu, J.J.; Wu, T.; Chou, C.; Feng, P.; Bu, X. Porous Indium–Organic Frameworks and Systematization of Structural Building Blocks. *Angew. Chem. Int. Ed.* **2011**, *50*, 8858–8862. <https://doi.org/10.1002/anie.201101957>.
78. Zheng, B.; Liang, Z.; Li, G.; Huo, Q.; Liu, Y. Synthesis, Structure, and Gas Sorption Studies of a Three-Dimensional Metal–Organic Framework with NbO Topology. *Cryst. Growth Des.* **2010**, *10*, 3405–3409. <https://doi.org/10.1021/cg100046j>.
79. Furukawa, H.; Miller, M.A.; Yaghi, O.M. Independent verification of the saturation hydrogen uptake in MOF-177 and establishment of a benchmark for hydrogen adsorption in metal–organic frameworks. *J. Mater. Chem.* **2007**, *17*, 3197. <https://doi.org/10.1039/b703608f>.
80. Kaye, S.S.; Dailly, A.; Yaghi, O.M.; Long, J.R. Impact of Preparation and Handling on the Hydrogen Storage Properties of Zn₄O(1,4-benzenedicarboxylate)₃ (MOF-5). *J. Am. Chem. Soc.* **2007**, *129*, 14176–14177. <https://doi.org/10.1021/ja076877g>.
81. Ng, M.S.; Wang, G.; Chakraborty, A.; Saha, B.B. Highly efficient hydrogen storage on porous materials under cryo-adsorption conditions. *Next Energy* **2025**, *9*, 100382. <https://doi.org/10.1016/j.nxener.2025.100382>.
82. Murugavel, R.; Rownaghi, A.A.; Rezaei, F. Improving hydrogen storage performance of UiO-67 and MOF-177 under temperature-pressure swing conditions via densification. *Int. J. Hydrogen Energy* **2025**, *127*, 362–373. <https://doi.org/10.1016/j.ijhydene.2025.01.325>.
83. Kim, H.; So, S.H.; Muhammad, R.; Oh, H. Comparing the practical hydrogen storage capacity of porous adsorbents: Activated carbon and metal-organic framework. *Int. J. Hydrogen Energy* **2024**, *50*, 1616–1625. <https://doi.org/10.1016/j.ijhydene.2023.10.160>.
84. Mirzaei, S.; LotfiKatoili, L.; Ahmadpour, A.; Niknam Shahrak, M.; Haghbin, M.R.; Arami-Niya, A. Enhancing energy carrier gas storage: Novel MOF-decorated carbons with high affinity toward methane and hydrogen. *Chem. Eng. Res. Des.* **2024**, *203*, 419–430. <https://doi.org/10.1016/j.cherd.2024.01.049>.
85. Garg, A.; Alması, M.; Bednarčík, J.; Sharma, R.; Rao, V.S.; Panchal, P.; Jain, A.; Sharma, A. Gd(III) metal-organic framework as an effective humidity sensor and its hydrogen adsorption properties. *Chemosphere* **2022**, *305*, 135467. <https://doi.org/10.1016/j.chemosphere.2022.135467>.
86. Salehi, K.; Rahmani, M.; Atashrouz, S. Machine learning assisted predictions for hydrogen storage in metal-organic frameworks. *Int. J. Hydrogen Energy* **2023**, *48*, 33260–33275. <https://doi.org/10.1016/j.ijhydene.2023.04.338>.
87. Rowsell, J.L.C.; Yaghi, O.M. Strategies for Hydrogen Storage in Metal–Organic Frameworks. *Angew. Chem. Int. Ed.* **2005**, *44*, 4670–4679. <https://doi.org/10.1002/anie.200462786>.
88. Aftabi, N.; Moradi, N.; Mahroo, F. Feed-Forward Neural Networks as a Mixed-Integer Program. 9 February 2024. Available online: <http://arxiv.org/abs/2402.06697> (accessed on September 2025).
89. Andersen, T.; Martinez, T. Cross validation and MLP architecture selection. In *Proceedings of the IJCNN'99. International Joint Conference on Neural Networks. Proceedings (Cat. No.99CH36339)*; IEEE: Piscataway, NJ, USA, 2003; pp. 1614–1619. <https://doi.org/10.1109/IJCNN.1999.832613>. Available online: <http://ieeexplore.ieee.org/document/832613/> (accessed on November 2025).
90. Alwosheel, A.; van Cranenburgh, S.; Chorus, C.G. Is your dataset big enough? Sample size requirements when using artificial neural networks for discrete choice analysis. *J. Choice Model.* **2018**, *28*, 167–182. <https://doi.org/10.1016/j.jocm.2018.07.002>.
91. Meduri, S.; Nandanavanam, J. Prediction of hydrogen uptake of metal organic frameworks using explainable machine learning. *Energy AI* **2023**, *12*, 100230. <https://doi.org/10.1016/j.egyai.2023.100230>.

92. Liashchynskiy, P.; Liashchynskiy, P. Grid Search, Random Search, Genetic Algorithm: A Big Comparison for NAS. 12 December 2019. Available online: <http://arxiv.org/abs/1912.06059> (accessed on November 2025).
93. Akiba, T.; Sano, S.; Yanase, T.; Ohta, T.; Koyama, M. Optuna: A Next-Generation Hyperparameter Optimization Framework. 25 July 2019. Available online: <http://arxiv.org/abs/1907.10902> (accessed on November 2025).
94. Specht, D.F. Probabilistic neural networks and general regression neural networks. In *Fuzzy Logic and Neural Network Handbook*; McGraw-Hill: Sydney, Australia, 1996; pp. 301–344.
95. Rasmussen, C.E.; Williams, C.K.I. *Gaussian Processes for Machine Learning*; The MIT Press: Cambridge, MA, USA, 2005; 248p. <https://doi.org/10.7551/mitpress/3206.001.0001>. Available online: <https://direct.mit.edu/books/book/2320/Gaussian-Processes-for-Machine-Learning> (accessed on November 2025).
96. Williams, C.K.I.; Rasmussen, C.E. Gaussian Processes for Regression. In *Advances in Neural Information Processing Systems 8* eds. D. S. Touretzky, M. C. Mozer, M. E. Hasselmo, MIT Press, 1996.
97. Chen, T.; Guestrin, C. XGBoost: A scalable tree boosting system. In *Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*; Association for Computing Machinery: New York, NY, USA, 2016; pp. 785–794. <https://doi.org/10.1145/2939672.2939785>.
98. Drucker, H.; Burges, C.J.C.; Kaufman, L.; Smola, A.; Vapnik, V. Support Vector Regression Machines. *Adv. Neural Inf. Process Syst.* **1997**, *28*, 779–784.
99. Laake, P.; Fagerland, M.W. Statistical Inference. In *Research in Medical and Biological Sciences: From Planning and Preparation to Grant Application and Publication*; Elsevier Ltd.: Amsterdam, The Netherlands, 2015; pp. 379–430. <https://doi.org/10.1016/B978-0-12-799943-2.00011-2>.
100. Makke, N.; Chawla, S. Interpretable Scientific Discovery with Symbolic Regression: A Review. *Artif. Intell. Rev.* **2024**, *57*, 2. <https://doi.org/10.1007/s10462-023-10622-0>.
101. Cranmer, M.D. *Interpretable Machine Learning for the Physical Sciences*; Princeton University: Princeton, NJ, USA, 2003.
102. PySR. PySR|Operators. Available online: <https://astroautomata.com/PySR/v1.5.9/operators> (accessed on September 2025).
103. Lundberg, S.; Lee, S.I. A Unified Approach to Interpreting Model Predictions. 25 November 2017. Available online: <http://arxiv.org/abs/1705.07874> (accessed on September 2025).
104. Kroeger, N.M.; Bindschaedler, V. Cluster Paths: Navigating Interpretability in Neural Networks. 8 October 2025. Available online: <http://arxiv.org/abs/2510.06541> (accessed on November 2025).
105. Montgomery, R.M. Overview of Clustering Techniques: From k-Means to Spectral Methods. 2024. Available online: <https://www.preprints.org/manuscript/202410.1397/v1> (accessed on November 2025).
106. scikit. Selecting the Number of Clusters with Silhouette Analysis on Kmeans Clustering. Available online: https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html (accessed on November 2025).
107. Rudin, C.; Chen, C.; Chen, Z.; Huang, H.; Semenova, L.; Zhong, C. Interpretable Machine Learning: Fundamental Principles and 10 Grand Challenges. 10 July 2021. Available online: <http://arxiv.org/abs/2103.11251> (accessed on September 2025).
108. Ali, S.; Abuhmed, T.; El-Sappagh, S.; Muhammad, K.; Alonso-Moral, J.M.; Confalonieri, R.; Guidotti, R.; Del Ser, J.; Díaz-Rodríguez, N.; Herrera, F. Explainable Artificial Intelligence (XAI): What we know and what is left to attain Trustworthy Artificial Intelligence. *Inf. Fusion* **2023**, *99*, 101805. <https://doi.org/10.1016/j.inffus.2023.101805>.

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