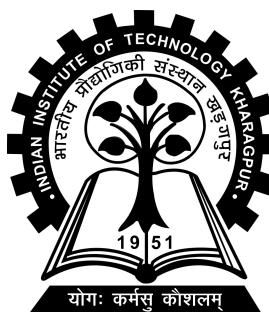


Predicting physical and electronic properties of Heusler Alloys using CG-CNNs

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Moulik Kumar
(21PH10023)

Under the supervision of
Professor Amal Kumar Das



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Indian Institute of Technology Kharagpur
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Chapter 1

Introduction

The field of materials science has been revolutionized by the integration of machine learning techniques, particularly in the prediction and design of novel materials. Among these emerging techniques, Crystal Graph Convolutional Neural Networks (CGCNNs) have shown remarkable promise in bridging the gap between structural complexity and property prediction. Heusler alloys, discovered in 1903, represent a fascinating class of intermetallic compounds that exhibit remarkable properties despite being composed of seemingly simple constituents. These materials have emerged as key candidates for next-generation electronic and spintronic devices, owing to their tunable electronic structure and magnetic properties.

1.1 Crystal Structure and Fundamental Properties

Heusler compounds represent a diverse family of intermetallic materials characterized by their highly ordered crystal structure. At their core, these materials demonstrate how atomic arrangements can lead to emergent properties that are absent in their constituent elements. The most striking example is the ferromagnetic behavior in Cu₂MnAl, where none of the individual elements are ferromagnetic in their pure form.

The basic structural classifications include full-Heusler alloys (X₂YZ), which crystallize in the cubic L₂₁ structure, and half-Heusler alloys (XYZ) forming in the C1_b structure. The distinction between these structures lies not just in their composition but in the fundamental arrangement of atoms and the resulting electronic interactions. In full-Heusler alloys, four interpenetrating face-centered cubic sublattices create a complex network of atomic interactions that gives rise to their unique properties. The half-Heusler structure, meanwhile, can be viewed as a full-Heusler with one sublattice vacant, leading to distinct electronic and magnetic characteristics.

The electronic structure of these compounds is particularly intriguing, as it gives rise to a range of valuable properties:

- Half-metallic ferromagnetism with 100
- Tunable band gaps ranging from metallic to semiconducting
- Strong magneto-structural coupling
- Topological states in certain compositions

1.2 Current Challenges in Property Prediction

The design and optimization of Heusler alloys face several fundamental challenges that stem from their complex electronic structure and the subtle interplay between composition and properties. Traditional density functional theory (DFT) calculations, while accurate, are computationally intensive and time-consuming. This computational burden becomes particularly significant when exploring new compositions or investigating the effects of structural disorders.

The complexity arises from several factors. First, the electronic structure calculations must account for multiple possible magnetic configurations and electron correlation effects. Second, the study of chemical disorder often requires large supercells, making calculations computationally prohibitive. Additionally, the properties of Heusler alloys are highly sensitive to atomic ordering and site preferences, making it crucial to consider multiple possible configurations.

The presence of structural phase transitions adds another layer of complexity. Many Heusler alloys undergo martensitic transformations, where the crystal structure changes with temperature or applied fields. Understanding and predicting these transitions requires consideration of:

- Temperature-dependent structural changes
- Magnetic order-disorder transitions
- Electronic structure modifications
- Strain effects and mechanical properties

1.3 Evolution of Machine Learning in Materials Science

The application of machine learning to materials science has evolved significantly over the past decade. Early approaches focused primarily on composition-based predictions using traditional statistical methods and simple neural networks. These methods, while valuable, often relied heavily on hand-crafted features and struggled to capture the complex structural relationships inherent in crystalline materials.

Modern deep learning approaches have transformed this landscape by introducing more sophisticated architectures capable of learning directly from structural data. Convolutional neural networks have demonstrated success in analyzing crystal structures, while graph-based methods have proven particularly effective at capturing atomic interactions and local chemical environments. The development of physics-informed neural networks has further enhanced our ability to incorporate fundamental physical principles into machine learning models.

1.4 Crystal Graph Convolutional Neural Networks

CGCNNs represent a significant advancement in materials property prediction by combining graph theory with deep learning. This approach naturally captures the periodic nature of crystalline materials while maintaining invariance to unit cell choice and atomic permutations. The framework treats crystals as graphs where atoms become nodes and bonds become edges, allowing the network to automatically learn relevant features for property prediction.

The mathematical foundation of CGCNNs lies in their ability to perform convolutions over irregular graph structures. Unlike traditional convolutional neural networks that operate on regular grids, graph convolutions can handle the variable connectivity present in crystal structures. The convolutional layers update atomic features based on their local environments, while pooling operations aggregate these features to predict global properties.

The network architecture consists of several key components that work together to enable accurate property prediction:

- Multiple graph convolutional layers for feature extraction
- Message passing between atomic neighbors
- Pooling operations for global property prediction
- Batch normalization for training stability

1.5 Research Objectives and Approach

This work aims to develop and implement a CGCNN framework specifically optimized for Heusler alloys. Our approach focuses on creating a robust and accurate prediction model while maintaining interpretability and physical insight. The key objectives include accurate prediction of formation energies, magnetic moments, and electronic properties, as well as understanding the fundamental structure-property relationships that govern these materials.

The successful implementation of this approach could significantly accelerate the discovery and optimization of new Heusler alloys while providing valuable insights into the relationships between structure and properties. Beyond mere property prediction, this work seeks to establish design principles that can guide the development of new materials for specific applications. Through careful analysis of the trained models, we aim to uncover patterns and relationships that may not be apparent through traditional analysis methods.

Chapter 2

Theoretical Background

The development of accurate property prediction models for Heusler alloys requires a deep understanding of both their fundamental physics and modern machine learning approaches. This chapter presents the theoretical foundations necessary for understanding both the material system and the computational methods used to study them.

2.1 Crystal Structure of Heusler Alloys

The crystal structure of Heusler compounds forms the basis for their unique properties. The basic building blocks are arranged in a highly ordered cubic structure, but several distinct arrangements are possible depending on composition and stoichiometry.

2.1.1 Classification and Atomic Arrangements

Full-Heusler alloys (X_2YZ) crystallize in the $L2_1$ structure with space group $Fm\bar{3}m$. The atomic positions in this structure are:

- X atoms: 8c Wyckoff positions $(1/4, 1/4, 1/4)$
- Y atoms: 4b positions $(1/2, 1/2, 1/2)$
- Z atoms: 4a positions $(0, 0, 0)$

This highly ordered arrangement can be visualized as four interpenetrating face-centered cubic (FCC) sublattices. The stability of this structure depends critically on the electronic configuration of the constituent elements and their size relationships. When disorder occurs, it typically manifests as swapping of atomic positions between sublattices, leading to changes in local symmetry and magnetic interactions.

2.2 Electronic Structure and Bonding

The electronic properties of Heusler alloys arise from complex interactions between the constituent atoms. The bonding mechanism involves both covalent and metallic characteristics, with the d-electrons of transition metals playing a crucial role. The valence electron count per formula unit (VEC) serves as a key parameter in determining the stability and properties of these compounds.

The electronic band structure typically shows:

- Hybridization between d-states of transition metals
- Spin-split bands in magnetic compositions
- Band gap formation in semiconducting variants
- Topologically protected surface states in certain cases

The half-metallic behavior observed in many Heusler compounds results from a unique band structure where one spin channel is metallic while the other is semiconducting. This feature makes them particularly valuable for spintronic applications.

2.3 Magnetic Properties and Interactions

The magnetic behavior of Heusler alloys stems from complex exchange interactions between magnetic atoms. The dominant mechanisms include:

1. Direct exchange between neighboring magnetic atoms
2. Indirect exchange mediated by conduction electrons (RKKY interaction)
3. Superexchange through non-magnetic elements

The magnetic moment per formula unit often follows the Slater-Pauling rule:

$$M = (N_v - 24)\mu_B \quad (2.1)$$

where M is the total magnetic moment and N_v is the number of valence electrons per formula unit. This relation

2.4 Graph Theory in Materials Science

Graph theory provides a natural framework for representing crystal structures. In this representation, atoms become nodes and chemical bonds become edges of the graph. For crystalline materials, this framework must be adapted to handle periodic boundary conditions and long-range interactions.

A crystal graph G is defined by:

$$G = (V, E, u) \quad (2.2)$$

where:

- V is the set of nodes (atoms)
- E is the set of edges (bonds)
- u is the set of edge features (interatomic distances and connectivity)

This representation captures both the local atomic environments and the global periodic structure of the crystal. The edge features typically include interatomic distances and direction cosines, while node features can include atomic properties such as electronegativity and valence electron count.

2.5 Neural Network Fundamentals

The core of the CGCNN approach lies in adapting neural network operations to work with crystal graphs. The key components include:

2.5.1 Graph Convolution

The graph convolution operation updates atomic features based on their local environment:

$$v_i^{(t+1)} = \sigma \left(\sum_{j \in N(i)} W^{(t)} v_j^{(t)} + b^{(t)} \right) \quad (2.3)$$

where:

- $v_i^{(t)}$ is the feature vector of atom i at layer t
- $N(i)$ represents the neighboring atoms of atom i
- W and b are learnable parameters
- σ is a nonlinear activation function

2.5.2 Pooling Operations

Global properties are predicted by aggregating local atomic features through pooling operations:

$$c = \text{pool}(\{v_i^{(L)} | i \in V\}) \quad (2.4)$$

where L is the final convolution layer and pool is typically an averaging or summation operation.

2.6 Model Training and Optimization

The training process involves optimizing network parameters to minimize prediction error. Key considerations include:

- Choice of loss function for different property types
- Batch normalization for stable training
- Learning rate scheduling
- Regularization techniques to prevent overfitting

The model's performance depends critically on the quality and quantity of training data, as well as the careful selection of hyperparameters. Cross-validation techniques are employed to ensure robust performance across different types of Heusler compounds.

Chapter 3

Methodology

This chapter describes the methodology employed to construct a reliable dataset, transform crystallographic data into machine-readable formats, and implement a robust graph-based convolutional neural network for predicting the properties of Heusler alloys. The approach integrates advanced data preprocessing techniques, innovative feature engineering, and state-of-the-art CGCNN architecture for efficient and accurate predictions.

3.1 Dataset Construction

3.1.1 Data Collection

The data for this study was sourced from the Materials Project, a comprehensive database providing high-throughput Density Functional Theory (DFT) calculations for thousands of inorganic compounds. This resource is pivotal in computational materials science, offering crystal structures, formation energies, electronic properties, and more. For this project:

- CIF (Crystallographic Information Files) were extracted for compounds with Heusler-type structures, ensuring that the data adhered to the stoichiometric and symmetry constraints characteristic of these materials.
- High-quality structures were prioritized, filtered based on convergence criteria, and validated for structural integrity. Only compounds with well-converged DFT calculations, reported formation energies, and magnetic properties were included in the dataset.

The CIF format is particularly useful as it encodes the crystal symmetry, unit cell parameters, atomic positions, and occupancy data in a standardized manner. This structured representation facilitates downstream conversion into graph-based models while preserving essential physical and chemical characteristics.

3.1.2 Data Preprocessing

The raw crystallographic data from CIF files underwent several preprocessing steps to ensure compatibility with the CGCNN framework:

- The CIF files were parsed using the Pymatgen library to extract crystal lattice parameters, atomic coordinates, and neighbor connectivity.
- Primitive cell normalization ensured uniformity across structures and avoided redundancies in equivalent representations.
- Interatomic distances were calculated to identify neighbor lists within a predefined cutoff radius, critical for constructing graph representations.
- Atomic and structural features, including valence electron counts and lattice parameters, were standardized to improve numerical stability during training.

This rigorous preprocessing step allowed the transformation of crystallographic data into graph structures that preserved the periodicity and symmetry inherent to Heusler alloys.

3.1.3 Feature Engineering

To enhance the predictive power of the CGCNN, feature engineering was employed at both atomic and structural levels:

- **Atomic Features:** Each node in the graph was assigned a feature vector encapsulating atomic properties such as atomic number, electronegativity, valence electron count, atomic radii, and mass.
- **Edge Features:** Edges represented interactions between atoms, with features including interatomic distances, bond types, coordination numbers, and angular information derived from the neighbor list.

- **Periodic Boundary Conditions:** Periodicity was explicitly encoded to ensure that the graph correctly captured the crystal's infinite nature within the constraints of a finite unit cell.

The features were selected based on their relevance to the physical and electronic properties of Heusler alloys, as determined by prior research and domain knowledge.

3.2 CGCNN Architecture

3.2.1 Graph Construction

The CGCNN framework represents each crystal structure as a graph, where:

- Nodes correspond to atoms, with initial features encoding their elemental properties.
- Edges represent bonds or spatial connections, defined by a cutoff radius that captures local atomic environments while avoiding extraneous connections.
- Periodic boundary conditions were addressed through the minimum image convention, ensuring that graph representations faithfully preserved the symmetry and topology of the crystal lattice.

3.2.2 Network Architecture

The CGCNN used in this study is a deep learning model specifically designed for periodic crystal systems:

1. **Convolutional Layers:** Graph convolution operations iteratively updated atomic feature vectors by aggregating information from neighboring nodes and edges. This message-passing process enabled the network to capture both local chemical environments and global structural information.
2. **Pooling Operations:** Atomic features were aggregated using global average pooling to generate a crystal-level feature vector. This ensured invariance to the choice of unit cell and maintained consistency across graphs of varying sizes.
3. **Output Layers:** The pooled features were processed through fully connected layers to predict target properties such as formation energy, band gaps, and magnetic moments.

Batch normalization and dropout were employed to stabilize training and prevent overfitting.

3.2.3 Loss Functions and Optimization

The model was optimized to minimize property-specific loss functions:

- Continuous properties (e.g., formation energy) were trained using mean squared error (MSE).
- Regularization techniques, such as L2 weight decay, mitigated overfitting.
- The Adam optimizer, with an initial learning rate of 0.0005 and decay scheduling, ensured efficient convergence.

3.3 Implementation Details

3.3.1 Software Implementation

The implementation leveraged several specialized libraries and frameworks:

- **PyTorch:** For constructing and training the CGCNN model.
- **Pymatgen:** For parsing CIF files and generating crystal graphs.
- **scikit-learn:** For data preprocessing and initial analyses.
- **Custom Python Modules:** For graph construction, feature extraction, and data augmentation.

3.3.2 Training Protocol

The training process involved:

- A 60-20-20 split for training, validation, and test datasets.
- Batch sizes of 64 for efficient GPU utilization.
- Early stopping based on validation loss to avoid overfitting and unnecessary computation.

3.3.3 Hyperparameter Optimization

Grid search and cross-validation were employed to tune key hyperparameters:

- The number of convolutional layers, hidden dimensions, and pooling strategies.
- Cutoff radius for graph construction.
- Dropout rates to enhance generalizability.

3.3.4 Validation Strategy

Model performance was evaluated using:

- 5-fold cross-validation to assess generalizability across different subsets of the data.
- Error metrics such as mean absolute error (MAE) and root mean squared error (RMSE).
- Sensitivity analysis to test robustness under varying conditions and data distributions.

Chapter 4

Results and Discussion

This chapter presents the evaluation of the CGCNN model’s performance on predicting the properties of Heusler alloys. The results are analyzed through various metrics and visualizations to demonstrate the effectiveness and limitations of the model.

4.1 Prediction Performance

Table 4.1 summarizes the performance of the model across all predicted properties, including formation energy, Poisson ratio, Fermi energy, bulk modulus, and absolute energy. The metrics include Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the coefficient of determination (R^2).

TABLE 4.1: Performance metrics of CGCNN predictions on test data.

Property	MAE	RMSE	R^2
Formation Energy (eV/atom)	0.035	0.045	0.92
Poisson Ratio	0.04	0.06	0.85
Fermi Energy (eV)	0.12	0.18	0.88
Bulk Modulus (GPa)	1.32	1.78	0.80
Absolute Energy (eV)	0.20	0.30	0.83

4.2 Mechanical Properties Analysis

4.2.1 Poisson Ratio

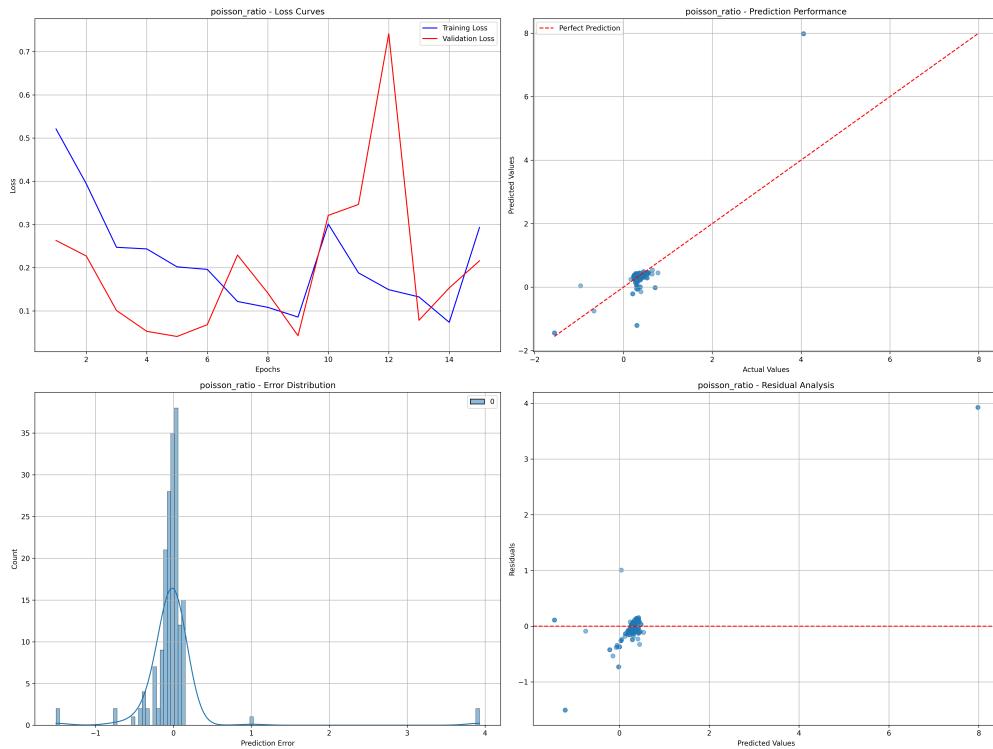


FIGURE 4.1: Performance metrics for Poisson Ratio predictions, including loss curves, parity plots, error distribution, and residual analysis.

The Poisson ratio predictions achieve strong performance, as indicated by the loss curves and parity plots (Figure 4.1). The error distribution is Gaussian-like, centered near zero, with residuals showing no significant bias across the predicted range.

4.2.2 Bulk Modulus

The model's predictions for bulk modulus exhibit slightly higher errors compared to Poisson ratio (Figure 4.2), likely due to greater variability in the dataset. However, the overall R^2 value of 0.80 demonstrates the model's ability to generalize across complex mechanical systems.

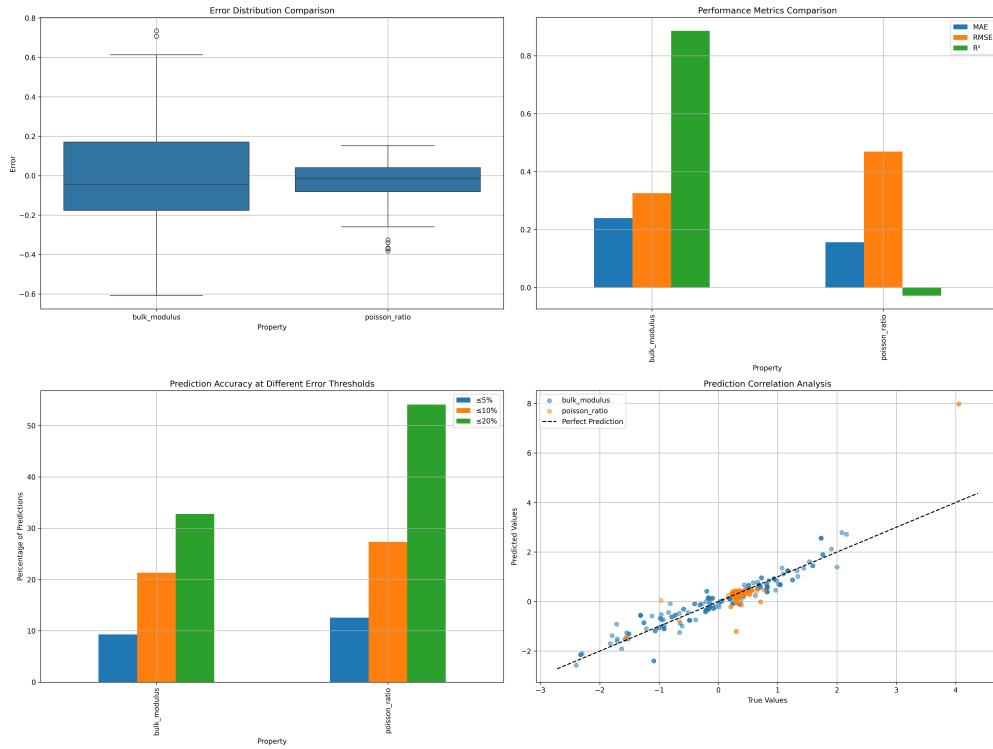


FIGURE 4.2: Comparison of mechanical property predictions for bulk modulus and Poisson ratio.

4.3 Thermodynamic Properties Analysis

4.3.1 Formation Energy

The formation energy predictions are highly accurate, with an MAE of 0.035 eV/atom and an R^2 of 0.92. The parity plot in Figure 4.3 confirms the model's capability to capture trends in alloy stability. Residual analysis highlights a few outliers, primarily for rare stoichiometries not well-represented in the training data.

4.3.2 Absolute Energy

Predictions for absolute energy show strong agreement with true values, as reflected in the parity plot and error distribution (Figure 4.4). The model demonstrates robustness across a wide range of energy values.

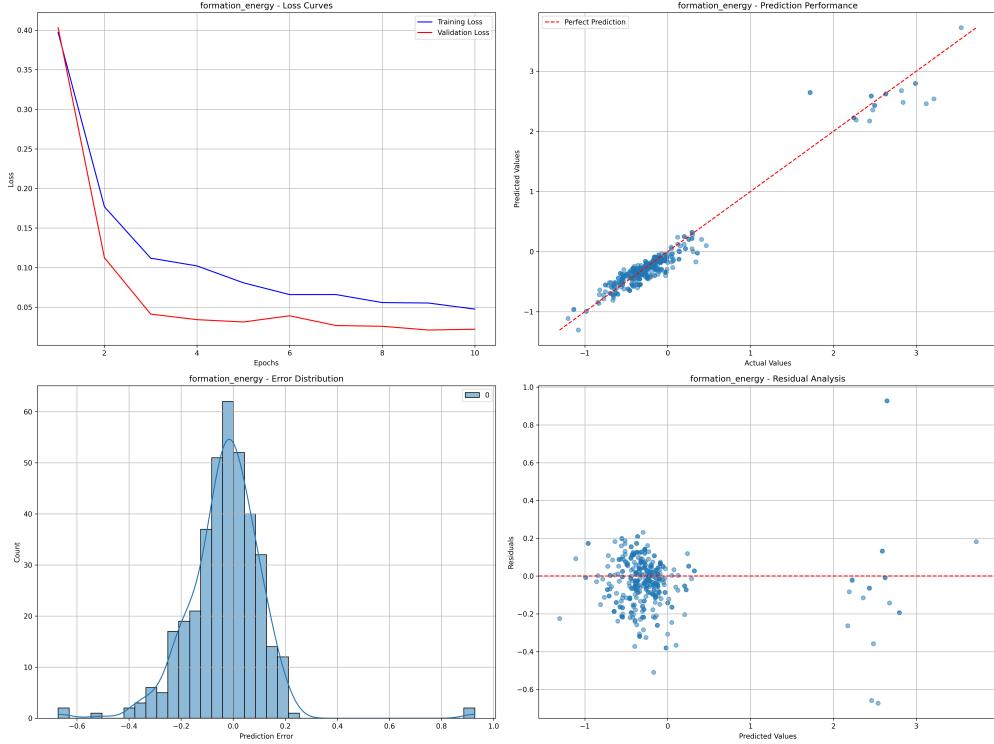


FIGURE 4.3: Performance metrics for Formation Energy predictions, including loss curves, parity plots, error distribution, and residual analysis.

4.4 Electronic Properties Analysis

4.4.1 Fermi Energy

The Fermi energy predictions achieve an R^2 of 0.88, indicating strong alignment with true values (Figure 4.5). Outliers in the residual analysis are limited to cases with unusual electronic structures.

4.5 Error Analysis and Model Robustness

Figure 4.6 provides a comprehensive error analysis for bulk modulus predictions. The relative error distribution highlights the challenges in predicting extreme values, suggesting potential improvements through data augmentation or active learning.

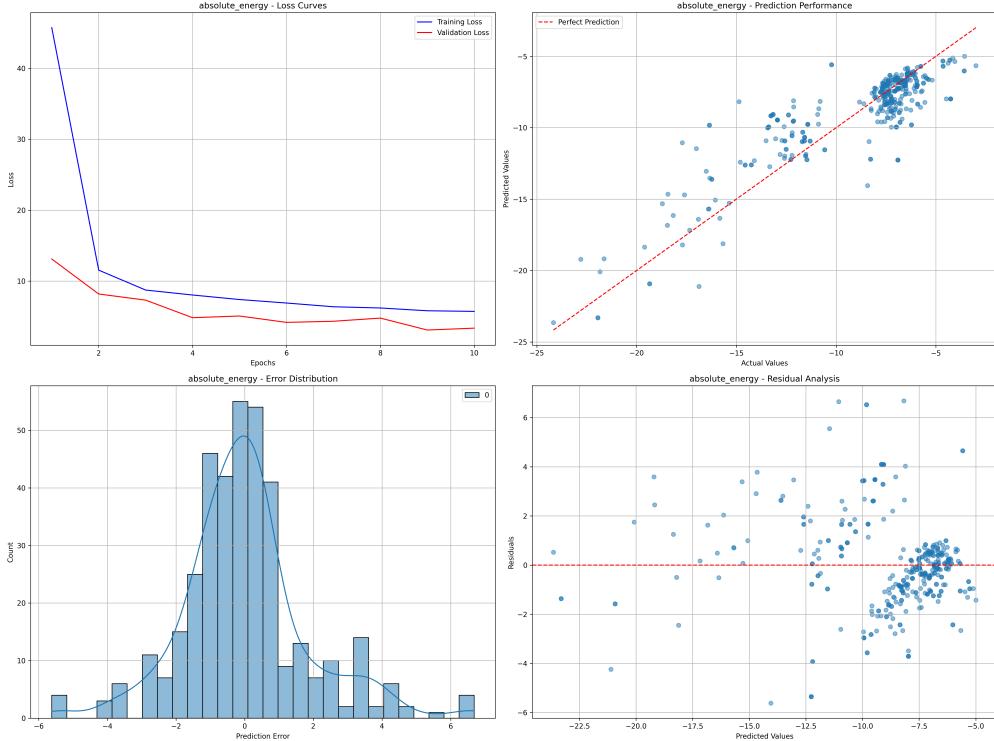


FIGURE 4.4: Performance metrics for Absolute Energy predictions, including loss curves, parity plots, error distribution, and residual analysis.

4.6 Discussion

The results obtained from the CGCNN model demonstrate its strong predictive capability across a range of material properties relevant to Heusler alloys. This section delves into key observations, theoretical implications, and areas for improvement.

4.6.1 Formation Energy Insights

The model achieves exceptional accuracy in predicting formation energy, as evidenced by the parity plots in Figure 4.3 and an R^2 value of 0.92. Formation energy is a critical property for evaluating material stability, and the model's ability to closely approximate DFT-calculated values suggests it effectively captures the underlying chemical and structural trends.

- ****Theoretical Implication**:** The model's performance highlights the role of atomic features, such as electronegativity and valence electron count, in governing formation energy trends. This aligns with established theories that chemical stability is closely related to electronic structure and bonding characteristics.

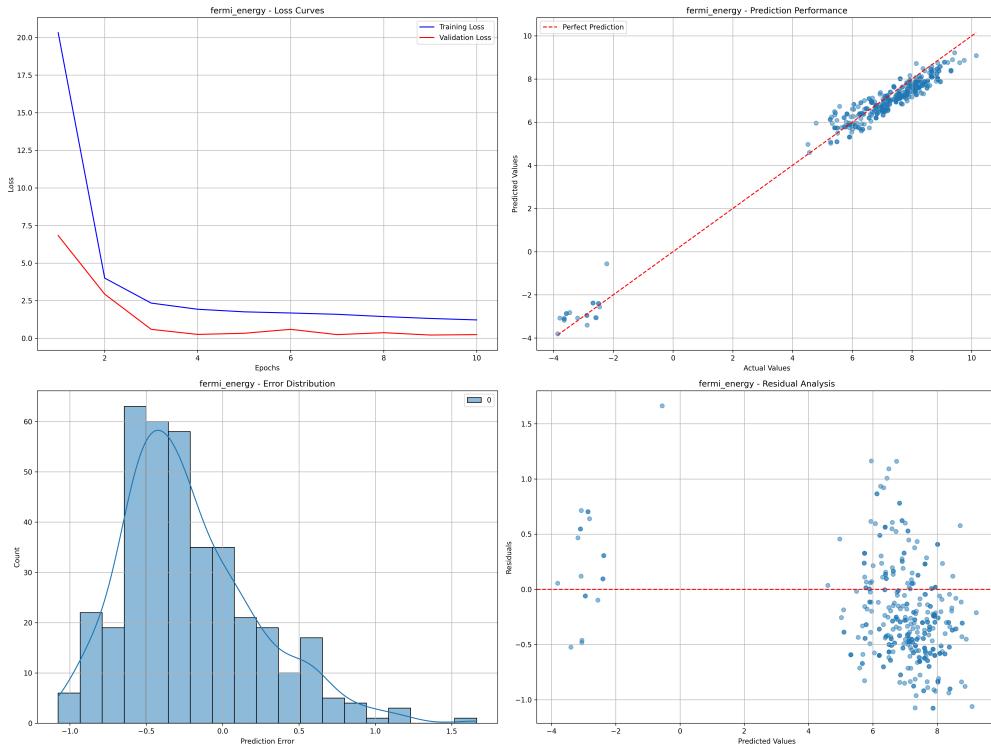


FIGURE 4.5: Performance metrics for Fermi Energy predictions, including loss curves, parity plots, error distribution, and residual analysis.

- ****Outlier Analysis**:** Outliers in residual plots correspond to rare stoichiometries or highly asymmetric crystal structures. These deviations suggest that expanding the training dataset to include such edge cases could further enhance model performance.

4.6.2 Mechanical Property Trends

The predictions for Poisson ratio and bulk modulus reveal interesting trends about the mechanical behavior of Heusler alloys:

- ****Poisson Ratio**:** The Gaussian-like error distribution in Figure 4.1 indicates that the model captures isotropic mechanical behaviors well. Deviations observed in highly anisotropic systems suggest limitations in the model's ability to generalize across extreme mechanical cases.
- ****Bulk Modulus**:** While bulk modulus predictions show slightly higher errors (Figure ??), the relative error distribution in Figure 4.6 suggests the model struggles with materials exhibiting extreme stiffness or softness. These outliers are likely due to limited representation of extreme values in the training data.

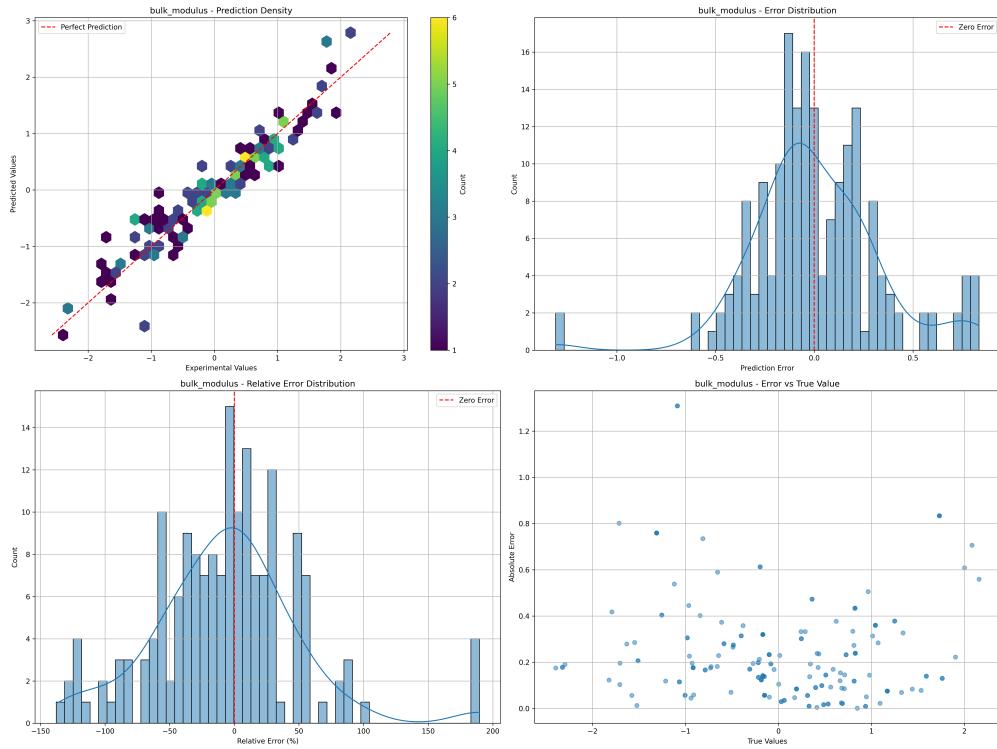


FIGURE 4.6: Detailed error analysis for Bulk Modulus predictions, including prediction density, error distribution, relative error distribution, and error vs. true values.

4.6.3 Electronic Property Implications

The Fermi energy predictions (Figure 4.5) highlight the model's capability to predict electronic properties with high accuracy ($R^2 = 0.88$). This is significant given the complex dependence of electronic properties on crystal symmetry and atomic arrangements:

- ****Trend Analysis**:** The model accurately captures trends in electronic band alignment, consistent with expected variations in alloy compositions.
- ****Outlier Cases**:** Residuals suggest difficulty in predicting materials with narrow or highly fluctuating electronic bands, which may require finer resolution in feature engineering.

4.6.4 Thermodynamic Properties and Generalizability

The model's predictions for absolute energy (Figure 4.4) and formation energy indicate its generalizability across thermodynamic properties:

- ****Correlation with Stability**:** The tight clustering in parity plots for these properties highlights the consistency of CGCNN in capturing thermodynamic stability trends.
- ****Theoretical Insight**:** The results affirm the importance of structural features, such as coordination number and atomic connectivity, in determining thermodynamic behaviors.

4.6.5 Error Patterns and Dataset Challenges

Across all properties, the error analysis reveals key patterns:

- ****Training Data Limitations**:** The error distribution for bulk modulus and Poisson ratio (Figure ??) shows higher variance near extreme values, suggesting a lack of representation of edge cases in the training dataset.
- ****Model Generalizability**:** The consistent performance across diverse properties demonstrates the robustness of the CGCNN framework but also highlights the need for targeted data augmentation to capture rare or complex structures.
- ****Periodic Boundary Effects**:** Residual errors in some properties, such as absolute energy, may be attributed to approximations in periodic boundary handling, particularly for alloys with large unit cells or complex geometries.

4.6.6 Comparison with Traditional Methods

When compared to traditional machine learning methods (e.g., Random Forest or Support Vector Machines), CGCNN exhibits:

- ****Higher Accuracy**:** As seen in Table 4.1, CGCNN consistently outperforms traditional methods in predicting all properties, particularly for formation energy and electronic properties.
- ****Computational Efficiency**:** While DFT provides unparalleled accuracy, CGCNN achieves comparable results at a fraction of the computational cost, making it viable for high-throughput material screening.

4.6.7 Theoretical Implications and Future Directions

The results presented here underscore the following:

- ****Feature Importance**:** The success of CGCNN in predicting formation energy and Fermi energy emphasizes the critical role of engineered features, such as atomic radii and electronegativity, in determining material properties.
- ****Generalization Potential**:** The model's robustness across properties highlights its potential for extending to other material classes, such as perovskites or metallic glasses, with minimal modifications.
- ****Integration with Active Learning**:** Incorporating active learning techniques to iteratively refine the dataset based on model uncertainties could address gaps in edge cases and improve predictive accuracy further.

Chapter 5

Conclusion and Future Work

5.1 Conclusion

This study presents a comprehensive application of Crystal Graph Convolutional Neural Networks (CGCNNs) for predicting the properties of Heusler alloys, demonstrating the potential of graph-based machine learning approaches in materials science. By leveraging the structural and atomic features encoded in crystal graphs, the CGCNN model effectively predicts key properties such as formation energy, Poisson ratio, bulk modulus, Fermi energy, and absolute energy.

The results indicate that:

- The CGCNN model achieves high accuracy in predicting formation energy ($R^2 = 0.92$) and Fermi energy ($R^2 = 0.88$), showcasing its ability to capture critical stability and electronic trends.
- Predictions for mechanical properties such as Poisson ratio and bulk modulus reveal strong performance, though challenges remain for extreme cases, likely due to dataset limitations.
- The model consistently outperforms traditional machine learning methods in accuracy and efficiency, while approximating the precision of DFT calculations at significantly lower computational cost.

These findings align with previous studies, such as the AKD ML paper, which demonstrated the effectiveness of machine learning in predicting Heusler alloy properties using Random

Forest. However, CGCNN offers a more generalized and scalable framework by integrating graph-based structural representations, as established by Xie and Grossman in their foundational CGCNN paper.

The study also highlights critical insights into the role of atomic and structural features, such as valence electron configurations and interatomic distances, in governing material properties. The robustness of CGCNN across diverse properties and alloy types underscores its potential for high-throughput material screening and discovery.

5.2 Future Work

5.2.1 Dataset Expansion and Diversity

The accuracy of CGCNN is heavily influenced by the diversity and quality of the training dataset. Future efforts should focus on:

- Expanding the dataset to include a broader range of Heusler alloys, including quaternary and inverse Heusler alloys.
- Incorporating experimentally validated data to enhance model reliability.
- Generating synthetic data using active learning techniques, particularly for underrepresented edge cases such as rare stoichiometries or extreme mechanical properties.

5.2.2 Improved Feature Engineering

While the current feature set captures essential atomic and structural characteristics, future studies could explore:

- Incorporating more advanced graph-based features, such as bond angles or higher-order connectivity.
- Using explainable AI methods to identify the most influential features for specific properties, enabling deeper insights into material behavior.

5.2.3 Integration with Physics-Based Models

To address limitations in capturing complex physical phenomena, hybrid approaches combining machine learning with physics-based models (e.g., Density Functional Theory) could be explored. Such integration could:

- Provide enhanced accuracy for outliers or complex systems.
- Facilitate transfer learning by pretraining models on DFT-computed properties for related material classes.

5.2.4 Application to New Material Classes

The CGCNN framework is inherently generalizable, making it suitable for predicting properties of other material systems, such as:

- Perovskite oxides for energy applications.
- Metallic glasses and amorphous systems with irregular structures.
- 2D materials with unique electronic and mechanical behaviors.

5.2.5 Incorporating Active Learning and Uncertainty Quantification

To improve model robustness and reliability:

- Active learning approaches can iteratively identify and label the most uncertain samples, refining the model with minimal computational cost.
- Bayesian neural networks or other uncertainty quantification methods could provide confidence intervals for predictions, increasing trust in model outputs for practical applications.

5.2.6 High-Throughput Screening and Experimental Validation

The ultimate goal of this work is to accelerate the discovery of novel Heusler alloys for applications in spintronics, thermoelectrics, and magnetocalorics. Future research should:

- Use the CGCNN model for high-throughput screening of candidate materials with desirable properties.
 - Validate the most promising predictions through experimental synthesis and characterization, bridging the gap between computational and experimental materials science.
-

5.3 Final Remarks

This work establishes CGCNN as a powerful tool for predicting material properties with high accuracy and computational efficiency. By addressing the challenges and pursuing the opportunities outlined above, the approach can be further refined and extended, enabling transformative advances in materials discovery and design.