SVOA Materials Science & Technology

ISSN: 2634-5331

ScienceVolks Open Access

Mini-Review

Advances in Machine Learning Applications in Material Science: From Non-2D to 2D Materials

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DOI: https://doi.org/10.58624/SVOAMST.2024.05.002

***Received:** September 05, 2024* ***Published:** September 23, 2024*

Abstract

This mini-review presents recent advancements in the application of machine learning to both non-2D and 2D materials. For non-2D materials, the main focus is on construction materials, energy and environmental materials, and advanced functional materials. In the case of 2D materials, the mini-review emphasizes the role of machine learning in predicting electronic and structural properties, as well as in identifying defects and phase preferences. The mini-review underscores the crucial role that machine learning plays in advancing materials science by enabling rapid screening of materials, predicting their properties, and significantly reducing the time required for such processes.

***Keywords:** Machine Learning (ML); 2D Materials; Model Prediction; Non-2D Materials*

Introduction

In recent years, the integration of machine learning (ML) with materials science has significantly improved the efficiency and accuracy of predicting material properties, synthesis routes, and performance characteristics, thereby accelerating advancements in the field. The fusion of ML enables materials scientists to explore a broader materials space and identify optimal candidates for different applications with unprecedented speed and precision. This mini-review aims to summarize the progress in the application of machine learning in both non-2D and 2D materials.

1. Advances in Machine Learning for Non-2D Materials Research

1.1. Construction Materials

Construction materials, particularly those used in large-scale infrastructure projects, require precise mechanical properties. Traditionally, determining these properties involves extensive and time-consuming experimental testing. The advent of machine learning (ML) offers a new avenue for efficiently predicting these properties. Babatunde Abiodun Salami et al.(2022)[1] employed 232 experimental results to apply ML models such as Artificial Neural Networks (ANN), Gene Expression Programming (GEP), and Gradient Boosted Trees (GBT) to predict the compressive strength of lightweight foamed concrete. They found that the GEP model outperformed the others in predicting the compressive strength of foamed concrete, and the developed model can be utilized to optimize mixture designs, thus accelerating the development process.

Through the use of extensive data and advanced algorithms, ML significantly enhances the ability to predict the compressive strength of construction materials. The effective application of ML in compressive strength prediction holds substantial potential for accelerating material design optimization in the construction sector.

1.2. Energy and Environmental Materials

Materials with specific properties are critical in the search for sustainable energy solutions and environmental remediation. For example, in thermoelectric materials, U.S. Vaitesswar et al. (2024)[2] successfully utilized ML models to predict thermoelectric materials with high power factors and identified four new half-Heusler compounds as promising thermoelectric materials. Their results demonstrated that the random forest (RF) model showed the best predictive performance and revealed that just ten key features were sufficient to predict the power factors of thermoelectric materials.

In environmental remediation, ML has enabled the design of biochar-based materials. Kumuduni Niroshika Palansooriya et al. (2022)[3] applied ML models including RF, Support Vector Regression (SVR), and ANN to predict the heavy metal immobilization efficiency of biochar in biochar-amended soils. They found that the hybrid SVM-ANN model performed best. The study identified significant features, such as the nitrogen content in biochar and biochar application rate, that influence heavy metal immobilization, providing insights for developing biochar-based remediation strategies.

ML enhances material development efficiency by identifying key features and utilizing minimal feature selection techniques. The availability of multiple ML models in material research offers researchers a variety of options to identify the most suitable and optimal model.

1.3. Advanced Functional Materials

Advanced functional materials, such as Metal-Organic Frameworks (MOFs) and photonic materials, are at the forefront of research due to their unique properties and wide-ranging applications. However, designing these materials for specific functions, such as gas separation or molecular property prediction, presents a complex challenge. ML has emerged as a key tool in this critical field. In the area of gas separation, Jian Guan et al.(2022)[4] used RF models to study the CO_2/CH_4 separation performance of MOF-based mixed matrix membranes (MMMs), finding that MOF type, polymer type, and loading significantly influence the ML model's performance. This research is valuable for the design and development of CO_2 capture MMMs.

In the field of molecular property prediction, Hui Zhang et al. (2022)[5] investigated the use of optical neural networks (ONN) on a chip, utilizing a complex-valued neural network optimized through genetic algorithms. The researchers found that complex-valued neural networks outperformed real-valued neural networks in predicting molecular properties. ML models enable the task of molecular property prediction to be performed with high accuracy and low power consumption, accelerating material design and development.

Additionally, Siyu Isaac Parker Tian et al. (2022)[6] explored advanced ML models including Roost, CrabNet, MEGNet, and CGCNN to compare composition-only models and composition-plus-structure models. They discovered that, for stable compounds, both models predicted properties, similarly, suggesting that composition alone is sufficient to predict many properties, while structure is a sufficient but not necessary condition for predicting stable compounds.

ML has greatly facilitated the design and optimization of advanced functional materials by focusing on key features and optimizing datasets. Researchers can now conduct more accurate and faster predictions, accelerating material development. Furthermore, for stable compounds, the emphasis on compositional features provides researchers with valuable insights for feature selection, expediting the overall research process.

2. Advances in Machine Learning for 2D Materials Research

2.1. Electronic Properties

Understanding the electronic properties of two-dimensional (2D) materials, such as work function, bandgap, and carrier concentration, is crucial for developing high-performance electronic and optoelectronic devices. The introduction of machine learning (ML) models has increasingly provided high-precision predictions of these properties, offering an alternative to traditional first-principles calculations and experimental methods.

For the prediction of work function, Pranav Roy et al. (2023)[7] found that non-linear ML models such as random forests and neural networks outperformed linear regression when predicting the work function of 2D MXenes using 15 features. The researchers also identified that the properties of surface termination, particularly electronegativity, were the most significant feature affecting the work function of MXenes. Ehsan Alibagheri et al. (2021)[8] used gradient boosting (GB) ML models with 15 input features to predict electronic and structural properties of 2D materials. The study showed that the prediction of metallic/non-metallic classification, bandgap, density of states, and work function exhibited high accuracy, highlighting the role of feature engineering in enhancing ML models' predictive power. These findings demonstrate the potential of ML to reduce computational costs and time in accelerating the discovery of ideal 2D materials.In the area of bandgap prediction, Yu Zhang et al. (2021)[9] developed an ML-based method to replace traditional first-principles calculations. Training their models on 2817 datasets, they found that gradient-boosted decision trees (GBDT) and random forest (RF) models outperformed support vector regression (SVR) and multilayer perceptron (MLP) models, with R^2 values greater than 90% and root mean square errors (RMSE) of 0.24 eV and 0.27 eV, respectively. Zhen

Zhu et al. (2020)[10] combined density functional theory (DFT) and ML to predict electronic properties of 2D semiconductors. They found that when elemental information was used as predictors, the SVR model accurately predicted electronic properties such as bandgap, valence band maximum (VBM), and conduction band minimum (CBM) with an RMSE below 0.15 eV. SVR models, which require no DFT calculations, are advantageous for quickly screening 2D semiconductor materials.

In the study of MoS_2, Yan Qi Huan et al. (2021)[11] used experimental current measurements to predict the breakdown mechanism and voltage of monolayer MoS_2 devices. The research utilized a deep neural network (DNN) classifier, achieving 79% accuracy in classifying breakdown mechanisms under bias currents below 20V. The study revealed that increasing the carrier concentration in monolayer MoS_2 devices reduced the occurrence of breakdown, offering a rapid and non-destructive method for characterizing the breakdown voltage of 2D materials.

2.2. Structural Properties

The structural properties of 2D materials, including thickness, mechanical stability, heterostructure, and binding energy, play a critical role in determining their performance and application. Machine learning enables the efficient prediction of these structural characteristics, improving our understanding and application of 2D materials.

In the study of thickness, C.E. Ekuma(2024)[12] introduced the THICK2D framework, based on ML models and large language models, which accurately predicts the thickness of 2D materials in the range of approximately 2Å to 13.5Å. When applied to well-known 2D materials such as graphene, GaN, and TiO_2, the predicted values were within 5% of the experimentally reported values. In the context of mechanical and thermal performance, Bohayra Mortazavi et al. (2022)[13] used ML interatomic potentials (MLIPs) and DFT to study the mechanical and thermal properties of BC_2N monolayers. They found that MLIP models outperformed empirical interatomic potentials in predicting lattice stability and revealed that BC_2N monolayers exhibit anisotropic mechanical properties and high thermal conductivity, making them ideal for thermal management applications. Furthermore, Bohayra Mortazavi et al. (2020)[14] employed a combined approach of DFT, AIMD, and MLIPs to predict the phononic properties of two-dimensional materials, revealing that AIMD and MLIPs exhibit remarkable agreement with DFPT results concerning phononic characteristics.

In heterostructure studies, Daniel Willhelm et al. (2022)[15] used ML and DFT models to predict the properties of van der Waals (vdW) heterostructures. Their findings showed that ML models accurately predicted critical descriptors, such as electronic properties, interlayer distances, and binding energy. The research also highlighted significant differences in equilibrium interlayer spacing between AA and AB stacking configurations in vdW heterostructures, aiding in the rapid screening of materials for optoelectronic applications. Sherif Abdulkader Tawfik et al. (2019)[16] had similar findings, showing that the combination of DFT and ML models could efficiently predict the interlayer distance and bandgap of bilayer heterostructures, significantly accelerating the prediction process.

Notably, Julia Fischer et al. (2020)[17] predicted the binding energies of adsorbates on graphene single-atom catalysts (SACs) by extracting topological structures from interatomic networks, such as lengths and angles, statistical features, and partial radial distances. Their models, based on RF and SVR, achieved R^2 values greater than 0.950 for both training and test sets, demonstrating the accuracy of ML-based prediction methods, which offer a fast and cost-effective way to discover suitable SACs.

2.3. Defects and Phase Preferences

Defects and phase preferences in 2D materials can significantly affect their electronic, optical, and mechanical properties. In defect studies, Pengru Huang et al. (2023)[18] developed an ML-integrated platform for material design, using datasets of pristine and defective materials to study the correlation between defect structures and properties. Their research revealed that the formation energy of defects in TMDCs is influenced by lattice perturbation and the introduction of mid-gap states. The sublattice structure affected the oscillation behavior of defect interactions. Additionally, Nathan C. Frey et al. (2020)[19] employed a combination of deep transfer learning, machine learning, and first-principles calculations to predict key characteristics of point defects in two-dimensional materials. In this study, the researchers found that machine learning models can effectively predict defect formation energies and energy levels without requiring detailed defect calculations. This provides insights for selecting materials for quantum computing and resistive memory applications.

In phase preference studies, Pankaj Kumar et al. (2022)[20] used high-throughput quantum calculations and ML algorithms to predict the phase preferences of transition metal dichalcogenides (TMDs). The study showed that ML models could accurately predict the phase preferences of TMDs based on their physical and chemical properties, identifying six key features that significantly influence phase formation energy and phase preferences.

Conclusions

The integration of machine learning (ML) into the study of both non-2D and 2D materials has significantly advanced the field of materials science. For non-2D materials, particularly in construction, energy, and environmental materials, ML models have demonstrated their ability to predict key properties such as compressive strength and thermoelectric performance with high accuracy, thereby accelerating material design and optimization processes. In advanced functional materials, ML models have been essential for optimizing properties like gas separation efficiency and molecular property prediction, offering new avenues for rapid discovery and development.

In 2D materials, ML has proven invaluable for predicting electronic properties, such as work function and bandgap, and structural properties, including thickness, mechanical stability, and heterostructure behavior. These capabilities allow researchers to bypass time-consuming experimental and first-principles methods, reducing computational costs and time while maintaining high accuracy. Moreover, ML's application to defect and phase preference studies in 2D materials has enhanced the understanding of how structural and electronic properties are affected, facilitating the design of materials with optimized performance for specific applications.

The use of machine learning in both non-2D and 2D material research is revolutionizing the discovery and optimization process, enabling faster, more efficient, and more accurate predictions of material properties. This marks a significant step forward in the development of next-generation materials for a wide range of technological applications.

Conflict of Interest

The author declares no conflict of interest.

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Citation: Wang Z. Advances in Machine Learning Applications in Material Science: From Non-2D to 2D Materials. SVOA Materials Science & Technology 2024, 5:1, 03-07. doi: doi.org/10.58624/SVOAMST.2024.05.002