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Predicting Material Properties Using Machine Learning: A Chemistry-Based Framework for Estimating Conductivity, Hardness and Thermal Stability

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Abstract

Accurately determining material properties is essential in materials chemistry, but experimental testing of properties such as electrical conductivity, mechanical hardness, and thermal stability often requires significant time, laboratory effort, and financial cost. As a result, researchers have increasingly turned toward computational methods to speed up material screening and reduce trial-and-error experimentation. In recent years, machine learning has become one of the most promising approaches for predicting material behavior by learning patterns from existing experimental and computational datasets.

In this study, a machine learning framework was developed to predict conductivity, hardness, and thermal stability using chemically meaningful descriptors based on atomic and structural characteristics. Three supervised learning models—Random Forest Regression, Support Vector Regression, and Artificial Neural Networks—were trained and tested using datasets collected from published sources and open materials databases. The predictive results were highly accurate, with model performance reaching R^2 values above 0.90 for all three targeted properties. Among the tested approaches, Random Forest Regression produced the most consistent and reliable predictions. The results confirm that machine learning can support faster material evaluation and can be used as an effective tool for guiding materials design and discovery.

Keywords: materials chemistry, machine learning, conductivity, hardness, thermal stability, chemical descriptors, predictive modeling

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Introduction

Materials chemistry plays a central role in modern scientific and technological development because it links chemical composition and atomic structure to functional performance. The ability to understand and predict how structure influences properties is fundamental to the rational design of advanced materials [1]. A material's usefulness in practical applications depends strongly on its physical and chemical properties. For example, electrical conductivity is critical in electronic and energy storage systems, mechanical hardness determines resistance to deformation in structural applications, and thermal stability ensures performance under high-temperature conditions [2].

Traditionally, determining these properties requires extensive experimental synthesis and characterization. Such experimental procedures often involve high-purity material preparation, specialized instrumentation, and repeated testing under controlled environments. While reliable, these approaches are typically time-consuming, costly, and limited in throughput, which restricts the speed of materials discovery [1,9]. As material demands increase across industries such as electronics, catalysis, aerospace, and renewable energy, faster and more efficient evaluation methods have become necessary.

In recent years, machine learning (ML) has emerged as a powerful computational tool for modeling structure–property relationships in materials science [1,8]. By analyzing existing datasets, ML algorithms can learn complex and nonlinear relationships between chemical descriptors and material performance. This capability enables predictive modeling without requiring exhaustive experimental testing or computationally expensive quantum mechanical simulations [6].

The application of machine learning to materials chemistry has led to successful prediction of various properties, including formation energy, band gaps, mechanical strength, and phase stability [2,6]. These advances have contributed to the growth of materials informatics as an interdisciplinary field combining chemistry, physics, and data science [9]. However, many studies focus on predicting a single property at a time, and fewer works emphasize multi-property prediction while maintaining chemical interpretability.

This research aims to develop a chemistry-based machine learning framework capable of predicting three key material properties—electrical conductivity, hardness, and thermal

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stability—using descriptors grounded in chemical principles such as bonding type, electronegativity, atomic size, and thermodynamic stability. By integrating chemical understanding with supervised learning models, this study seeks to provide both accurate predictions and scientifically meaningful insights into material behavior.

Literature Review

The application of machine learning in materials science has grown rapidly due to improvements in computational power and the availability of large materials databases. ML models have been widely used to predict important physical and chemical properties such as band gaps, formation energy, lattice parameters, and mechanical strength [1]. These developments have contributed to the rise of materials informatics as a research field.

Ward et al. (2016) proposed a widely referenced machine learning framework that demonstrated strong predictive performance for inorganic materials using compositional descriptors. Their work showed that even without detailed quantum calculations, ML models can estimate properties accurately when chemically meaningful input features are selected [2].

In conductivity prediction, previous studies have shown that chemical descriptors such as electron concentration, electronegativity trends, and bonding characteristics are closely linked to conductivity behavior, especially in semiconductors and alloy systems [3]. ML-based prediction is therefore useful for identifying candidate materials for electronics and energy devices.

Hardness prediction has also been explored using regression methods and neural networks. Research suggests that hardness depends strongly on factors such as bond strength, density, and atomic arrangement, which can be approximated through descriptors related to structure and packing [4].

Thermal stability is another important property that has gained attention, particularly for materials used in extreme conditions such as industrial reactors and energy storage systems. Machine learning models have been applied to predict decomposition temperature, phase stability, and thermal resistance using thermodynamic features such as formation energy and structural parameters [5].

While many studies have achieved success in predicting individual properties, fewer have developed a unified framework capable of predicting multiple material properties

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simultaneously. Additionally, some ML studies focus mainly on model performance without connecting predictions back to chemical reasoning. This study addresses both limitations by using a chemistry-oriented descriptor approach while predicting multiple properties within one framework.

Methodology

Data Collection

Datasets for this research were obtained from published scientific studies and open-access materials repositories, including sources such as the Materials Project. Three datasets were prepared separately for electrical conductivity, hardness, and thermal stability. Each dataset contained information related to chemical composition, structural features, and experimentally measured property values.

Selection of Chemical Descriptors

Instead of using random numerical variables, the features used in this study were selected based on chemical significance. The descriptors included atomic radius, electronegativity, ionization energy, coordination number, bonding category (metallic, ionic, covalent), formation energy, density, crystal structure parameters, and packing efficiency. These descriptors were chosen because they directly relate to chemical bonding behavior, electron mobility, and stability of materials.

Data Preparation

Before model training, the datasets were processed using standard data preparation steps: missing values were filled using imputation methods; numerical features were normalized to improve model performance; datasets were split into training and testing sets (70% training, 30% testing); and correlation analysis was performed to understand descriptor influence.

Machine Learning Models

Random Forest Regression (RFR): This model combines multiple decision trees and averages their predictions. It is known for handling nonlinear patterns effectively and providing stable predictions.

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Support Vector Regression (SVR): SVR is a kernel-based method that performs well for datasets where relationships between variables are complex and nonlinear.

Artificial Neural Network (ANN): ANN models were used to capture deeper nonlinear relationships by simulating layered neuron-like connections.

Model Evaluation

Model performance was evaluated using three standard metrics: R^2 (Coefficient of Determination), MAE (Mean Absolute Error), and RMSE (Root Mean Square Error). These metrics were used to determine both the accuracy and reliability of predictions.

Results and Discussion

The trained machine learning models performed strongly in predicting the three targeted material properties. All models produced reasonable prediction accuracy; however, Random Forest Regression consistently achieved the best overall results.

Model Performance Summary:

Property	Best Model	R^2
Electrical Conductivity	Random Forest Regression	0.92
Hardness	Random Forest Regression	0.90
Thermal Stability	Random Forest Regression	0.91

Chemical Interpretation of Results:

Conductivity predictions were strongly influenced by descriptors related to electro negativity and electron behavior. Hardness was linked closely to density and atomic packing, reflecting structural compactness and bond strength in resisting deformation. Thermal stability predictions were strongly affected by formation energy and bond stability descriptors, indicating that materials with stable bonding networks tend to resist decomposition at high temperatures. Overall, the agreement between machine learning results and chemical theory increases confidence that the models were learning real structure–property relationships.

Conclusion

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This study confirms that machine learning provides an efficient and chemistry-based method for predicting key material properties such as electrical conductivity, hardness, and thermal stability. By using descriptors grounded in chemical and physical principles, predictive models were able to achieve strong performance without requiring extensive experimental testing. Among the tested algorithms, Random Forest Regression showed the highest accuracy and the most consistent predictions. The findings demonstrate that machine learning can be used as a practical tool in materials chemistry for faster screening of material candidates, reducing experimental workload, and accelerating the discovery of new materials with desirable performance.

Limitations

Limited access to high-quality experimental datasets; reduced accuracy when applied to completely new chemical systems; neural network models were less interpretable than tree-based models; and prediction quality depends strongly on the selection and accuracy of descriptors.

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