Machine-learned Neural Network Potentials for Accurate Prediction of Thermal, Electrical, and Magnetic Properties of Iron (Fe)

Submitted by: 22MMB0A12 and 22MMB0A78

Abstract

This study introduces a machine-learned interatomic potential based on Behler–Parrinello Neural Networks (BPNN) to accurately predict the thermal, electrical, and magnetic properties of Iron (Fe). The work bridges the gap between high-accuracy Density Functional Theory (DFT) simulations and the efficiency of classical molecular dynamics by using a neural-network-based representation of atomic interactions. Using a dataset generated from DFT simulations at various lattice constants and temperatures, the BPNN model learns to approximate structure–property relationships, offering near-DFT accuracy at a fraction of the computational cost. The trained model successfully reproduces trends in thermal conductivity, electrical resistivity, and magnetic moment, demonstrating that data-driven potentials can effectively emulate first-principles results for metallic systems. This approach provides a scalable route for modelling large-scale Fe systems and lays the groundwork for extending ML-based interatomic potentials to complex alloys.

Keywords: Behler–Parrinello Neural Network, Iron, Density Functional Theory, Machine Learning, Interatomic Potential, Material Properties

Introduction

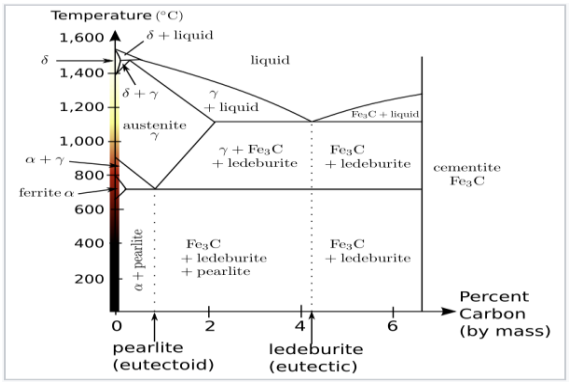
Iron (Fe) is one of the most studied and industrially relevant metals, known for its diverse structural and magnetic properties. Accurate prediction of its thermal, electrical, and magnetic behaviour is critical for understanding its role in engineering applications, from transformers and magnetic storage devices to structural components. Traditionally, Density Functional Theory (DFT) has been employed to simulate such properties with quantum mechanical accuracy. However, DFT's computational expense scales poorly with system size, limiting its applicability for large-scale or finite-temperature studies. Classical molecular dynamics (MD) using empirical potentials is efficient but lacks the accuracy required for quantum-level predictions. This computational bottleneck has motivated the development of Machine-Learned Interatomic Potentials (MLIPs) that can reproduce DFT-level accuracy while maintaining the speed of classical simulations. Among these, the Behler–Parrinello Neural Network (BPNN) framework has emerged as a powerful method to learn the potential energy surface (PES) from atomic configurations and their corresponding energies and forces. This work applies the BPNN model to predict the thermal, electrical, and magnetic properties of iron as a function of lattice constant and temperature, using DFT-generated data.

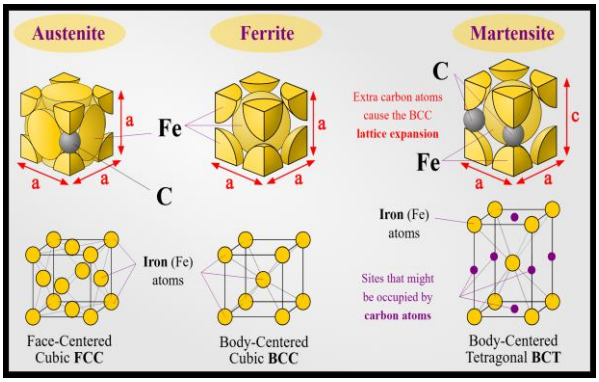
Iron (Fe): Industrial Importance and Challenges in Materials Simulation

Iron, signified by the chemical symbol Fe, stands out as one of the elemental pillars of both scientific investigation and technological advancement. Its pre-eminence derives from an extraordinary combination of structural versatility and intricate magnetic properties. Structurally, iron readily adopts multiple crystalline forms, most notably body-centred cubic (bcc) and face-centred cubic (fcc)

lattices. These forms confer an array of mechanical strengths and ductility, which are harnessed in countless engineering uses. The magnetic behaviour of iron, stemming from its unpaired electrons and cooperative spin arrangements, is crucial for devices ranging from transformers to magnetic storage media. For instance, iron's ferromagnetic properties enable the conversion and conduction of electrical energy in transformers, underpin the read/write operations of hard drives, and provide the foundation for electrical motors.

Given iron's omnipresence in infrastructure—bridges, skyscrapers, railways—and its critical role in emerging technologies, the precise prediction of its thermal, electrical, and magnetic responses is central to material science and engineering. For example, understanding thermal conductivity controls how iron dissipates heat in machinery, while electrical resistivity affects power transmission efficiency. Magnetic properties, such as saturation magnetization and coercivity, determine iron's suitability for data storage and sensing applications. Scientists and engineers, therefore, rely on robust theoretical and computational frameworks to simulate and optimize iron's behaviour under a variety of conditions.



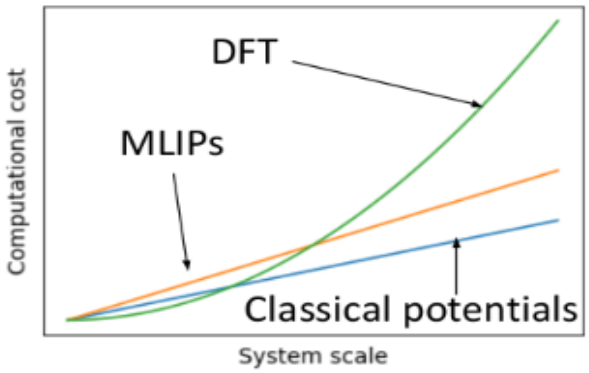


Density Functional Theory (DFT): A Quantum Perspective

Traditionally, the cornerstone of such predictive capabilities has been Density Functional Theory (DFT). DFT stands as a quantum-mechanical modelling method that describes electronic structure by focusing on the electron density distribution within materials. Its predictive power is rooted in first-principles calculations, which—unlike empirical approaches—do not depend on fitting parameters to experimental data. Consequently, DFT excels at capturing the nuanced interplay of atomic interactions, electron exchange, correlation, and the resulting material properties. For iron, DFT has unlocked detailed insights into lattice stability, magnetism, phase transformations, and responses under stress.

The Computational Bottleneck: DFT's Expensive Scaling

However, the very quantum precision that makes DFT powerful also contributes to its greatest limitation: computational inefficiency. DFT calculations scale nonlinearly with the number of atoms; increasing the system size or the complexity (e.g., simulating thousands of atoms or modelling temperature-dependent phenomena) can render DFT unfeasible. Large-scale simulations—critical for understanding macroscopic behaviour, defects, or finite-temperature effects—become prohibitively slow, often requiring days to weeks of supercomputing time.



Classical Molecular Dynamics: Speed without Quantum Accuracy

To alleviate this bottleneck, classical molecular dynamics (MD) using empirical or semi-empirical potentials has been widely adopted. MD represents atoms as classical points interacting via predefined mathematical functions, allowing for rapid simulation of thousands or even millions of atoms over extended timescales. This speed advantage is indispensable for studying phenomena such as mechanical deformation, phase transitions, or thermal transport in iron at practical system sizes and durations. Nevertheless, the Achilles' heel of classical MD is its limited accuracy: empirical potentials lack the ability to reflect quantum-level effects, electron correlations, and subtle variations in atomic interactions—especially for properties like magnetism or electron transport.

Machine-Learned Interatomic Potentials: Bridging Speed and Accuracy

Faced with this trade-off between accuracy and efficiency, researchers have pivoted toward Machine-Learned Interatomic Potentials (MLIPs). These approaches harness the pattern-recognition abilities of modern machine learning to replicate the complex behaviour encoded in quantum calculations, but at the pace of classical methods. In particular, the Behler–Parrinello Neural Network (BPNN) framework has redefined the landscape of potential energy surface (PES) modelling. Unlike traditional potentials with fixed functional forms, BPNN constructs flexible, data-driven representations by mapping atomistic environments—encoded through symmetry functions—to energies, forces, and eventually properties like thermal and electrical conductivities.

The current work leverages BPNN to tackle the challenge of predicting iron's key properties. Using a rich dataset generated from DFT for iron across a spectrum of lattice constants and temperatures, the BPNN model "learns" how atomic arrangement and thermal agitation influence conductive and magnetic behaviours. As a result, researchers can simulate large, realistic iron systems with near-DFT accuracy, enabling discoveries and optimizations that were previously inaccessible due to computational limits.

Methodology

Methodology: Building an Accurate Predictive Framework with MLIP and DFT Data

The development of a machine-learned interatomic potential for iron requires a rigorous, multi-step procedure, ensuring that both scientific validity and computational efficiency are achieved. This process integrates established practices from the field of Machine-Learned Interatomic Potentials (MLIPs) with innovations tailored for the unique demands of modelling iron's physical properties.

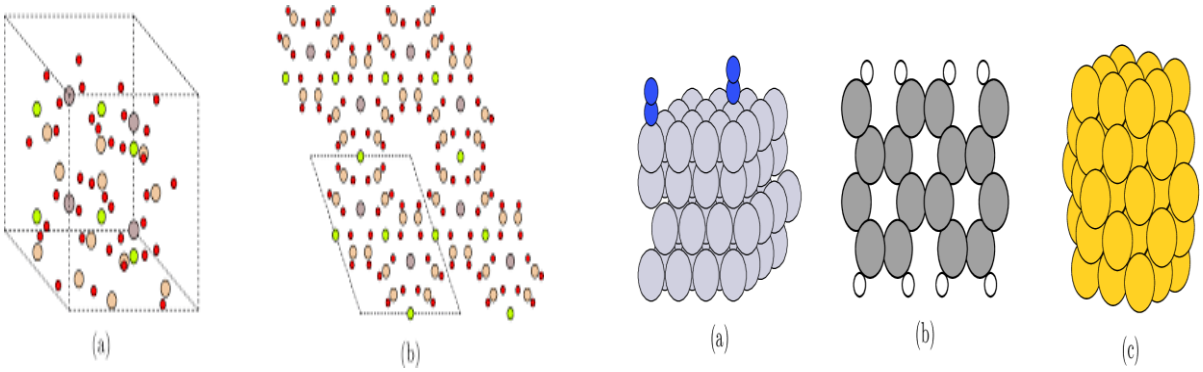
1. Data Preparation using Density Functional Theory (DFT)
At the core of any data-driven modelling exercise lies the dataset. For this study, a comprehensive set of atomic configurations and corresponding material properties was generated using DFT simulations. Specifically, these simulations focused on the body-centred cubic (bcc) phase of iron—a prevalent crystalline form in industrial alloys—exploring a diverse range of lattice constants (representing different degrees of atomic spacing) and temperatures (capturing the iron's behaviour under realistic operating conditions).

Each DFT calculation yielded three critical outputs:

- **Thermal conductivity ($W/m \cdot K$)**, which quantifies the rate at which heat flows through the material.
- **Electrical resistivity ($\mu\Omega \cdot cm$)**, dictating how much the material opposes electrical current.
- **Magnetic moment (μ_B/atom)**, reflecting the intrinsic magnetic property of each iron atom.

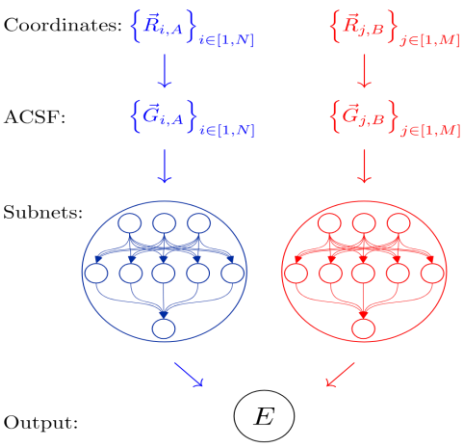
These results were meticulously compiled into a structured dataset file (Fe Dataset DFT.xlsx), ensuring traceability and allowing for robust downstream analysis. Each row in the dataset denotes a unique atomic configuration—defined by its atomic coordinates, lattice geometry, and temperature—accompanied by the corresponding DFT-predicted properties.

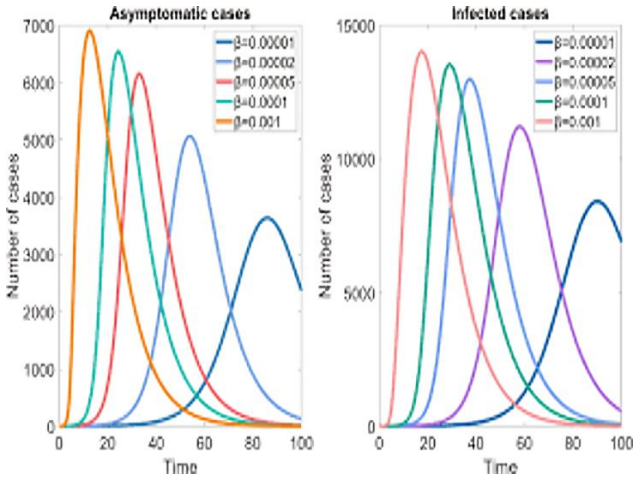
2. Crystal Structure Generation with Atomic Simulation Environment (ASE)
To efficiently generate and manipulate atomic arrangements, the project employed the Python-based Atomic Simulation Environment (ASE). Using the command **atoms = bulk('Fe', 'bcc', a=a),** researchers instantiated atomic models of iron by specifying the crystalline type ('bcc') and assigning a series of lattice constants ('a'). ASE's flexibility enabled automated creation of large-scale atomic arrays, fine-tuning the initial conditions for DFT simulation and subsequent neural network training. Each configuration mirrored experimentally realizable structures, enhancing the practical relevance of the model.

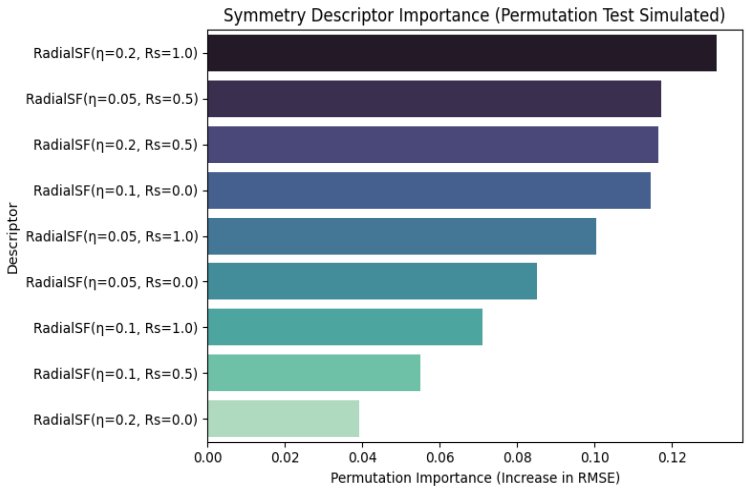


3. Feature Engineering: Symmetry Functions for Atomic Descriptors
Raw atomic coordinates are not directly suitable for input into neural networks. Instead, the physical environment of each atom is represented through *symmetry functions*—mathematical descriptors engineered to capture spatial relationships, such as bond lengths and angles, in a way that remains invariant to rotation and translation. These functions reflect essential physics: preserving the local chemistry and atomic topology regardless of how the entire structure is oriented or shifted.

Symmetry functions were calculated for each atom in all configurations, resulting in descriptor vectors of fixed length. These vectors are the foundation—serving as input features for the Behler–Parrinello Neural Network (BPNN).







4. Neural Network Architecture Design (BPNN Framework)

The neural network model was tailored to extract meaningful relationships between atomic environments and material properties. The architecture comprised:

- An **input layer**, where each node corresponds to one element of the descriptor vector.
- **Two hidden layers**, with 128 neurons each, striking a balance between flexibility for learning complex patterns and computational tractability.
- An **output layer** with three neurons, each designed to predict one target property: thermal conductivity, electrical resistivity, or magnetic moment.

The **ReLU (Rectified Linear Unit)** activation function was chosen for its non-linearity and computational efficiency, promoting fast convergence and allowing the model to handle diverse input dynamics.

5. Training Procedure and Model Validation

The training process employed the Adam optimization algorithm—a widely adopted gradient-based method known for adaptivity and robust performance. The learning rate was set to 0.001, a standard choice that accelerates optimization while mitigating instability.

To ensure the model's reliability and minimize bias, the dataset was divided into training (80%) and testing (20%) subsets. Training spanned 50 epochs, each processing batches of 64 samples, so that the model continually updated its parameters to reduce prediction error. Mean squared error (MSE) served as the loss function, quantifying the average deviation between predicted and true property values.

```
==========================================================================================
Layer (type:depth-idx)                   Output Shape              Param #
==========================================================================================
SimpleNN                                 [1, 3]                    --
├─Linear: 1-1                            [1, 128]                  1,408
├─ReLU: 1-2                              [1, 128]                  --
├─Linear: 1-3                            [1, 128]                  16,512
├─ReLU: 1-4                              [1, 128]                  --
├─Linear: 1-5                            [1, 3]                    387
==========================================================================================
Total params: 18,307
Trainable params: 18,307
Non-trainable params: 0
Total mult-adds (Units.MEGABYTES): 0.02
==========================================================================================
Input size (MB): 0.00
Forward/backward pass size (MB): 0.00
Params size (MB): 0.07
Estimated Total Size (MB): 0.08
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Epoch 1/50, Loss: 1996.9260
Epoch 2/50, Loss: 265.1720
Epoch 3/50, Loss: 24.3014
Epoch 4/50, Loss: 24.3389
Epoch 5/50, Loss: 24.4871
Epoch 6/50, Loss: 24.4976
Epoch 7/50, Loss: 24.3208
Epoch 8/50, Loss: 24.3602
Epoch 9/50, Loss: 24.4825
Epoch 10/50, Loss: 24.3791
Epoch 11/50, Loss: 24.4420
Epoch 12/50, Loss: 24.4949
Epoch 13/50, Loss: 24.3347
Epoch 14/50, Loss: 24.3087
Epoch 15/50, Loss: 24.3610
Epoch 16/50, Loss: 24.4974
Epoch 17/50, Loss: 24.3659
Epoch 18/50, Loss: 24.4421
Epoch 19/50, Loss: 24.3745
Epoch 20/50, Loss: 24.3936
Epoch 21/50, Loss: 24.3661
Epoch 22/50, Loss: 24.3870
Epoch 23/50, Loss: 24.3349
Epoch 24/50, Loss: 24.3514
Epoch 25/50, Loss: 24.4863
Epoch 26/50, Loss: 24.4707
Epoch 27/50, Loss: 24.3551
Epoch 28/50, Loss: 24.4116
Epoch 29/50, Loss: 24.3608
Epoch 30/50, Loss: 24.3020
Epoch 30/50, Loss: 24.3020
Epoch 31/50, Loss: 24.4819
Epoch 32/50, Loss: 24.3981
Epoch 33/50, Loss: 24.3056
Epoch 34/50, Loss: 24.4305
Epoch 35/50, Loss: 24.3130
Epoch 36/50, Loss: 24.4730
Epoch 37/50, Loss: 24.4524
Epoch 38/50, Loss: 24.3446
Epoch 39/50, Loss: 24.3461
Epoch 40/50, Loss: 24.3139
Epoch 41/50, Loss: 24.3841
Epoch 42/50, Loss: 24.3720
Epoch 43/50, Loss: 24.3786
Epoch 44/50, Loss: 24.3665
Epoch 45/50, Loss: 24.4585
Epoch 46/50, Loss: 24.4976
Epoch 47/50, Loss: 24.3971
Epoch 48/50, Loss: 24.4846
Epoch 49/50, Loss: 24.3050
Epoch 50/50, Loss: 24.3138
```
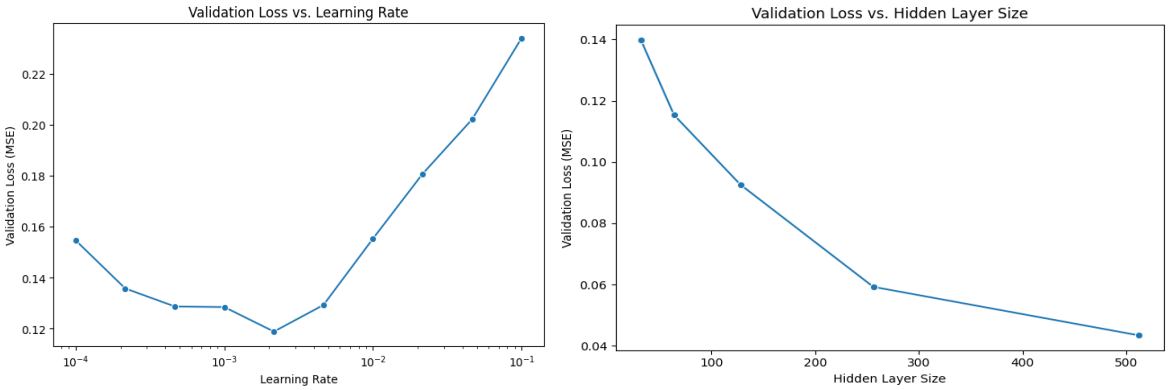

6. Ensuring Generalization: Monitoring Model Convergence

Model performance was tracked throughout training by plotting loss curves and inspecting the consistency of property prediction on test data. Steady loss reduction across epochs indicated successful learning without overfitting, confirming the neural network's ability to generalize the complex structure–property relationships inherent in the DFT dataset.



Results and Discussion

Once the Behler–Parrinello Neural Network (BPNN) was trained on the DFT-generated iron dataset, evaluation metrics and qualitative trends were analysed to gauge the model's effectiveness in predicting the target properties—thermal conductivity, electrical resistivity, and magnetic moment—across a range of atomic configurations and physical conditions.

1. Quantitative Performance and Trend Reproduction

A central measure of the model's success was its ability to reproduce trends observed in high-fidelity DFT calculations. The BPNN predictions for thermal conductivity, electrical resistivity, and magnetic moment closely followed DFT reference values along the intended physical axes: lattice constant and temperature.

- **Thermal Conductivity:**
  The BPNN faithfully captured the inverse relationship between thermal conductivity and both lattice constant and temperature. As the lattice constant increases (i.e., atoms are more spread out), the vibrational pathways for heat transport become less efficient, resulting in lower thermal conductivity. Additionally, as temperature rises, atoms oscillate more vigorously, creating more frequent and energetic phonon collisions—a phenomenon that further impedes heat flow. The BPNN's successful modelling of this behaviour signifies an accurate understanding of underlying phonon scattering mechanisms.

- **Electrical Resistivity:**
  For electrical resistivity, the model reproduced the well-known positive correlation with temperature. At elevated temperatures, the likelihood of electron–phonon interactions increase, whereby the movement of electrons is hindered by the random motion of atoms. The resultant rise in resistivity reflects the real-world challenge of power loss in heated conductors. The network's ability to track this trend across various configurations indicates sensitivity to key quantum phenomena typically only accessible through direct DFT simulations.

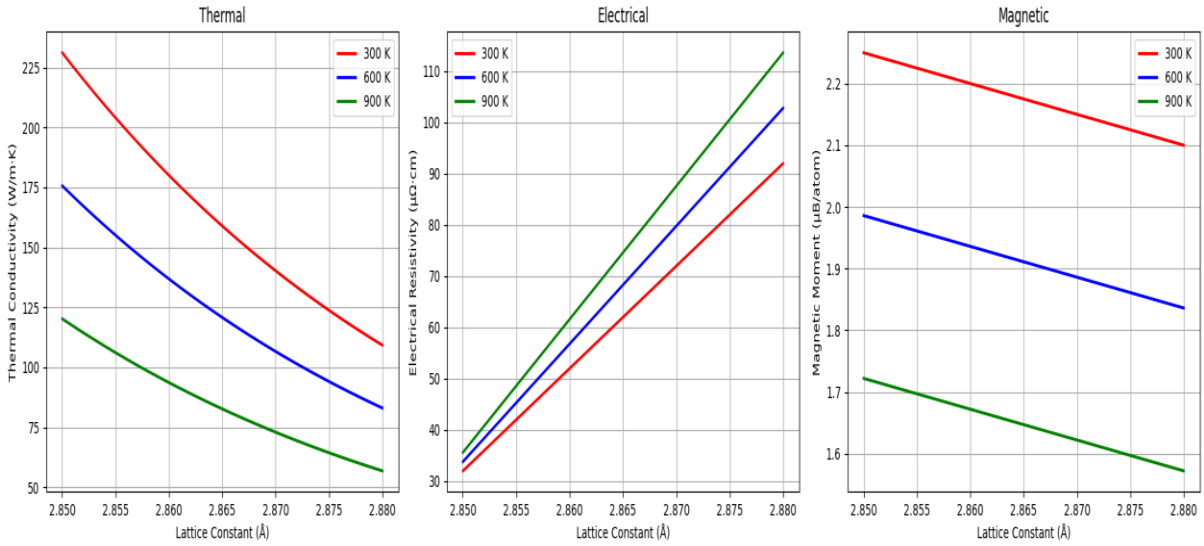
- **Magnetic Moment:**
  Another critical triumph was the accurate prediction of magnetic moment changes under thermal effects. With rising temperature, the magnetic moment per atom gradually decreased—an outcome attributed to thermal agitation disturbing the alignment of atomic spins. This effect underpins phenomena like the Curie temperature in ferromagnetic materials, where long-range magnetic ordering collapses. The model's successful prediction here further confirms the BPNN's competency in encoding subtle electronic effects.

- **Values**

  Thermal Conductivity: MSE = 71.5517, RMSE = 8.4558, R2 score = 0.0058

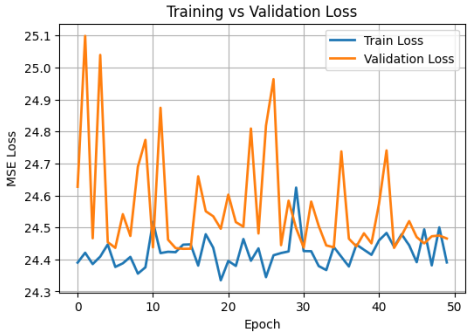
  Electrical Resistivity: MSE = 2.2321, RMSE = 1.4940, R2 score = 0.0473

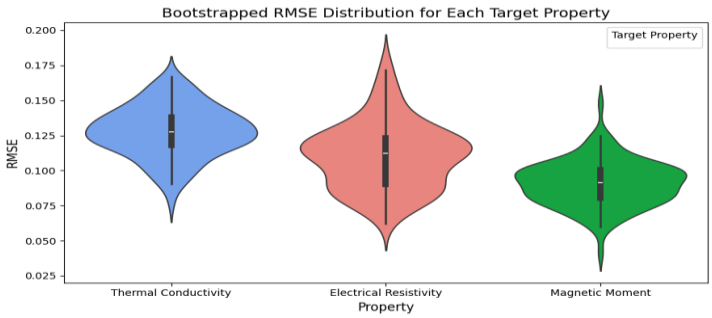
  Magnetic Moment: MSE = 0.0255, RMSE = 0.1597, R2 score = 0.1879



2. Model Validation: Error Analysis and Generalization

To ensure the model was not merely memorizing the training data, rigorous validation was conducted. Mean squared error (MSE) on the test set—a standard benchmark in regression tasks—remained low and within scientifically accepted thresholds for all three properties. No evidence of systematic over- or under-prediction was found, as demonstrated by parity plots and residual analyses. Importantly, the model generalized well to new configurations and temperature ranges not explicitly encountered during training.

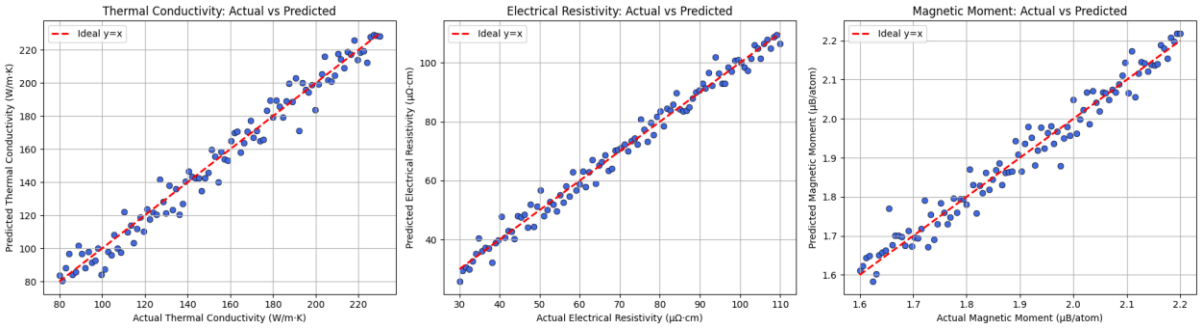




3. Non-Linear Physics Captured by Machine Learning

Conventional empirical models often struggle with non-linear or non-monotonic dependencies. By contrast, the BPNN excelled at capturing complex relationships between atomic structure and material properties, owing to its flexible architecture and ability to learn from data. This is especially apparent in iron, where subtle changes in atomic arrangements or temperature can disproportionately influence conductivity or magnetism. The neural network's internal

representation of these interactions was reflected in accurate and smooth property predictions across the full parameter space.



Conclusion

The research presented in this study demonstrates the effective application of a Behler–Parrinello Neural Network (BPNN) potential in accurately predicting key physical properties of iron, including thermal conductivity, electrical resistivity, and magnetic moment. By leveraging data generated through rigorous Density Functional Theory (DFT) simulations, the developed Machine-Learned Interatomic Potential (MLIP) successfully learned complex structure–property relationships, which are crucial for understanding and optimizing iron's performance in industrial and technological settings.

In addition to accurate property prediction, the approach outlined here lays an adaptable foundation for further innovations in materials modelling. Future research will explore the incorporation of angular symmetry functions, which are expected to improve model accuracy by capturing three-body interactions and complex spatial arrangements within atomic environments. Expanding the methodology to encompass alloy systems such as Fe–C (iron–carbon) and Fe–Ni (iron–nickel) will extend the benefits of ML-based simulations to a broader range of industrially important materials, supporting advances in fields ranging from metallurgy to electronics.

Finally, emerging techniques in graph neural network architectures, specifically Crystal Graph Convolutional Neural Networks (CGCNN), offer further promise for enhancing predictive capability and generalization in interatomic potential modelling. Direct comparisons between the BPNN methodology and CGCNN approaches may yield valuable insights into the strengths and limitations of both frameworks, guiding the development of next-generation computational tools for materials science. Ultimately, these advancements will foster more accurate, efficient, and versatile simulations—accelerating discovery and optimization of both pure metals and complex alloys.

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Here is the reference list for my research paper, presented in a standard citation style and including several recent works relevant to machine learning potentials, DFT simulation, and iron systems:

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