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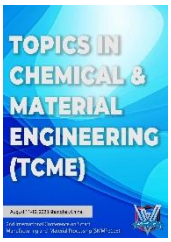

RESEARCH ARTICLE

EXPERIMENTAL STUDY ON THE APPLICATION OF MACHINE LEARNING METHOD IN CATALYTIC MATERIALS

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ABSTRACT

Machine learning has emerged as a powerful tool for analyzing complex data sets and making predictions in a wide range of applications, including catalysis. Bycombining statistical methods, algorithms, and computational power, machine learning can help identify patterns and relationships in catalytic systems that are difficult or impossible to discern using traditional approaches. This can lead to more efficient and effective catalyst design, optimization, and prediction of catalytic activity. Machine learning has already been successfully applied to various aspects of catalysis, including catalyst discovery, reaction mechanism identification, and kinetic modeling. The continued integration of machine learning with catalysis research holds great promise for advancing our understanding of catalytic systems and developing new and improved catalysts for important industrial processes.

KEYWORDS

Machine Learning, catalytic materials, chemistry, efficiency, catalytic.

1. INTRODUCTION

The background of catalytic materials can be traced back to ancient times when people started using catalytic materials in the production of pottery. However, the understanding of catalytic reactions did not begin to develop until the 18th century. At that time, it was discovered that some chemical reactions required high temperatures to occur, but under certain conditions, these reactions could occur at lower temperatures, which is the basic concept of catalytic reactions. Catalytic materials are substances that can promote chemical reactions, accelerate reaction rates, improve efficiency and yield, and reduce energy requirements and costs. Catalytic materials are widely used in fields such as chemistry, medicine, energy, and others, such as automotive emission control, chemical production, pharmaceuticals biotechnology, batteries, and fuel cells. Machine learning is a branch of artificial intelligence aimed at allowing computer systems to automatically learn and improve task performance without explicit programming (Mitchel, 2007; Zhou, 2021; Jordan and Mitchell, 2015). The history of machine learning dates back to the 195os and 196os, when computer scientists began using algorithms and statistical methods to enable computer systems to automatically learn patterns and rules from data (Mahesh, 2020; Carleo, 2020). However, the application of machine learning was severely limited by hardware and algorithm capabilities at that time. It wasn't until the 198os that machine learning began to gain wider usage with the development of computer hardware and algorithms. With the explosive growth of data, machine learning has become increasingly important in the 21st century. The development of big data, cloud computing, and deep learning technologies have enabled the implementation of more accurate and efficient algorithms and models for machine learning (El Waqa and Murphy, 2015). Machine learning is now widely applied in various fields such as natural language processing, image and video processing, speech recognition, medicine, finance, e-commerce, and intelligent transportation, among others (Aladdin, 2021). Machine learning is a branch of artificial intelligence that aims to improve task performance by allowing computer systems to learn and improve automatically without explicit programming. The history of machine learning can be traced back to the 1950s and 1960s, when computer scientists began experimenting with algorithms and statistical methods to enable computer systems to learn patterns and rules from data. However, the application of machine learning was limited by hardware and algorithm capabilities at that time (Bi, 2022). It wasn't until the 198os that machine learning began to gain more widespread use as computer hardware and algorithms improved. With the explosion of data in the 21st century, machine learning has become increasingly important. The development of big data, cloud computing, and deep learning technologies have enabled more accurate and efficient algorithms and models to be developed for machine learning (Bell, 2022). Machine learning is now widely used in various fields, such as natural language processing, image and video processing speech recognition, medicine, finance, e-commerce, and intelligent transportation. Catalytic descriptors link structures and properties, enabling experimentalists to quickly screen materials from databases and optimize existing catalysts. The combination of theoretical and experimental descriptors provides a more reasonable method for catalyst design. However, identifying descriptors and discovering how they determine the activity and selectivity of electrocatalysts is a challenge and largely underexplored. In situ characterization combined with high throughput computing and machine learning is expected to break the bottleneck of HER catalyst development. In recent years, two-dimensional MXenes as HER catalysts have received attention in both experimental and theoretical calculations, but they mainly focus on the regulation of catalytic activity of perfect materials and are relatively lacking in the design of catalytic performance and the construction of catalytic descriptors for single atom doped and ordered alloy two-dimensional MXenes materials, which play an important role in the field of catalysis.

2. METHODOLOGY

Based on Density Functional Theory of quantum mechanics, the crystal structure and physical properties of materials such as force, heat, light,

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electricity and magnetism can be determined by self-consistent calculation. With the rapid development of high-performance computing technology and various professional computing software, DFT computing has been deeply applied in condensed matter physics, materials science (design, simulation computing and virtual synthesis) and biochemistry. There is no doubt that DFT calculation, as a conventional research model, has become a bridge and supplement to theoretical and experimental research. And combined with high-throughput, artificial intelligence and big data, it is expected to play a wider role in computational physics, chemistry and materials. The theoretical basis of density functional theory is based on two basic mathematical theorems proved by two scientists, Kohn and Hohenberg, and a set of equations deduced by Kohn and Sham in the mid-197os. The first theorem proved by Kohn and Hohenberg shows that there is a one-to-one correspondence between the ground-state wave function and the ground-state charge density. The specific content can be described as: the ground state energy obtained from the Schrodinger equation is the only functional of charge density. The second theorem proved by Kohn and Hohenberg is that under the condition that the number of particles remains constant, the energy functional takes the minimum of the correct charge density, and the minimum is the ground state energy of the system. According to the Hohenberg-Kohn theorem, the total non-relativistic Hamiltonian for a multiparticle system can be written Formula 1

$$H = -\frac{h^2}{2m}\sum_i \emptyset^2 + V_{ext}(r) + \frac{1}{2}\sum_{i\neq L}\frac{e^2}{|r_i - r|} \quad (1)$$

The energy form of the corresponding system is as follows Formula 2:

$$E_{HK}[P(r)] = T[p(r)] + \mathrm{U}[p(r)] + \mathrm{Ex}[p(r)] \quad (2)$$

On the right side of the equation, the kinetic energy, the potential energy, and the exchange correlation function (including all other interactions) are represented in turn.

Although Hohenberg-Kohn Theorem I rigorously proves the existence of a charge-density functional that can be used to solve the Schrodinger equation, the exact form of the functional is still uncertain. Fortunately, Hohenberg-Kohn Theorem II gives an important feature of this functional, which is that the charge density that minimizes the global functional is the true charge density corresponding to a complete solution of the Schrodinger equation. If the form of this "true" functional is known, the charge density can be adjusted until the energy determined by the functional is minimized, and the corresponding charge density can be found. In practical applications, the variational principle is often used in approximate expressions of functional. In the process of finding the minimum energy solution of the total energy functional, Kohn and Sham gave the following result: Solving the correct charge density can be expressed as solving a set of equations, each of which is related to only one electron. Then the electron density function can be expressed as Formula 3:

$$p(r) = \sum_{i=1}^{a} |\emptyset(r_i)|^2 \quad (3)$$

The total energy of the hypothetical system can be expressed as Formula 4:

$$E_s = T_s[p(r)] + U_H[p(r)] \quad (4)$$

Combined with Hohenberg-Kohn Theorem I, the exchange interaction terms can be obtained by simultaneous equations Formula 5:

$$E_{xc}[p(r)] = T[p(r)] - T_S[P(r)] + U[p(r)] - U_H[p(r)] \quad (5)$$

Therefore, all complex interacting parts and unknown terms are divided into exchange dependent terms. Therefore, finding suitable exchange correlation function is the key to density functional theory.

Machine learning descriptors accurately predict HER catalytic activity from the above electronic structure analysis and Fermi level and directly interacting with. It was found that the electronic structure of Ti2Co2-STM played a dominant role in HER catalytic activity. The prediction accuracy of Spz to the target value is less than 75%. Moreover, in Ti2Co2-STM system doped with the same metal monatomic, the A values of the active sites & and & are the same, and the catalytic activity of different active sites cannot be distinguished. Therefore, more advanced methods are needed to build accurate descriptors.

Machine learning (ML) is becoming increasingly popular as a new research tool for semi-automated and quantitative data correlation discovery in materials science. In this work, 18 kinds of atomic information, crystal parameters, electronic structure and other characteristic parameters with physical significance that are initially related to HER catalytic activity are selected. By analyzing the importance of the characteristic parameters to the catalytic activity of the target value HER and the correlation between the parameters, the dimension of the characteristic parameters is constantly reduced. Table 1 It is found that when the characteristic parameter is reduced to 5 dimensions, the accuracy and 2 can still be maintained to 0.93, the error and MM: is only 79eV.

Table 1: The number and type of machine learning characteristic parameters, and the corresponding prediction accuracy and error.

Number	Feature	R2	Rmse
5	[dM1-00 dM0-00 Med EFerml Bm]	0.931	0.079
4	[dM1-00 EFerm Med Rm]	0.926	0.083
3	[dM1-00 EFerm CHM]	0.9	0.09
2	[dM1-00 EFerm]	0.86	0.11
1	[EFerml]	0.746	0.153

3. Experiment

More significantly, the characteristic parameters from dimension 1 to dimension 5 all contain Fermi level, which is consistent with the key parameter affecting HER catalytic activity revealed in the above analysis. It shows that the key parameters of catalytic performance can be found through machine learning. Further analysis shows that starting from the second characteristic parameter, it contains the information of the local structural distortion of the reaction, which is the bond length between the doped metal single atom and the surface oxygen atom. It just verified our qualitative analysis above that the more far away from metal single atom doping position electronic structure description porphyrite, the better the prediction effect. The above machine learning shows that in addition to the Fermi level, the bond length between the doped metal single atom and the surface oxygen atom is the secondary factor. In addition, it can be seen from Figure 1 (a-b) that with the increase of the dimension of characteristic parameters, the accuracy keeps improving and the error keeps decreasing. When the dimension reaches 5, the growth of accuracy gradually slows down and the error reduction gradually becomes stable. Further Figure 1 (c-d) shows that for different catalytic active sites &, & and &, the prediction accuracy is greatly improved after taking into account the characteristic parameter of the information about the local structural distortion of the reaction, which is the bond length between the doped metal single atom and the surface oxygen atom. The prediction accuracy was up to o.99, indicating that the machine learning model captures the key parameters regulating HER catalytic activity of Ti2Co2-STM. The above analysis indicates that machine learning is an effective means to find accurate descriptors for the regulation of multiple factors on HER catalytic activity.

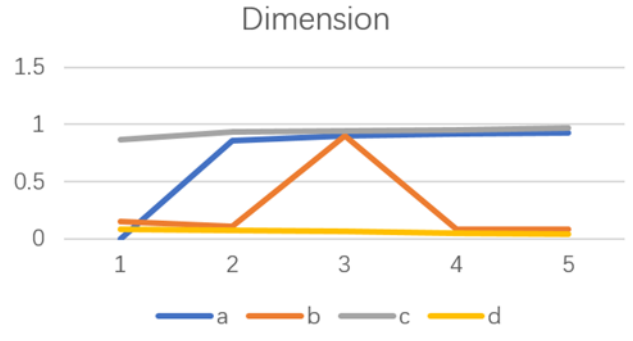

Figure 1: The variation of prediction accuracy and error with the increase of characteristic parameters for different equivalent catalytic active sites.

Under acidic conditions, HER has two different reaction mechanisms: Volmer-Tafel and Volmer-HeyrovskyE67 '. In both mechanisms, the first step involves the adsorption and reduction of protons, known as the Volmer reaction. When a hydrogen atom is adsorbed on the surface of the electrocatalyst, there are two possible reactions in the second step: 1) react with another adsorbed hydrogen atom to produce hydrogen; 2) or react with solvated protons and surface electrons to form oxygen. The first is a Langmuir-Hinshelwood-type mechanism involving Tafel reactions. The second is the Eley-Rideal type mechanism, which involves the Heyrovsky reaction. The main difference between the Tafel reaction and the

Heyrovsky reaction is that the Tafel reaction does not involve electron transfer, while the Heyrovsky reaction does. Thus, the Heyrovsky reaction can be driven by potential, while the Tafel reaction is potential-independent and needs to be activated by heat (Bell, 2022). According to the Bronsted-Evans-Polanyi relation, the activation energy of HER is linearly correlated with the adsorption energy of hydrogen. Therefore, the adsorption capacity of hydrogen is an important index to evaluate the catalyst. Exchange current density j ○ is one of the most important catalytic indexes that can be directly measured in experiments. As shown in Figure 2, if the current density i2 is large enough (red curve), the system can provide a large current even at very low overpotential, which means that the whole reaction is very easy to activate, and the electrode dynamics are very fast. As the jo decreases, as in the green and blue curves, there is no significant current unless a large activation overpotential is applied. As shown in Figure 3, CN ties are highest on both sides and lower in the middle (Shavlik et al., 1990). PD is the highest at -0.4, up to 4.5. Mos is the highest at 0.8, up to 6. When drawing the relationship curve between the experimentally measured exchange current density CN and the Gibbs free energy AGH of hydrogen adsorption for various catalyst materials, it is found that there is a volcanic model relationship. The PD value at the maximum reaction rate is close to 1.5. It is shown that if the binding of hydrogen to the surface is too weak, the Volmer step will limit the overall reaction rate. However, if the binding is too strong, the desorption (Heyrovsky/Tafel) step limits the reaction rate. Therefore, the necessary condition for the activity of hydrogen evolution catalyst is Mos. The results also reflect Sabatier's principle, which states that the best catalysts should bind atoms and molecules with optimal binding strength: not too weak to activate reactants and not too strong to desorb products.

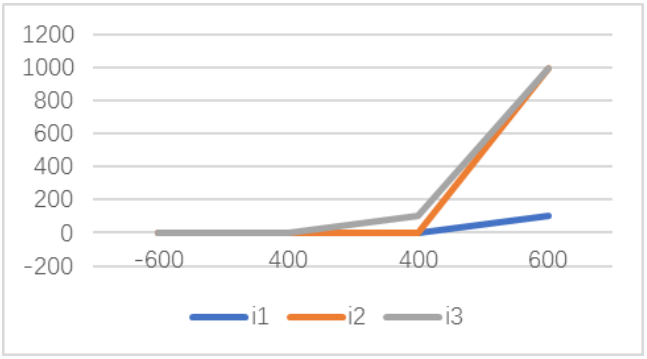

Figure 2: Exchange current density

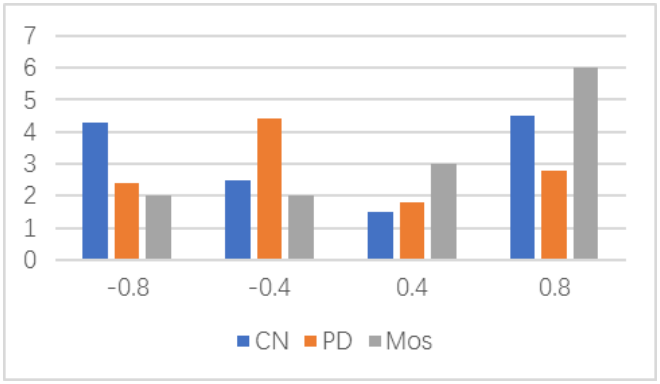

Figure 3: Kahn adsorbs Gibbs free energy

4. Discussion

HER catalytic properties of ft two-dimensional NM- Ti2Co2MXenes with large surface area and corrosion resistance were investigated. 14 kinds of nonmetallic atoms with different valence electron numbers and periods were selected by DFT theory, and their catalytic properties were controlled by surface doping. The results show that surface nonmetallic doping can optimize the catalytic activity and band gap of catalyst while maintaining the relative stability of the catalyst. (More importantly, the valence electron and charge transfer descriptor can accurately predict: The trend of HER catalytic activity of NM- Ti2Co2MXenes has shifted the design of catalysts from traditional trial and error to rational theoretical guidance. Systematic analysis of the electronic structure of two-dimensional NM-Ti2Co2MXenes not only explains the rationality of this simple coupling description, but also reveals the origin of the regulation of catalytic activity of two-dimensional NM- Ti2Co2MXenes. The e study provides theoretical basis for the design and high throughput screening of HER catalysts. Screening and study of HER properties of gold doped Ti2Co2 by Occhuan observation method / 3d, 4d, 5di. ter. The adsorption energy of two-dimensional MXenes-OBAs was calculated using an automatic process of feature engineering. We developed machine learning process code based on Scikit-leam and published it in the open source MGEdata. As shown in Figure 4, this workflow consists of three parts: (a) Functional design. According to our knowledge of the origin of HER activity, 41 characteristics were selected, including electronic and geometric parameters of elements. We extended the main features to a total of 63 by simple summary statistics (mean and standard deviation) as initial features to train a machine learning model predicting H adsorption energy based on 420 sets of DFT calculated data. (b) Feature selection. In this paper, a comprehensive feature search strategy based on reverse selection is designed based on feature importance and feature correlation. AdaBoost model and Pearson correlation coefficient were used to calculate the significance and correlation of features. After the importance and correlation of the features are obtained, the features with lower rank and higher correlation coefficient than the threshold are removed from the feature group. AdaBoost was used to re-model the retained features with low threshold correlation coefficient to further reduce the number of features. In this way, the resulting features can remain both independent and modeling accurate. In this work, the initial threshold is 0.9 and the rate 0f decline is 0.1. (c) Multi-perspective evaluation. To test the validity of the selected features, we used a variety of schemes to evaluate the features. Firstly, different segmentation data are used to evaluate the modeling results of the features. Secondly, 1o-fold cross-validation was carried out on the data to further check the stability of the features. Finally, using support vector regression , gaussian process regression (GPR), P ex-wife-to-be machine return to forest, a. a. (RFR) model and AdaB AdaB multipleine learning methods, such as the universality of the characteristics of the test.

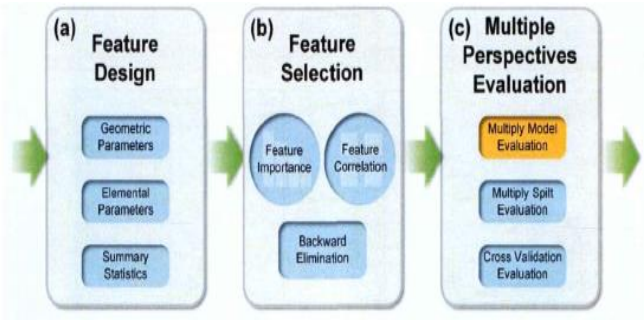

Figure 4: Machine learning processes.

The study found that single atom metal doping can improve its ehrs do M | catalytic activity and electrical conductivity, thus make Ti2Co2 - V, Nb, Mo, W and Re performance of catalyst optimal Ti2Co2. Special foot Ti2Co2 - W: U have good catalytic activity, electrical conductivity, and stability. The electronic structure level understanding of HER regulation of Ti2Co2-STM is analyzed by using the theory of electron structure. The results show that the change of HER catalytic activity is caused by the rearrangement of electric f structure near the Fermi level caused by the hybridization of P and P-D orbitals (Sar et al., 2012). The origin and trend of HER catalysis of Ti2Co2-STM were revealed by qualitative analysis of the electron structure at the Fermi level and Opz orbital band center. Machine learning method was used to construct a high precision HER catalytic activity descriptor with clear physical significance, which could reveal the difference of catalytic activity of + with the same active site. This paper provides a theoretical basis for the design of Ti2Co2-STM or other doped two-dimensional MXene-STM catalysts, which is conducive to the synthesis and application off ideal non-precious metal HER catalysts.

5. Conclusion

Hydrogen evolution plays a key role in electrochemistry and energy conversion technology. The key to promote the industrial application of electrolytic hydrogen evolution is to find catalysts with low price and superior performance. Catalytic descriptors can link the structure and properties of catalysts, enabling rapid screening of new materials and optimization of existing catalyst performance. This work focuses on HER catalytic properties of complex two-dimensional MXenes materials and explores potential excellent HER catalysts by integrating DFT high-throughput computing with machine learning methods. The catalytic activity was predicted by using descriptors and the origin mechanism of the catalytic activity at the electronic structure level was revealed. Above work not only for the synthesis of various complex two-dimensional MXenes provides data reference material, with a clear physical meaning

and use of descriptors for more two-dimensional MXens - its ehrs catalyst design provides a theoretical guidance. High-throughput computing combined with machine learning and integration way of the descriptor is expected to become efficient design is an effective means of its ehrs catalyst in the future. In the future, machine learning and descriptor methods could quickly screen ideal electrode materials. While doping or alloying may break the linear correlation between adsorption energy and diffusion barrier, machine learning can be used to give full play to the advantages of being good at dealing with complex materials or correlation.

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