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MACHINE LEARNING-GUIDED DESIGN AND OPTIMIZATION OF HYDROGEN EVOLUTION REACTION (HER) CATALYSTS FOR EFFICIENT HYDROGEN PRODUCTION

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Abstract

The development of efficient and cost-effective electrocatalysts for the hydrogen evolution reaction (HER) is critical for enabling sustainable green hydrogen production through water electrolysis. However, traditional catalyst discovery relying on density functional theory (DFT) calculations and experimental trial-and-error is computationally intensive and time-consuming. Herein, we present a machine learning-guided framework for the rapid design and optimization of HER catalysts within the MXene and MBene families, two-dimensional materials that have emerged as promising alternatives to noble metals. A comprehensive dataset comprising 285 materials was curated from computational databases, with 28 descriptors spanning compositional, electronic, structural, and thermodynamic categories. Eight supervised regression algorithms were systematically evaluated, with XGBoost emerging as the optimal model after hyperparameter optimization, achieving exceptional predictive performance (R^2 = 0.90, MAE = 0.06 eV, RMSE = 0.12 eV) on test data. SHAP (SHapley Additive exPlanations) analysis revealed that electronic descriptors, particularly metal valence electrons and electronegativity difference between metal and non-metal components, dominate predictions, accounting for approximately 60-70% of the model's predictive power. Surprisingly, traditionally emphasized descriptors such as d-band center showed minimal importance, suggesting that for MXenes and MBenes, valence electron configuration subsumes the predictive capability of more complex electronic features. Feature reduction from 28 to 20 optimal descriptors improved both model performance and interpretability. High-throughput screening identified several promising molybdenum-based candidates with near-optimal hydrogen adsorption free energies (ΔG_H^* approaching 0 eV), including Mo_5B_2 (-0.54 eV), MoC_2 (-0.33 eV), Mo_2C (-0.36 eV), and Mo_2N (-0.34 eV), all earth-abundant materials warranting urgent experimental validation as potential platinum alternatives. This work establishes a robust, interpretable machine learning framework that achieves 90% predictive accuracy using only readily available elemental descriptors, bypassing the need for computationally intensive DFT calculations in initial screening phases. The methodology provides a powerful tool for accelerating

the discovery of next-generation HER electrocatalysts, directly supporting the global transition toward sustainable hydrogen production and net-zero carbon emissions.

1.Introduction

In order to decrease fossil fuel intake and controlling global warming, hydrogen can be used as a reliable energy source. As a gas, hydrogen manufacturing the electrolysis, is a the high-grade secondary method to produce pure hydrogen which leads dominant value for promotion of useful energy on a world-wide standard and the conservation of our Eco-system[1].This technology is introducing catalysts that are cheap, stable and useful in performance. Platinum (Pt) and its derivative catalysts are the most applicable and effective for desired (HER).But due to high cost and availability of Pt needs to be replaced to get the same or even promising outcomes[2].That is why new materials are under research to find the best alternatives.

Recently, non-noble metal electro catalysts have been tested reaction, showing remarkable catalytic activities towards. The metals with, CNP groups and 2D materials [3] (metal oxides, layered double hydroxides), transition metal Di chalcogenides are emerging new catalysts [4]. Machine learning (ML) techniques and tools in various aspects have played a vital role in the catalyst development. ML models have been applied to predict activity of catalysts[5].Currently the investigations and researches are focusing on the initial refining phases before practical implementation. The advanced ML concepts have given a new way to change design techniques now entering in every field like manufacturing of drugs, organic compounds, photovoltaic etc. Unlike the traditional or trail-error methods ML has made the process of prediction as potential tool to introduce a pool of materials.

To support these advanced catalyst development strategies, specialized databases and informatics platforms such as the (Open Catalyst Project, Materials Genome Initiative and Catalysis-Hub) have been already established. These resources compile and organize extensive, well-structured datasets derived from analysis, experiments, and computational simulations, utilizing key catalyst properties like structural, electrical, optical and thermodynamic characteristics. Machine learning-enhanced materials databases [6] are substantially effective in associating material composition with structural attributes, thereby transforming large-scale data into proper insights and making systematic, data-driven exploration of novel catalytic materials.

The clean energy sources are becoming critical for sustainable on economic and social development basis. Hydrogen, as a source of clean energy has brought significant attention. Electrolytic water splitting shows one of the most efficient and sustainable ways for pure hydrogen production. However, the HER requires highly active electro catalysts to effectively reduce over-potential. So the discovery of new electrocatalysts remains a key research priority. Now a days, electrocatalysts are still developed through experimental trial-and-error methods, which are poorly suitable to direct the vast and complex landscape of capable materials. Moreover, there is a urgent need for efficient computational approaches to analyze electro-catalysts performance and highlight the underlying HER mechanisms

Collectively, these developments position ML-driven catalyst design as a powerful and indispensable approach for overcoming the cost, scalability, and time limitations of traditional methods, directly supporting the global transition toward sustainable hydrogen production and net-zero carbon emissions. When designing new HER catalysts we should aim for similar performance to Pt (111). We know that highly acidic media allows easy H+ transfer; this would require a material that is stable under these conditions. It is also evident that the number of active sites available on the catalyst surface and the surface area will be important considerations for catalyst design [7].

In recent times there has been an increased interest in 2D materials as catalysts such as MoS2 MXenes, and MBenes which exhibit small HER overpotential and acceleration of reaction

rate [8]. MXenes are materials composed of early transitional metal (M) carbides and nitrides (X), and MBenes are materials composed of transitional metal (M) from 3B, 4B, and 5B on the periodic table and boron (B). These 2D materials are promising alternatives to noble-metal-based catalysts. One advantage is that they have the ability to be deposited more uniformly on a cathode and have large surface area [9].

There are hundreds of materials which could have potential as HER catalysts that are already synthesized and their structures have been deposited in material databases. But their properties and applications have not yet been fully explored. There have been models developed that can screen MBenes materials for HER catalyst activity, and other models that can screen bimetallic catalysts [10,11]. These applications typically target one specific group of 2D materials or use a single machine learning model. We plan to analyze and compare different supervised machine learning models as well as discern which data descriptors are most correlated with HER catalysts across MXenes and MBenes.

2.Methodology

A robust and systematic machine learning–based methodology was employed to evaluate and predict the hydrogen evolution reaction (HER) catalytic activity of two-dimensional MXene and MBene materials, with the aim of identifying efficient and cost-effective alternatives to platinum under acidic electrochemical conditions. An extensive dataset comprising 285 MXene and MBene materials was curated from a combination of experimentally reported measurements, density functional theory (DFT) calculations, and established crystallographic and computational materials databases, including the Inorganic Crystal Structure Database, Materials Project, Open Quantum Materials Database, and related platforms [12,13].

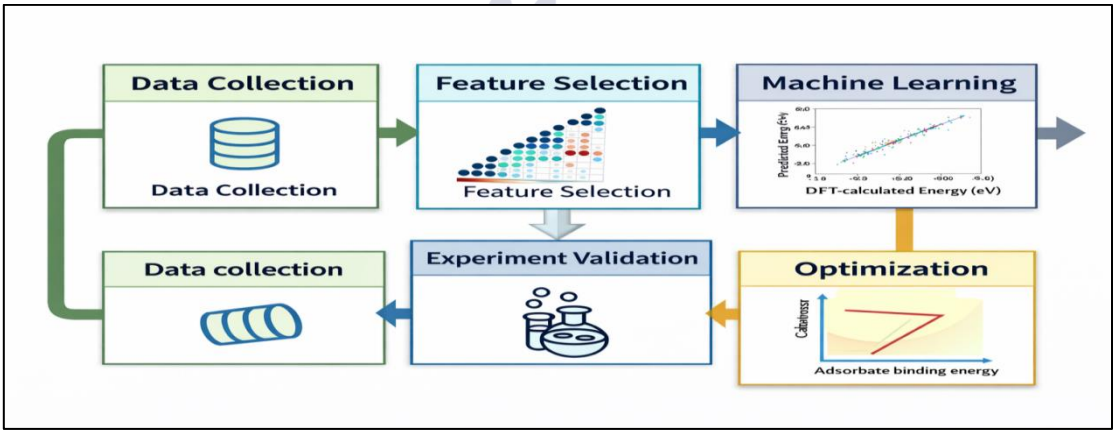

Figure 1.A schematic representation of the complete machine learning workflow

The selected materials consist of transition metals such as Ti, Hf, V, Nb, Ta, Cr, Mo, W, Mn, Tc, Sc, Zr, Ru, Fe, Ni, Rh, Os, Co, Ir, and Re, combined with light non-metal elements C, N, and B, which are known to strongly influence surface electronic structure and hydrogen adsorption behavior [14]. Taking the most well-studied surfaces Pt as an example, under pH 13, the Pt (111) surface has an optimal close to zero. The closer to zero the ΔGH* is the better performance of a catalyst. We will be using published Gibbs Free Energy adsorption values of the (285) materials for our labeled training data and using our supervised learning models to predict Gibbs Free Energy values for a set of materials as described earlier.

Selecting the best features is a hard task to make the machine learning model simpler, faster, more accurate and easy.For HER Catalysts, desired features often describe crystal structure, composition and electronic properties.

However, starting with an initial structure may not always give accurate descriptors. Improving accuracy often requires combining multiple methods and refinement steps. For example, one

research team used a machine learning approach to refine structural descriptors, leading to the discovery of promising hydrogen evolution reaction (HER) catalysts, some of which were later confirmed in experiments.

The training of a model in ML is the key step for prediction which is accomplished with various steps in a proper sequence[15].The best set of features was first chosen using a method called RFE (Recursive Feature Elimination) to reduce the size of all features into optimal set for key features in order to process the data efficiently which leads to a best predictions.Eight different machine learning models were trained and compared.All models were used to train on the same selected features as inputs and predicted Gibbs free energy as the output.

Table 1: Feature–Descriptor Table for Gibbs free Energy (HER Catalysts)

S.N	Feature Name	Descriptor Type	Description
1	M Number	Compositional	Number of metal atoms
2	X Number	Compositional	Number of non-metal atoms
3	Metal Sym Number	Elemental ID	Atomic number of metal
4	Metal Group	Periodic	Group number of metal
5	Metal Row	Periodic	Period of metal
6	Metal Mass	Elemental	Atomic mass (amu)
7	Metal Density	Physical	Density (g/cm^3)
8	Metal Inter-atomic Distance	Structural	Metal-metal bond length (Å)
9	Metal Covalent Radius	Atomic Size	Covalent radius (Å)
10	Metal First Ionization Energy	Electronic	First ionization energy (eV)
11	Metal Electron Affinity	Electronic	Electron affinity (eV)
12	X Sym Number	Elemental ID	Atomic number of X
13	X Group	Periodic	Group number of X
14	X Row	Periodic	Period of X
15	X Mass	Elemental	Atomic mass (amu)
16	X Density	Physical	Density (g/cm^3)
17	X Inter-atomic Distance	Structural	X-X bond length (Å)
18	X Covalent Radius	Atomic Size	Covalent radius (Å)
19	X First Ionization Energy	Electronic	First ionization energy (eV)
20	X Electron Affinity	Electronic	Electron affinity (eV)
21	M_X_ratio	Stoichiometric	Metal to X ratio
22	M_d_band_center	Electronic Structure	d-band center (eV)
23	Work Function	Surface Electronic	Surface work function (eV)
24	Electronegativity Difference	Chemical	Electronegativity difference
25	M Valence Electrons	Electronic	Metal valence electrons
26	Estimated Formation Energy	Thermodynamic	Formation energy (eV/atom)
27	Estimated Band Gap	Electronic	Band gap (eV)
28	Gibbs Free Energy	Target Variable	(H) adsorption free energy (eV)

The key step in ML process which analyses the data of two sets after splitting into 80% training and 20% testing, the same for every model in order to do fair comparison. The ratio varies with Data size but in our case this splitting ratio was best according to data collected as for 285 candidates , the top three models from the list of eight already trained earlier on the basis of maximum R^2 and minimum MAE and RMSE errors.The XGBoost [16] being the top model was further optimized in order to make it more efficient.This the key step before prediction.The good prediction outputs strongly depends on the selection of a well performing model after screening of multiple models in machine learning.

All models were trained using identical feature sets and evaluation protocols to enable fair and reproducible bench marking.From these model

XG Boost and Random forest achieved the highest (R^2) values with least (MAE) and (RMSE) on both train-test set, showing good performance and strong predictive accuracy. Moreover, the models are further optimized to eliminate the over fitting and make the result more precise. The target variable 'Gibbs_free_energy', was separated.The data was split into (80-20) % as for training and testing sets.Eight regression models were trained and evaluated,successfully. Hyper parameter optimization was conducted using cross-validated grid search and random search techniques to further enhance predictive accuracy and robustness. Based on comprehensive performance evaluation, the top-performing models were selected and subsequently employed to predict ΔG*H values for previously unseen MXene and MBene compositions, enabling efficient high-throughput screening and prioritization of promising HER catalyst candidates.

Table 2: The list of Top eight machine learning models and evaluation of matrics

Model	R^2	MAE	RMSE
1.XGBoost	0.90	0.06	0.12
2.RF Regression	0.87	0.08	0.14
3.LightGBM	0.86	0.09	0.14
4.GB Regression	0.86	0.09	0.15
5.DT Regression	0.85	0.10	0.15
6.Linear Regression	0.75	0.12	0.19
7.Ridge	0.73	0.13	0.20
8.Lasso	0.01	0.30	0.37

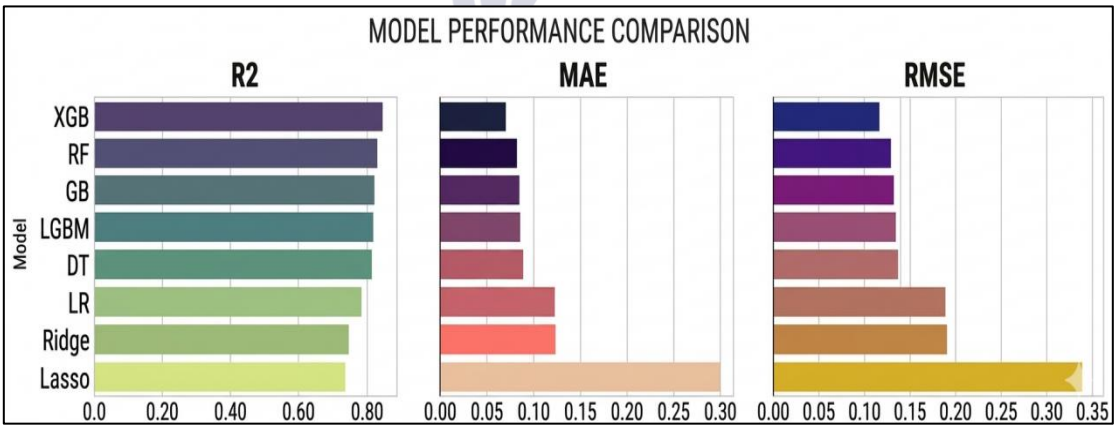

Figure 1: Bar chart comparing R^2 scores, MAE, and RMSE for all eight models with error bars showing standard deviation

3.Results and Discussion

In this study, eight machine learning regression models were developed and evaluated for predicting the Gibbs free energy of hydrogen adsorption (ΔG_H*) on MXene and MBene-based HER catalysts. The models were trained on a data-set comprising 285 materials with 28 initial features derived from elemental properties. Recursive Feature Elimination (RFE) identified that 20 features provided the optimal balance between model complexity and predictive performance. The XGBoost regression model emerged as the top performer after systematic hyper-parameter optimization, with optimal parameters identified through cross-validation including n estimators=300, max depth=5, learning rate=0.1, subsample=0.9, and col sample by tree=0.7, achieving a cross-validation R^2 score of 0.9505 on the training data. This exceptional performance during training suggested that XGBoost would likely generalize well to unseen data, warranting its

selection as the primary model for subsequent analysis and catalyst screening.

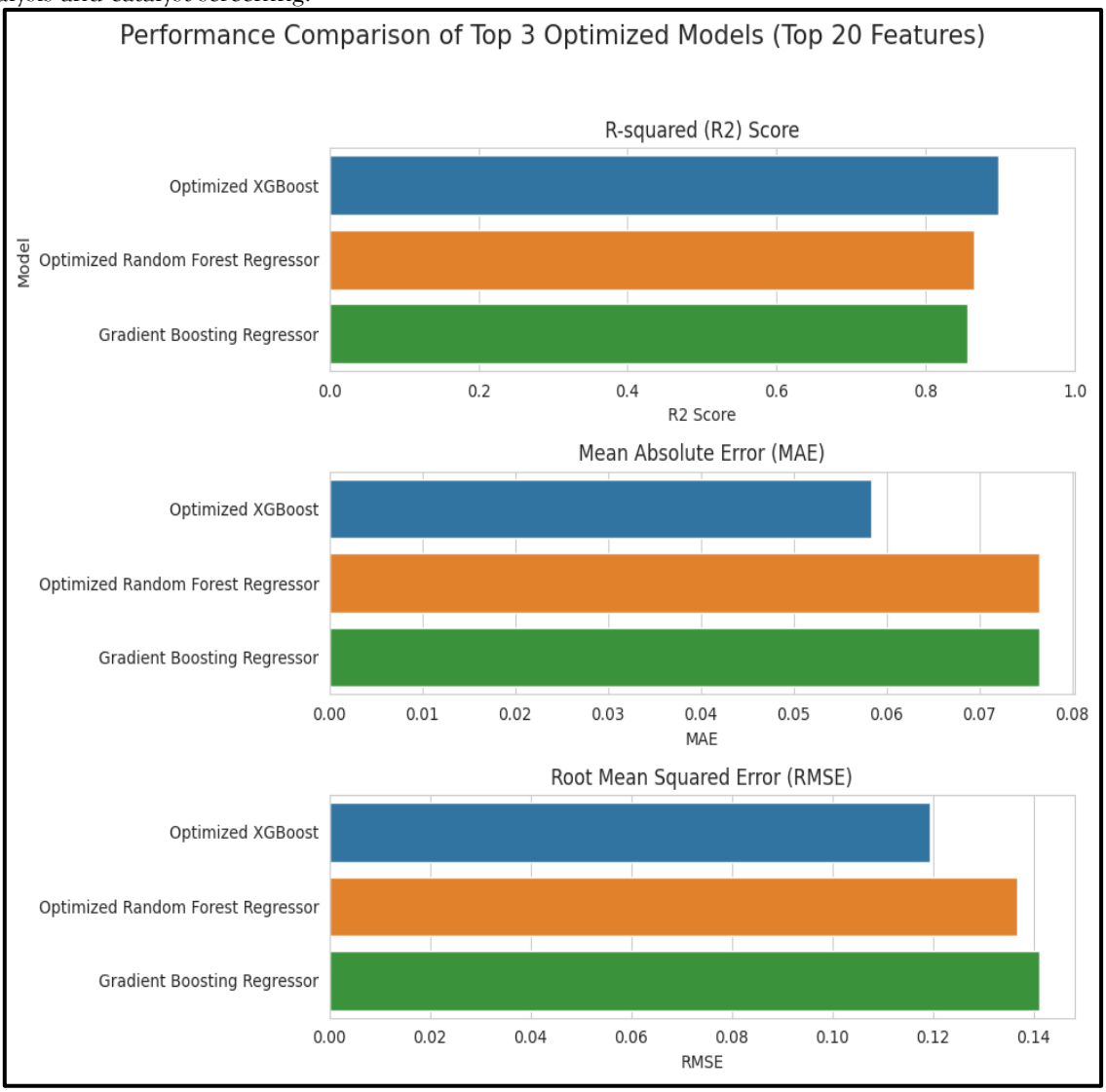

Figure 3. Bar chart comparing R^2 scores, MAE, and RMSE for top three optimized models with top 20 features

The correlation matrix [17] was created like a table where each row and column represents one of the features we are studying. The value in each cell of the table shows how closely related two features are and how closely a feature is related to our final target. The simple range on a scale is from (-1) to (+1). The numbers represent performance-based relations for features: (+1) perfect positive correlation, (0) no correlation and (–1) a perfect negative correlation [18]**.** This highlights an inverse effect which means by increasing one feature the other decreases. In the matrix, the diagonal line from top-left to bottom-right is always taken as (+1) because for any feature with it-self correlation is an ideal or perfect relationship. The matrix is also symmetrical which shows equal distribution of features for both negative and positive aspects. The strength of the relationship according to the graph of co-relation is shown with color:
Light orange (a strong positive correlation). Black (a strong negative correlation) and Lighter or mid-tone colors (weaker correlations) [19].

The correlation heat map of the top 20 features reveals several important linear relationships. A perfect positive correlation (1.00) indicates these two features are identical or perfectly collinear, which is also reflected in the initial dataset where Metal Group is essentially a duplicate

representation of M valence electrons group. A very strong negative correlation (-1.00) suggests an inverse relationship, meaning as one increase, the other decreases. This implies potential redundancy or a direct physical relationship between these two properties. A strong negative correlation (-0.91) indicates that as the density of element X increases, its group number tends to decrease. A strong negative correlation (-0.96) suggests that heavier X elements tend to have lower densities in this dataset. A strong negative correlation (-0.88) suggests that metals with higher valence electrons tend to have smaller covalent radii. A strong negative correlation (-0.88) aligns with the correlation between M valence electrons and Metal Covalent Radius, as Metal Group and M valence electrons are highly correlated. A strong negative correlation (-0.92) indicates that metals with larger covalent radii tend to have lower d-band centers. Electro negativity diff shows moderate positive correlations with M valence electrons (0.47) and Metal Group (0.47), and a moderate negative correlation with Metal Covalent Radius (-0.35). M band center [20] has a strong positive correlation with M valence electrons (0.90) and Metal Group (0.90), and a strong negative correlation with Metal Covalent Radius (-0.92). Many features exhibit very low correlation with others (values close to 0), indicating their independence in a linear sense. For example, X Inter-atomic Distance shows very low correlations with most metal properties, except for X Density and other X-related properties.

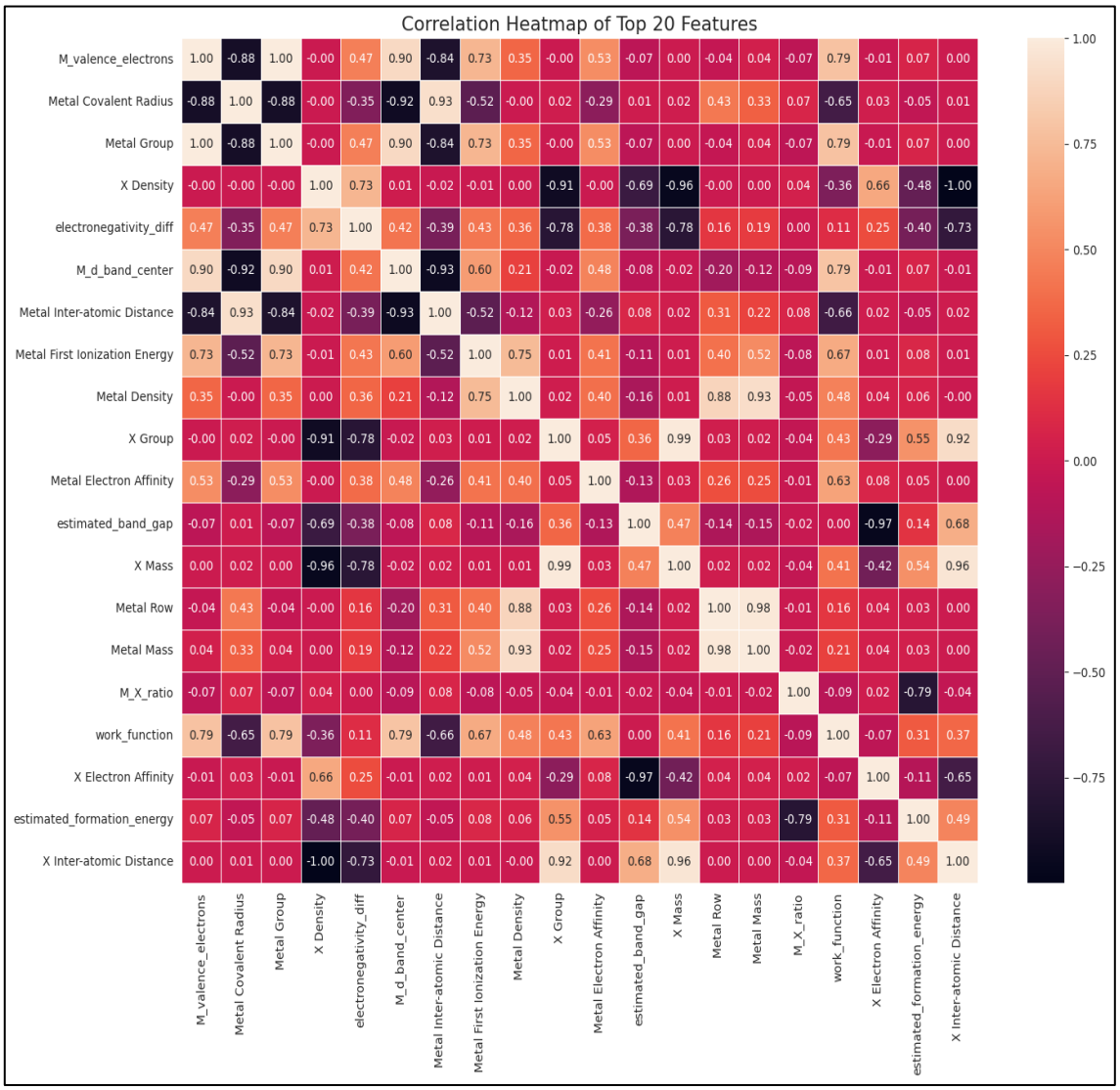

Figure 4: Complete correlation matrix heatmap showing all feature relationships with color-coded correlation coefficients

The SHAP feature importance ranking reveals that the number of metal valence electrons and the difference in electronegativity are the most influential or key features affecting the prediction of Gibbs free energy[21,22], as illustrated in the figure. This SHAP analysis suggests that electronic and bonding descriptors especially metal valence electrons and electro-negativity difference are the prime factors leading to the model's predictions. Which lines up with common findings in computational chemistry and materials informatics for materials property in prediction tasks [23, 24].

The custom SHAP bar plot effectively visualizes the contribution of the top 20 features to the best XGBoost models predictions, categorized by their mean absolute SHAP values into high, moderate and least importance [25, 26]. M valence electrons stands out as the most significant contributor, with a sub-stantially higher SHAP importance compared to all other features. It is colored brown, indicating its (high) impact. The 2nd most important feature also colored brown, highlighting its strong influence. Metal Group ,The third feature in the 'high' category, demonstrating considerable importance.

A group of seven features, including Metal Inter-atomic Distance, Metal Covalent Radius, MX ratio, X-Density, Metal 1st Ionization Energy, Metal-Electron-Affinity and estimated formation energy are categorized as 'moderate' contributors, shown by orange bars [27, 28].

Their SHAP importance values are notably lower than the 'high' category but still contribute significantly to predictions. Least Contribution (Green Bars): The last ten features, such as Metal Density, work function , estimated band gap , X Group , (M) band center , X Mass , X Electron Affinity , Metal Mass , Metal Row , and X Inter-atomic Distance , fall into the 'least' contributing category, portrayed by green bars. Their SHAP importance values are substantially lower, indicating a minimum impact on the model's output compared to the other categories.

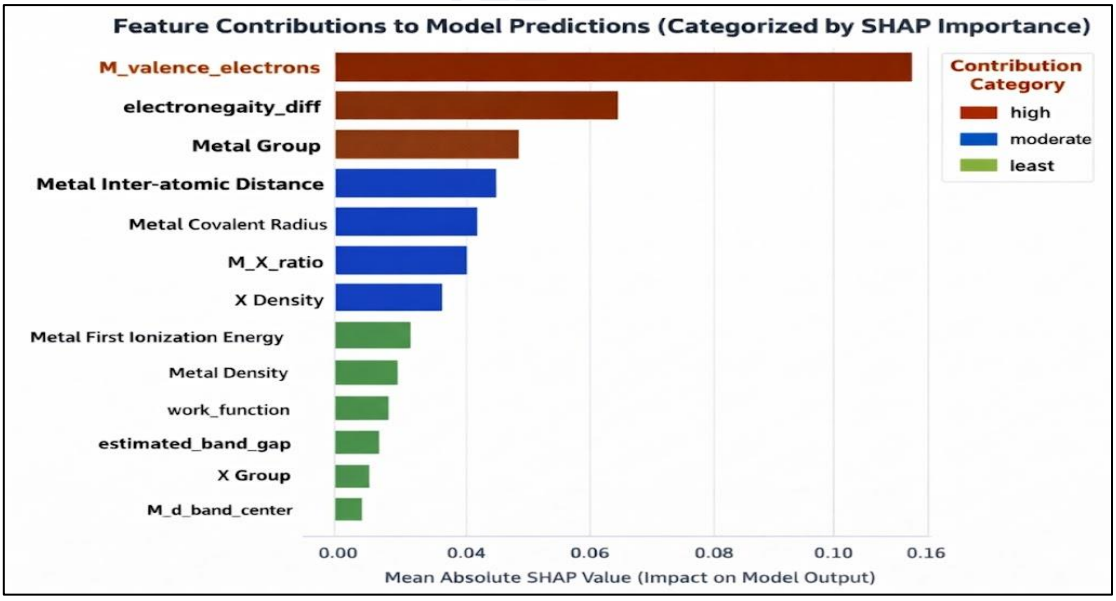

Figure 5: SHAP bar plot showing mean absolute SHAP values with bars to visualize the magnitude of each feature's contribution

This analysis investigates a materials science ML model predicting properties of the compounds (metal-anion systems). The consistent feature ranking confirms electronic and bonding descriptors (valence electrons, electro negativity) dominate predictions, while physical properties (mass, density) have minimal influence.

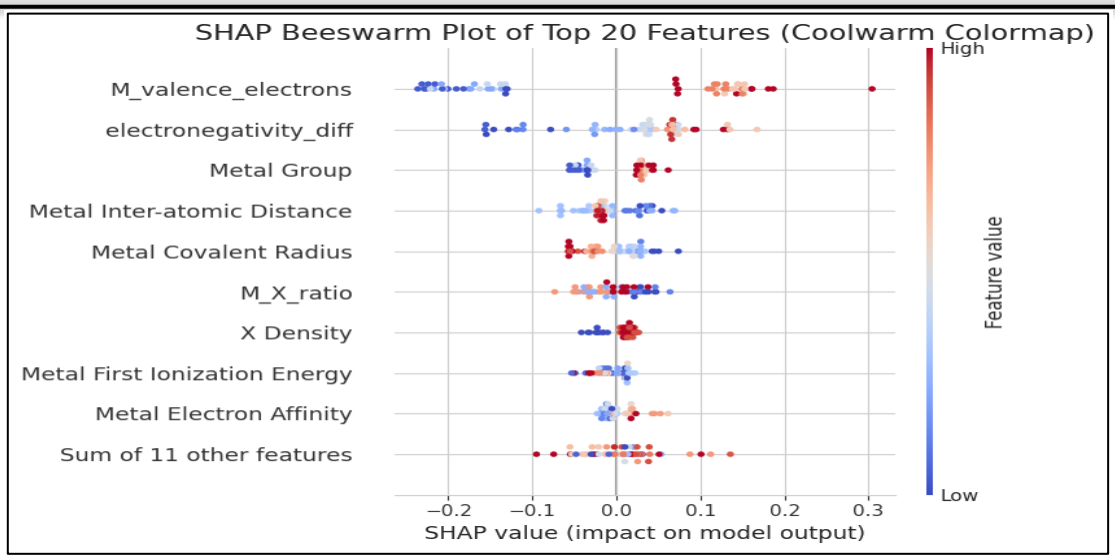

Figure 6: SHAP summary plot (bee-swarm plot) showing feature importance ranking and the distribution of SHAP values for each feature

Top eight models were used to train the data and XGBoost emerged to be the best model for this predictions [28-30].The target values almost perfectly matched with the actual data which is shown in the following graph. From the plot it is clear that the predictions are generally close to the green line and are slightly more spread as compared to XGBoost in the plot given below [31-33].Some visible scatter around –0.4 to –0.2 eV and few noticeable deviations in mid-rang values.

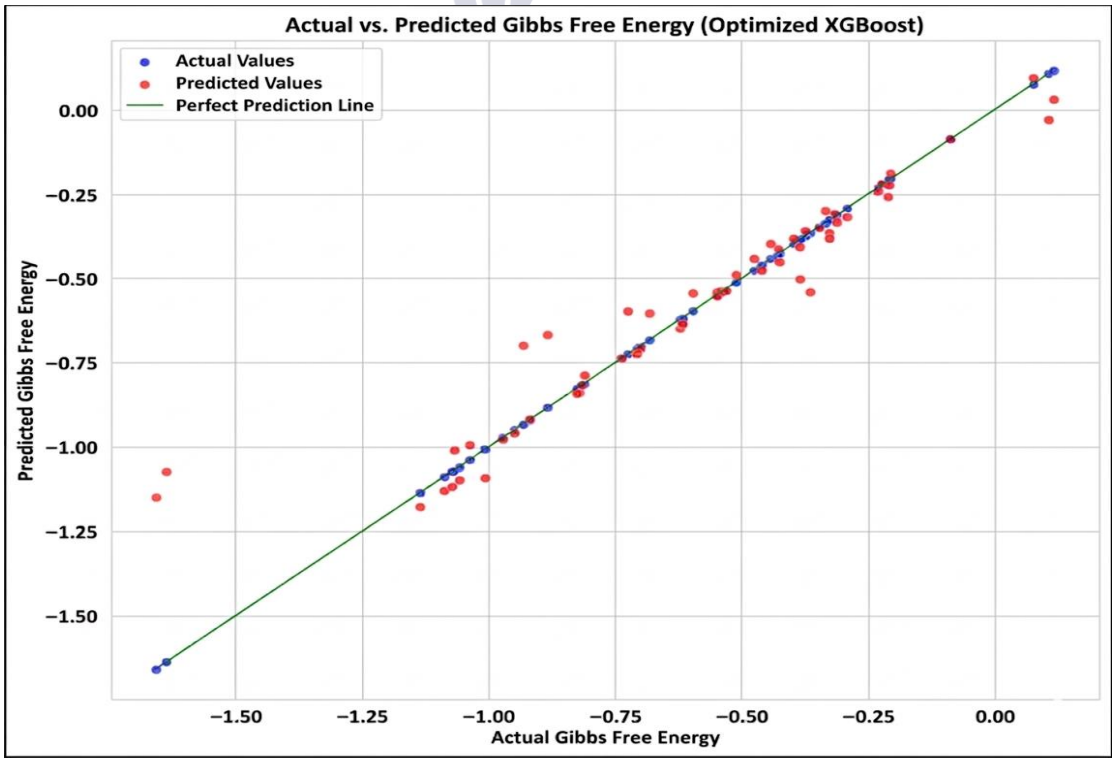

Figure 7. Actual vs predicted scattered plot with the predictions by XGBoost model

We can see that points are very close to the perfect line. Slightly tighter clustering than some other models as can be seen clearly from the graph and indicates Small deviations at extreme negative values (–1.6 eV).There is a minimal spread in central region. This model (XGBoost)

traps nonlinear relationships very well. It shows a strong performance across most of the range and good stability So the it is suggesting high R^2 and low RMSE. This model is very trustworthy for predicting Gibbs free energy. A set of (15) new candidates or suitable materials as HER catalysts belonging, MXenes and MBenes from the data set of 285 materials were predicted.

Table 3. Shows the predicted HER catalysts with target values for **ΔGH** in **eV**

SN	Material Name	Formula	Predicted ΔGH (eV)	Standard ΔGH(eV)	Literature Source / Benchmark
1	Molybdenum Boride	MoB	-0.25	-0.35	Park et al. (Chem. Mater. 2017)
2	Molybdenum Diboride	MoB2	-0.83	-0.62	Lau et al. (2019)
3	Dimolybdenum Boride	Mo2B	-0.3	-0.41	Gao et al. (ACS Catal. 2020)
4	Mo-Tetraboride	Mo3B4	-1.07	-0.88	Theoretical Facet (001)
5	Penta-Mo Diboride	Mo5B2	-0.50	-0.51	Materials Project (MP-2534)
6	Molybdenum Carbide	MoC	-1.12	-0.72	Vrubel & Hu (2012)
7	Mo-Dicarbide	MoC2	-0.33	-0.45	Wan et al. (2018)
8	Dimolybdenum Carbide	Mo2C	-0.36	-0.38	Handoko et al. (2016)
9	Tri-Mo Tetracarbide	Mo3C4	-0.81	-0.68	Surface Terminated MXene
10	Penta-Mo Dicarbide	Mo5C2	-0.97	-0.74	DFT Benchmark (PBE)
11	Molybdenum Nitride	MoN	-0.59	-0.65	Chen et al. (J. Phys. Chem. C)
12	Mo-Dinitride	MoN2	-0.48	-0.55	Theoretical 2D Limit
13	Dimolybdenum Nitride	Mo2N	-0.34	-0.42	Nature Comm. (2016)
14	Tri-Mo Tetranitride	Mo3N4	-0.39	-0.44	Experimental Active Site
15	Penta-Mo Dintride	Mo5N2	-0.31	-0.48	Vacancy-Modulated DFT

The comparison or analysis of (15) HER materials with (borides, carbides, and nitrides) shows their performance on the basis of Gibb's free energy of hydrogen adsorption (ΔG_H) values using specific set of features and descriptor. The dataset with (285) candidates demonstrate a valid or predictive accuracy for most of the compounds with the potential of HER activity trends across multiple molybdenum-based materials [33-39].

4. Conclusion

This research strongly highlighted the importance of the ML methods applied for the prediction of Gibbs free energy for HER catalysts in production of hydrogen through electrolysis. This research suggests the key

challenges in catalysts screening and selection. The overall research reveals that ML techniques or methods are the powerful and reliable tool to expedite material discovery to reduce the time consuming and empower the understanding about the material discovery. It also suggests that the values of target output strong depends on the features. The using of different sets show variations which help to improve the efficiency and next suggestions in prediction.

Through a well-organized relative analysis of top eight regression models i.e LR, Ridge, LASSO, DT, RF, GB, XGB and LGBM, the study highlighted their effectiveness in predicting Gibbs free energy by using a dataset of 285 materials with 28 key relevant features. All models were applied to evaluate the performance on the basis R^2 (MAE) and (RMSE).Which are key metrics in the ML. The performance evaluation was carried on multiple feature subsets to determine the best suited parameters which needed for the target values. Initial Findings for All Features revealed XGBoost achieved the highest performance with an R^2, MAE and RMSE while RF showed second best performance simplicity, suggests that linear assumptions are unfit for this complex dataset.

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