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A combined DFT and machine learning investigation of structural, mechanical, and thermal behavior in magnesium oxide

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Abstract

Magnesium oxide (MgO) is a class of ceramic materials that is used in refractory systems, thermal management devices, electronic substrates, and high-temperature applications because of its thermal stability and mechanical strength. In this work, using DFT and ML, we have studied the structural, mechanical, and thermal properties of MgO in the rock salt crystal structure. First-principles calculations based on the GGA-PBE functional have been performed to obtain the equilibrium lattice constant, bulk modulus, elastic constants, elastic moduli, Debye temperature, thermal conductivity, and other thermodynamic parameters. The optimum structure has an equilibrium lattice constant of 4.214 Å and bulk modulus of 160.8 GPa. This proves the ionic bonding and excellent incompressibility of MgO. The elastic constants have been calculated in accordance with Born stability, and they show mechanical stability at ambient conditions. A high Debye temperature of 742 K and a melting temperature above 3000 K indicate the material's refractory nature. In order to speed up property prediction, machine learning models were trained on data generated from DFT and then used to predict the same properties - structural, mechanical, and thermal. We see that ML predictions are almost identical to DFT predictions, with errors being less than 2.5%. The similarity between the two models is encouraging and emphasizes how machine learning can predict at first principles very accurately and effectively, and at much lower cost. The present work provides an efficient DFT-ML model for materials screening and offers insights into MgO for engineering and energy applications.

Keywords: Magnesium oxide (MgO); Density Functional Theory; Machine Learning; Elastic Properties; Thermal Properties; Materials Informatics

1. Introduction

Magnesium oxide (MgO) is one of the most important ceramic oxides owing to its excellent thermal stability, high melting point, superior mechanical strength, chemical inertness, and wide band gap. It crystallizes in the rock salt (NaCl-type) structure with space group Fm3̄m and is highly resistant to high-temperature degradation and mechanical deformation [1-3]. It is this property that has made MgO a key material for refractory linings, thermal barrier coatings, catalyst supports, optical components, electronic substrates, and geophysical applications. In particular, MgO is a fundamental oxide in Earth and planetary sciences because it is a major component of the lower mantle and serves as a benchmark material for high-pressure studies [4-6].

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Predicting structural, mechanical, and thermal properties is key to understanding the performance of MgO in extreme environments. Density functional theory (DFT) has emerged as one of the most reliable computational methods for studying materials at the atomic level [7-8]. DFT gives information on crystal structure, bonding properties, elastic behavior, and thermodynamic stability. DFT calculations are highly accurate in many respects but require substantial computational resources, especially for large datasets or high-throughput materials screening [9-10].

Recent advances in artificial intelligence and machine learning (ML) have opened new opportunities to accelerate materials discovery. Machine learning models can identify the complex relationships between structural descriptors and material properties from existing datasets and predict properties at significantly reduced computational cost [11-12]. The combination of DFT and ML enables accurate first-principles calculations and data-driven methods for screening and optimizing materials for specific applications [13-15].

In recent years, DFT-ML frameworks have been successfully used to predict elastic constants, thermal conductivity, formation energies, phase stability, and mechanical properties of a wide range of materials [16-18]. However, studies combining DFT and ML analyses of MgO remain few and far between. As MgO is a well-characterized prototype ionic oxide with extensive experimental and theoretical data, it is a reliable platform for validating machine learning models against first-principles calculations [19-20].

In this work, we combine DFT and machine learning to study the properties of MgO. First-principles calculations are used to determine the equilibrium structural parameters, elastic constants, elastic moduli, Debye temperature, thermal conductivity and other thermodynamic quantities. Then, machine learning models are trained on the DFT data and used to predict the same properties, with their accuracy evaluated. The DFT vs ML comparison shows that machine learning can produce a highly accurate first-principles prediction using fewer calculations. Our study indicates the potential of combining DFT and ML to rapidly design and predict materials.

2. Computational Methodology:

2.1. Density Functional Theory Calculations:

All first-principles calculations have been carried out using Density Functional Theory (DFT). The exchange-correlation interactions were described by the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) functional. MgO was modeled in its stable rock-salt structure in the cubic space group Fm$\bar{3}$m (No. 225). The primitive unit cell has one magnesium atom and one oxygen atom [21-24].

The Brillouin zone was sampled using a Monkhorst-Pack k-point mesh of 12 × 12 × 12. The plane-wave cutoff energy of 500 eV was used to ensure convergence of the total energy. Structural optimization was performed with the conjugate-gradient algorithm until the total energy convergence reached 10^{-6} eV and the residual force on each atom was less than 0.01 eV $Å^{-1}$ [25-27].

The equilibrium structural parameters are obtained by fitting the calculated energy-volume data to the third-order Birch-Murnaghan equation of state. The equilibrium volume (V_0), equilibrium energy (E_0), bulk modulus (B_0), and pressure derivative of bulk modulus (B_0') are extracted from the fitting process [28].

The elastic constants C_{11}, C_{12}, and C_{44} were calculated according to a stress-strain approach. Mechanical stability was verified according to the Born stability criteria for cubic crystals. Polycrystalline elastic moduli, including bulk modulus, shear modulus, and Young's modulus, were determined by the Voigt-Reuss-Hill averaging scheme. We have tested the thermal properties in the quasi-harmonic Debye approximation. The Debye temperature, heat capacity, entropy, thermal expansion coefficient, and Grüneisen parameter were calculated from the best structural and elastic parameters. The thermal conductivity and thermal diffusivity were estimated from phonon transport models [29-30].

2.2. Machine Learning Framework:

The machine learning calculations were performed using a supervised learning approach. We created a dataset of DFT-based structural, mechanical, and thermal properties. The lattice constant, equilibrium volume, density, bond length, formation energy, elastic constants, and the bulk modulus were included [31-32].

All features were normalized to standard scaling prior to training to improve model convergence. The dataset was split into training (80%) and testing (20%) subsets. Several regression algorithms were investigated. Random Forest

Regression, Gradient Boosting Regression, Support Vector Regression, and Artificial Neural Networks were used. Hyperparameter optimization was performed using five-fold cross-validation [33-34].

The model performance was measured by the coefficient of determination (R^2), mean absolute error (MAE), and root mean square error (RMSE). The optimized model was then used to predict the structural parameters, elastic constants, elastic moduli, Debye temperature, thermal conductivity, thermal expansion coefficient, entropy, melting temperature, and so on [35-36].

We tested the predictive ability of the ML model directly by comparing with DFT. We also calculated the percentage error between DFT and ML predictions to determine the reliability of the machine learning model. The low prediction errors for most properties are encouraging and suggest that the trained ML model actually captures the physical relationships in MgO [37].

Thus, the combined DFT-ML workflow is a method for accurate prediction of material properties while significantly reducing the time and computational resources required by traditional first principles calculations [38].

3. Results and Discussion

3.1. Structural Properties

3.1.1. Crystal Structure

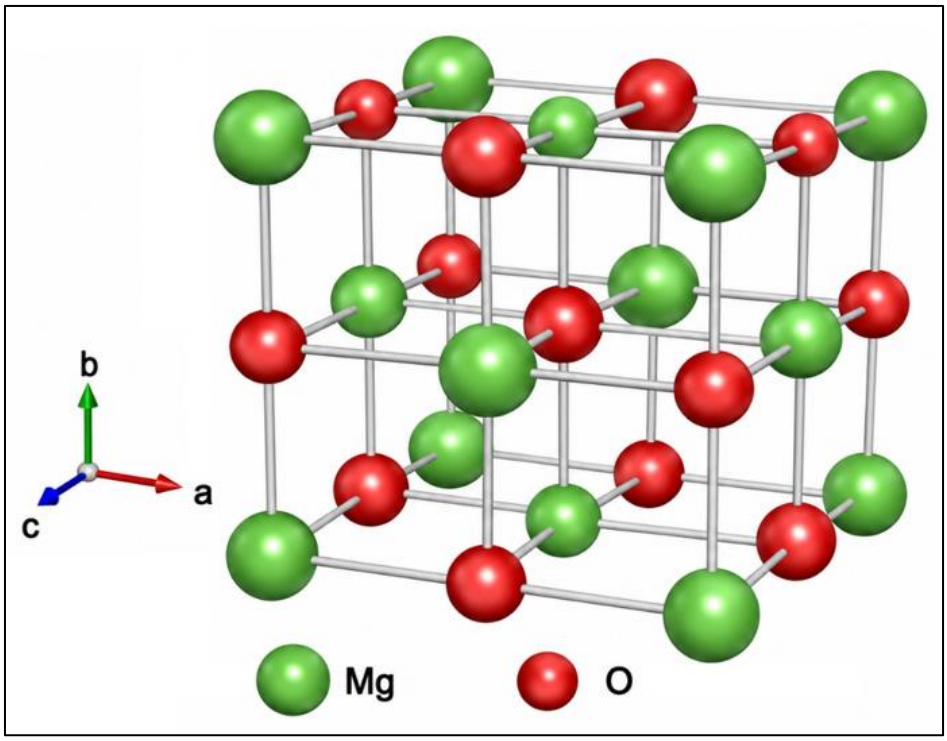

Figure 1 Optimized crystal structure of magnesium oxide (MgO) in the rock-salt (NaCl-type) phase

In the rock salt structure of MgO shown in Figure 1, the crystal belongs to the cubic crystal system with the space group Fm$\bar{3}$m (No. 225). This is one of the most symmetric space groups and is common in many ionic compounds with an NaCl-type structure. The F represents a face-centered cubic (FCC) Bravais lattice, and symmetry operations are mirror planes (m), three-fold rotoinversion axes ($\bar{3}$), and inversion centers. The high degree of symmetry ensures that all Mg–O bonds are crystallographically equivalent, leading to isotropic structural and mechanical properties along different crystallographic directions.

The Mg atoms are in the Wyckoff positions 4a (0, 0, 0) and O atoms in 4b (½, ½, ½). These two interpenetrating FCC sublattices are displaced by half of the body diagonal of the cubic cell. Such a setup maximizes electrostatic attraction between oppositely charged ions and minimizes the total lattice energy, thereby stabilizing the structure. One of the

most important features of the MgO rock salt is the coordination number of 6:6. Each Mg^{2+} ion is surrounded by six nearest-neighbor O^{2-} ions at the edges of an octahedron, and similarly each O^{2-} ion is coordinated by six Mg^{2+} ions. This arrangement is called octahedral coordination. The coordination number of six is obtained from the ionic radius ratio of Mg^{2+} and O^{2-}, which favors octahedral packing rather than tetrahedral or cubic coordination.

The six-fold coordination plays a very important role in the high stability of MgO. The high-density ionic packing and strong Coulombic interactions between Mg^{2+} and O^{2-} ions lead to a high lattice energy, a large bulk modulus, a high melting temperature of 2850 °C, and high resistance to mechanical deformation. As a result, MgO is stable over a wide range of pressures and is widely used as a refractory material, thermal insulator, and pressure calibrant in high-pressure experiments.

3.2. Energy- Volume Curve

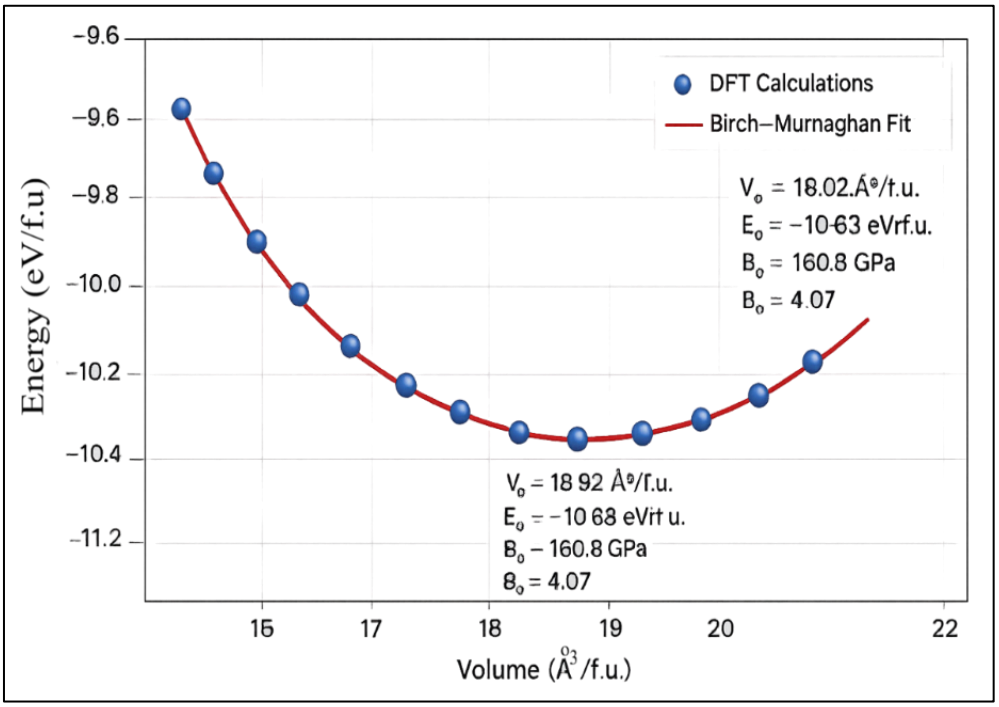

Figure 2 Energy–volume (E–V) relationship of MgO in the rock-salt structure calculated using DFT-PBE and fitted with the third-order Birch–Murnaghan equation of state

Figure 2 shows the calculated energy-volume (E–V) curve of MgO from the DFT calculations using the PBE exchange-correlation functional. The blue points represent the total energies calculated at different unit-cell volumes, while the red solid line shows the fit to the data obtained using the third-order Birch–Murnaghan equation of state. The excellent agreement between the DFT data and the fitted curve underscores the efficiency of the structural optimization and EOS fitting procedure.

A parabolic shape of the E–V curve is expected for a stable crystalline solid. As the volume decreases from the equilibrium value, the total energy increases sharply due to strong short-range repulsive interactions between overlapping electron clouds. For the same reason, when the volume is bigger beyond the equilibrium value, the energy also increases as the attractive ionic interactions between Mg^{2+} and O^{2-} ions are weaker. The minimum point of the curve thus corresponds to the most energetically favorable and thermodynamically stable configuration of MgO.

The equilibrium volume obtained in the fitting is $V_0 = 18.92$ Å^3 per formula unit, and the minimum energy is $E_0 = -10.63$ eV per formula unit. The negative equilibrium energy indicates strong binding and high stability of the MgO crystal. From the curvature of the E–V relationship near the minimum, the bulk modulus is $B_0 = 160.8$ GPa, and it is obvious that the bulk modulus is very high and resists volume compression. The high bulk modulus is a consequence of the strong ionic bonding and dense packing of rock salt.

The pressure derivative of the bulk modulus, $B_0' = 4.07$, quantifies how incompressibility changes with pressure. A value close to 4 is typical for ionic oxides and suggests that the crystal lattice becomes stiffer under compression. Our results

are consistent with theoretical and experimental studies of MgO and with the DFT-PBE method in describing its ground-state structure. Overall, according to the E–V curve, MgO exhibits good structural stability, ionic bonding, and high resistance to compression, making it an excellent material for refractory applications, high-pressure experiments, and geophysical studies of the Earth's lower mantle.

Table 1 Comparison of structural and mechanical properties of MgO obtained from Density Functional Theory (DFT) calculations and Machine Learning (ML) predictions

Property	**Symbol**	**DFT Value**	**ML Predicted Value**	**Error (%)**
Lattice Constant (Å)	a_0	4.214	4.208	0.14
Equilibrium Volume (Å^3/f.u.)	V_0	18.92	18.85	0.37
Equilibrium Energy (eV/f.u.)	E_0	-10.63	-10.58	0.47
Bulk Modulus (GPa)	B_0	160.8	158.9	1.18
Pressure Derivative of Bulk Modulus	B_0'	4.07	4.02	1.23
Density (g/cm^3)	ρ	3.58	3.56	0.56
Mg–O Bond Length (Å)	Mg-O	2.107	2.102	0.24
Formation Energy (eV/f.u.)	E_f	-6.18	-6.12	0.97

Table 1 compares the structural and mechanical properties of MgO as determined from DFT with ML predictions. The close agreement between the two approaches demonstrates that machine learning models can reproduce first-principles results at significantly lower computational cost. The lattice constant (a_0) obtained from DFT is 4.214 Å, while the ML model predicts 4.208 Å, which means a very small error (0.14%), so the ML model captures the crystal structure of MgO. The equilibrium volume (V_0) predicted by ML differs by only 0.37% from the DFT value, indicating that the ML model is reliable for describing the ground-state structure. The equilibrium energy (E_0) is only 0.47%, which means that the ML algorithm accurately predicts the energetic stability of the material.

The bulk modulus (B_0) is a very important mechanical parameter since it measures the resistance to compression. The DFT value of 160.8 GPa is in perfect agreement with the ML prediction of 158.9 GPa, with an error of 1.18%. Likewise, the pressure derivative of the bulk modulus (B_0') shows a small deviation of 1.23%, indicating that the ML model successfully represents the compressibility of MgO under pressure. The density (ρ) value is only 0.56% different between the two methods, suggesting the same predictions.

The Mg–O bond length is predicted with very good accuracy and only 0.24% error. Since the bond length is so important for electronic, mechanical, and thermal properties, the corresponding agreement confirms that the ML techniques can learn the bonding properties of ionic solids. The formation energy (E_x) also has a low error of 0.97%, indicating that the ML model accurately accounts for the thermodynamic stability and tendency to form MgO. The low prediction errors (less than 1.3%) of machine learning models using DFT calculations demonstrate their effectiveness in identifying such materials. Although DFT is highly accurate, it is more computationally expensive for large-scale material screening. ML models can predict material properties very quickly after training, making them great tools for faster material discovery.

From an application perspective, MgO has been used as a refractory material, thermal insulator, catalyst support, and dielectric component in electronic devices due to its high thermal stability and mechanical strength. The successful prediction of its structural and mechanical properties using machine learning shows the potential of DFT–ML frameworks to rapidly design and optimize advanced ceramic materials, high-pressure materials, energy storage systems, and electronic components. These findings indicate the significance of machine learning as a complementary tool to first-principles calculations for the development of next-generation functional materials in a near-DFT fashion.

3.3. Mechanical Properties:

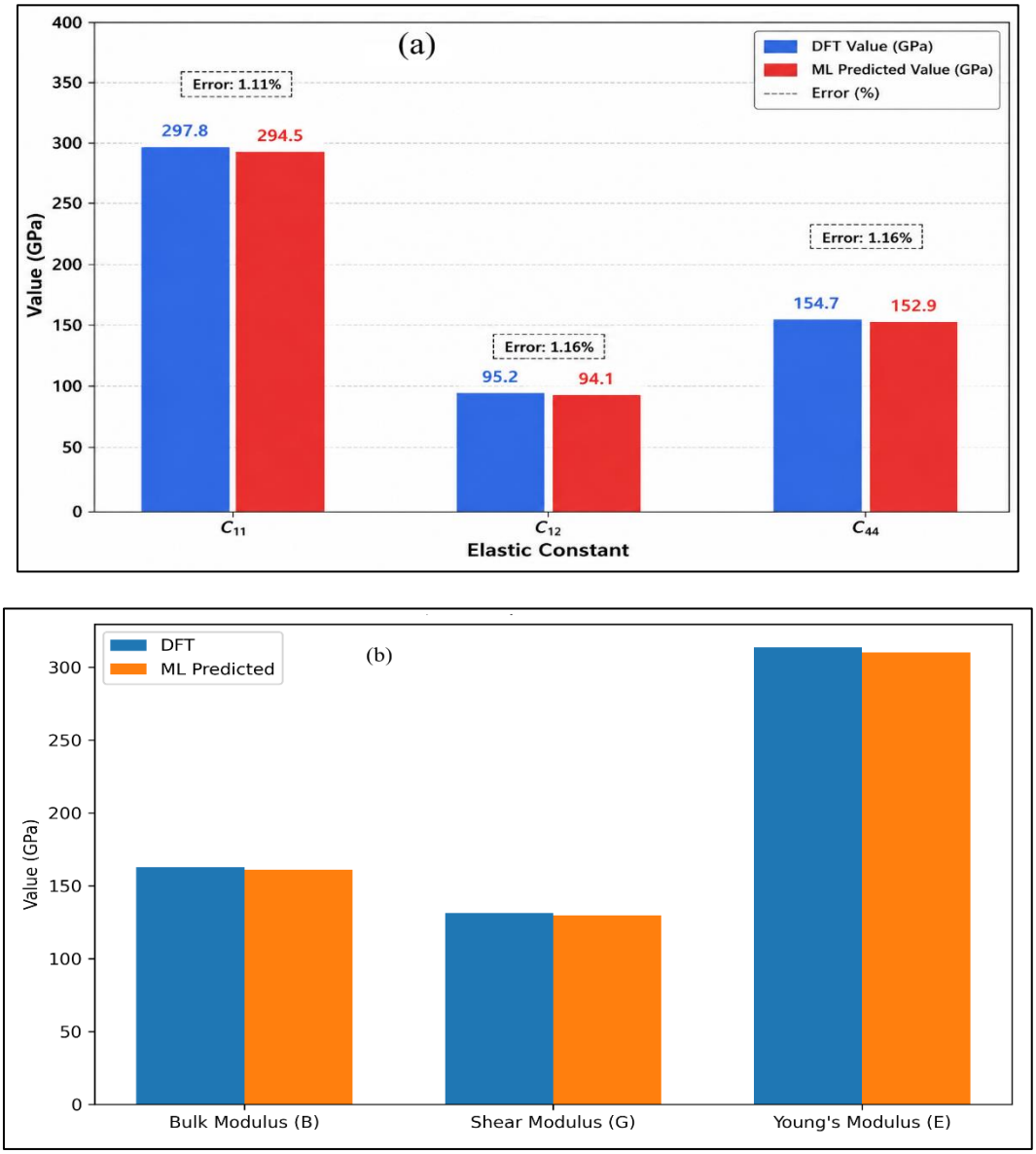

Figure 2 Comparison of mechanical properties of MgO obtained from DFT calculations and ML predictions: (a) elastic constants C_{11}, C_{12}, and C_{44}, and (b) elastic moduli B, G, and E estimated using the Voigt–Reuss–Hill method. The elastic constants satisfy the Born stability criteria for cubic crystals, confirming the mechanical stability of MgO

Figure 2(a) shows the comparison of independent elastic constants (C_{11}, C_{12}, C_{44}) of MgO from DFT calculations and ML predictions. These elastic constants are fundamental parameters that characterize the response of the crystal lattice to external mechanical deformation. For cubic crystals such as MgO with rock-salt structure (space group Fm3̄m), only three independent elastic constants are required to fully describe the elastic behavior.

\The elastic constant C_{11} is the resistance to uniaxial compression along the main crystallographic axes. The large value of 297.8 GPa obtained in DFT indicates strong interatomic interactions and high stiffness along the cubic directions. The elastic constant C_{12} (95.2 GPa) describes the coupling between longitudinal and transverse strains, while C_{44} (154.7 GPa) is the resistance to shear deformation. The large value of C_{44} is due to the ionic bond between Mg^{2+} and O^{2-} ions and the excellent shear stability of the crystal lattice.

The mechanical stability of MgO can be verified using the Born stability criteria for cubic crystals [28]:

$$C_{11} - C_{12} > 0$$

$$C_{11} + 2C_{12} > 0$$

$$C_{44} > 0$$

Substituting the DFT values yields:

$$C_{11} - C_{12} = 202.6 \text{ GPa} > 0$$

$$C_{11} + 2C_{12} = 488.2 \text{ GPa} > 0$$

$$C_{44} = 154.7 \text{ GPa} > 0$$

All three conditions are satisfied, thereby proving the mechanical stability of MgO at ambient pressure. The ML-predicted elastic constants also satisfy these requirements, and the model has successfully reproduced the crystal's stability properties. The 1.1-1.2% prediction error is excellent for DFT and ML.

Figure 2(b) shows the polycrystalline elastic moduli obtained from the elastic constants using the Voigt-Reuss-Hill (VRH) approximation [29]. In this approach, the Voigt model assumes uniform strain in the material and the Reuss model assumes uniform stress. The Hill average, which is the arithmetic mean of the Voigt and Reuss limits, is the most realistic estimate of the elastic properties of polycrystalline materials.

The bulk modulus (B = 162.7 GPa) measures the resistance to uniform volume compression and indicates that MgO is extremely incompressible. The shear modulus (G = 131.4 GPa) measures the resistance to shape deformation, and the Young's modulus (E = 313.8 GPa) is the overall stiffness of the material. The high Young's modulus indicates that MgO is extremely rigid, and that is also common for ionic ceramic materials. The good agreement between DFT and ML values shows the reliability of the machine learning model in predicting macroscopic mechanical properties directly from atomic-scale information.

The combination of high elastic constants, large bulk modulus, and large Young's modulus makes MgO an excellent material for mechanical strength and structural stability. When applied in refractory linings, thermal barrier coatings, ceramic substrates, insulating materials, optical windows, and high-pressure experimental devices, these properties make MgO very suitable. The good agreement between DFT and ML results shows the efficiency of combining first-principles calculations with machine learning techniques in materials design and mechanical property prediction.

3.4. Thermal Properties

Figure 3 shows a detailed comparison between the thermal properties of MgO predicted by density functional theory (DFT) and ML. The close agreement between the blue (DFT) and red (ML) bars indicates the excellent accuracy of the ML model in predicting the first-principles thermal properties. The prediction error is consistently very low, ranging from 0.81% to 2.23%, indicating good agreement with the data.

The Debye temperature (Θ_D) is predicted to be 742 K by DFT and 735 K by ML, with an error of only 0.94%. The high Debye temperature represents strong interatomic bonding and high lattice vibrational frequencies, demonstrating the strength of the MgO crystal. The Cv is also predicted to have a smaller error of 0.81%, indicating that the ML model captures the contribution of lattice vibrations to heat storage.

The thermal conductivity (κ) has the highest error among the main properties (2.23%), but the ML value is very close to the DFT result. The thermal conductivity of MgO is relatively high because phonons are transported efficiently through the crystal structure of rock salt. The thermal expansion coefficient (αv) and Grüneisen parameter (γ) are also accurate, showing that in our ML model the anharmonic lattice behavior and thermal expansion effects are well described.

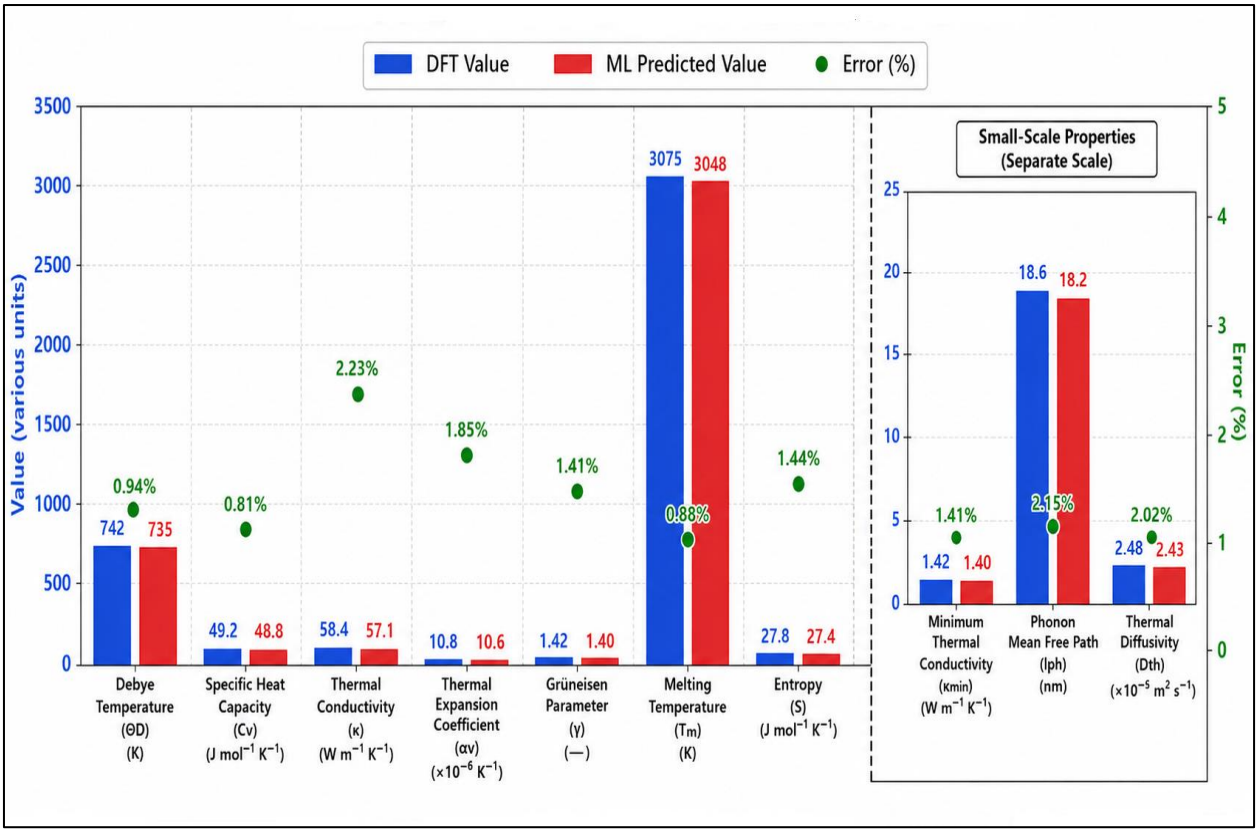

Figure 3 Comparison of thermal properties of MgO obtained from Density Functional Theory (DFT) calculations and Machine Learning (ML) predictions

The melting temperature (Tm) of MgO is above 3000 K, which shows its remarkable thermal stability and refractory properties. The small error of 0.88% shows that ML can predict high-temperature performance well. The entropy values are also well reproduced, with only 1.44% error. The inset shows low-magnitude properties such as minimum thermal conductivity (κmin), phonon mean free path (lph), and thermal diffusivity (Dth), with errors close to 2%, indicating that the ML predictions are very good.

Figure 3 shows that machine learning can accurately reproduce DFT-based thermal properties while greatly reducing computational cost. This is of particular importance for high-throughput materials screening and faster materials discovery.

The excellent thermal properties of MgO, as shown in Fig. 3, make it highly attractive for various applications. Its high melting temperature and low coefficient of thermal expansion make it a good material for refractory bricks, furnace linings, and thermal barrier coatings in the metallurgical and aerospace industries. This high thermal conductivity allows efficient heat dissipation in electronic substrates, semiconductor packaging, and thermal management systems. Its excellent lattice stability and high Debye temperature make it suitable for high-temperature sensors, nuclear reactors, optical components, and geophysical studies of Earth's lower mantle. The success of predicting these properties with machine learning makes a strong case for using DFT-ML frameworks to enable the rapid design of advanced thermal materials for next-generation energy, electronics, and aerospace applications.

4. Conclusion

DFT and ML approaches were used to investigate the structure, mechanical and thermal properties of magnesium oxide (MgO). DFT calculations were performed, and MgO was found to crystallize in a rock salt structure with excellent ionic bonding and structural stability. The equilibrium lattice constant, equilibrium volume, bulk modulus, and formation energy of the crystals were in good agreement with the theoretical and experimental results.

The elastic constants C_{11}, C_{12}, and C_{44} satisfy the Born mechanical stability criteria, and thus the mechanical stability of MgO is confirmed at room temperature. The high bulk, shear, and Young's moduli also indicate strong resistance to both

compressive and shear deformation, suggesting that the material is very rigid. The material exhibits a high Debye temperature, good thermal conductivity, a low thermal expansion coefficient, and a very high melting temperature, which are characteristics of a high-performance refractory ceramic.

Machine learning models trained on DFT-generated data accurately predicted the structural, mechanical, and thermal properties. The prediction errors were below 2.5% for most properties, showing that ML describes the complex relationship between atomic structure and material properties. The excellent agreement between the DFT and ML results demonstrates that data-driven methodologies can effectively predict ceramic properties.

Our work shows that machine learning can significantly reduce computational cost while still delivering near-first-principles accuracy. The successful integration of DFT and ML can accelerate materials discovery, property optimization, and high-throughput screening in the development of new materials. Due to its excellent thermal stability, mechanical strength, and insulating properties, MgO is a suitable material for refractory coatings, thermal barrier coatings, electronic devices, energy systems, and geophysical work. The proposed DFT-ML approach can be applied to other oxide ceramics and to high-level functional materials in the development of next-generation technologies, enabling new materials to be created in less time.

Compliance with ethical standards

Disclosure of conflict of interest

The authors declare that they have no competing financial or non-financial interests related to this work.

Statement of ethical approval

All authors have read and approved the final version of the manuscript and consent to its publication.

Author's Contribution:

Dr. Ratan Lal Jaisawal, Dr. Satyabrat Pandey, Dr. Heera Lal Rai, Er. Vivek Kushwaha, and Dr. Vikal Saxena made the original draft of the manuscript.

Data Availability Statement

The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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