

Stability of MgCO_3 throughout the lower mantle: Phase diagram and wave velocity of a deep carbon reservoir

ZhongShan He¹, XiLong Dou^{1*}, Yuan Guo², RunFu Liu¹, ZiJiang Liu^{1,3}, and XiaoWei Sun^{1,3}

¹School of Mathematics and Physics, Lanzhou Jiaotong University, Lanzhou 730070, China;

²School of Information Engineering, Lanzhou City University, Lanzhou 730070, China;

³School of Mechanical Engineering, Lanzhou Jiaotong University, Lanzhou 730070, China

Key Points:

- The melting curve of MgCO_3 has been accurately predicted by constructing a deep potential model, in agreement with the experimental results.
- Magnesite is highly stable under pressure and is identified as a key deep carbon reservoir in the mantle.
- Its seismic velocity signature provides direct evidence for the deep mantle carbon cycle.

Citation: He, Z. S., Dou, X. L., Guo, Y., Liu, R. F., Liu, Z. J., and Sun, X. W. (2026). Stability of MgCO_3 throughout the lower mantle: Phase diagram and wave velocity of a deep carbon reservoir. *Earth Planet. Phys.*, 10(4), 648–658. <http://doi.org/10.26464/epp2026057>

Abstract: Carbonate minerals are key carriers of carbon into the Earth's interior, yet their stability and melting behavior under lower mantle conditions remain incompletely constrained. Here, we develop a high-accuracy machine learning interatomic potential for MgCO_3 based on the deep potential framework, trained on an extensive *ab initio* molecular dynamics dataset spanning 0–140 GPa and 300–5000 K. Using large-scale two-phase coexistence molecular dynamics simulations, we determine the melting behavior of MgCO_3 across the pressure range of the entire lower mantle. At ambient pressure, the predicted melting temperature of 1857 K agrees with experiments within 0.3%, validating the potential. We show that the high-pressure $\text{C2}/m$ phase exhibits a substantially higher melting temperature and a steeper Clapeyron slope than the low-pressure phase, leading to a pronounced increase in melting temperature across the structural transition. The resulting melting curve lies approximately 400 to 1100 K above representative lower mantle geotherms, indicating that crystalline MgCO_3 can remain thermodynamically stable under idealized anhydrous, Mg-end-member conditions. Calculated elastic wave velocities display a pressure-dependent high–low–high deviation relative to the PREM (Preliminary Reference Earth Model), reflecting changes in crystal structure and elastic softening near phase transitions. These results provide quantitative constraints on the phase stability, melting behavior, and elastic properties of MgCO_3 at deep-mantle conditions and offer a reference framework for evaluating the role of carbonates in deep Earth carbon storage when coupled with more realistic multicomponent mantle compositions.

Keywords: magnesite; deep potential; melting behavior; deep carbon cycle

1. Introduction

Carbon storage and carbon cycling have always been central topics in Earth science research. Carbonates represent the primary carbon-bearing phase on the Earth's surface and are transported into the mantle through subduction zones. Within these zones, decarbonation reactions release carbon into ascending fluids and melts, which are subsequently emitted at the surface via volcanic eruptions, thus participating in the deep carbon cycle of the Earth (Plank and Manning, 2019). In this process, part of the carbon reacts with silicate minerals in the lower mantle, forming carbonates that can stably exist within the lower mantle section of

subducting slabs. Existing research indicates that carbonate minerals—such as magnesite and ferromagnesite $[(\text{Mg,Fe})\text{CO}_3]$ —are likely the principal hosts for deep carbon in the lower mantle (Tsuchiya et al., 2020). Previous reports indicate that, following reaction, CO_2 present in peridotite is sequestered in dolomite $[\text{CaMg}(\text{CO}_3)_2]$ at pressures exceeding 1.5 GPa. Subsequently, dolomite converts to magnesite (MgCO_3) under pressures ranging from 2.5 to 5 GPa (Katsura and Ito, 1990). Concurrently, magnetotelluric sounding surveys have revealed significant electrical conductivity anomalies in the mantle transition zone (MTZ), which have been attributed to enhanced proton mobility in hydrous silicate phases such as ringwoodite (Zhou XY et al., 2025). Such findings demonstrate that atomic-scale dynamic processes in mantle minerals can profoundly influence large-scale geophysical signatures, motivating an extension of similar mechanistic investigations to carbonate systems in the deeper mantle.

Magnesite (MgCO_3) demonstrates higher stability at elevated

First author: Z. S. He, hezsljtu@163.com

Correspondence to: X. L. Dou, xilongdou369@163.com

Received 28 JAN 2026; Accepted 20 MAY 2026.

First Published online 26 JUN 2026.

©2026 by Earth and Planetary Physics.

temperatures and pressures than other carbonate minerals (Isshiki et al., 2004; Rohrbach and Schmidt, 2011; Maeda et al., 2017). For instance, calcite (CaCO_3) experiences several phase transitions (Bayarjargal et al., 2018), whereas siderite (FeCO_3) tends to decompose under the pressure and temperature conditions characteristic of the mantle (Cerantola et al., 2017). Remarkably, magnesite maintains its stability under ultra-high-pressure and ultra-high-temperature conditions, remaining intact at pressures of at least 80 GPa and temperatures as high as 3000 K (Fiquet et al., 2002; Isshiki et al., 2004; Solopova et al., 2015). Previous studies have shown that MgCO_3 undergoes multiple structural transitions as the pressure increases, exhibiting a complex multi-stage evolution under high-pressure environments. X-ray diffraction (XRD) analyses performed in the early 2000s have shown that magnesite maintains its structural integrity at pressures up to 80 GPa (Fiquet and Reynard, 1999; Isshiki et al., 2004), with the onset of a high-pressure phase transition occurring only at 115 GPa (Isshiki et al., 2004). From a theoretical perspective, Pickard and Needs (2015) utilized *ab initio* random structure searching to predict that, upon compression, MgCO_3 initially transforms into the $P\bar{1}$. The stability field of this phase is rather limited, mainly occurring near 80 GPa. This prediction was later independently verified by the research groups of Zhang and Santos (Zhang ZG et al., 2018; Santos et al., 2019). Universal Structure Predictor: Evolutionary Xtallography (USPEX) simulations (Oganov et al., 2008) have further demonstrated that the $C2/m$ phase is stable over a pressure range of 82 to 130 GPa, in agreement with the XRD data from Maeda et al. (2017) and the Raman spectroscopic analyses performed by Binck et al. (2020). To achieve a more accurate interpretation of the high-pressure XRD patterns of magnesite, Boulard et al. (2011) introduced the $P2_1/c$ phase. However, later Gibbs free energy calculations indicated that the stability of this phase is restricted to a narrow pressure window near 130 GPa. At higher pressures, it transitions to the $P2_12_12_1$ structure, which had previously been predicted by Pickard et al. (Zhang ZG et al., 2018; Li Z and Stackhouse, 2020). Pickard and Yao, along with their respective teams (Pickard and Needs, 2015; Yao X et al., 2018), jointly discovered that at approximately 150 GPa, the $P2_11_11$ phase undergoes a further transition to the $P2_1$ phase. Recently, Li Z and Stackhouse (2020) provided a systematic summary of the phase transition sequence of MgCO_3 within the pressure range of 0 to 160 GPa as follows: $R\bar{3}c \rightarrow P\bar{1} \rightarrow C2/m \rightarrow P2_1/c \rightarrow P2_12_12_1$. Given that both the $P\bar{1}$ and $P2_1/c$ phases are stable only within a very narrow temperature–pressure window, their impact on the physical properties of MgCO_3 in the lower mantle is considered negligible. Consequently, this study does not provide a detailed analysis of these phases.

Carbon cycling in the deep mantle is strongly modulated by melting processes. Investigations into the melting behavior of recycled oceanic crust indicate that, in the mantle transition zone, subducted slabs experience partial melting and liberate their carbonate constituents. This phenomenon acts as a barrier, restricting the transfer of carbon into the deeper mantle. Currently, static high-pressure experiments have determined the melting temperature of magnesite at 84 GPa (Solopova et al., 2015). Using first-principles calculations in combination with the

quasi harmonic approximation (QHA), Yao C et al. (2018) elaborated on the thermodynamic and seismic properties of magnesite under lower mantle conditions. Utilizing these results, Sun WD et al. (2018) linked magnesite formation to carbon cycling at the base of the mantle transition zone, providing a compelling pathway or perspective for understanding key mantle anomalies. More interesting, recent *in situ* ultrasonic and synchrotron X-ray measurements on a natural magnesite have provided direct evidence for its density and elastic wave velocity at conditions up to ~ 8 GPa–1073 K (Xu M et al., 2024), yielding thermoelastic properties that are consistent with the theoretical predictions of Yao C et al. (2018). In contrast, studies on magnesite at the extreme temperatures of the deep mantle remain relatively limited. Notably, the effect of intrinsic anharmonicity, driven by direct phonon–phonon interactions but neglected by the QHA method, may increase with temperature and pressure. In addition, the melting temperature of the high-pressure $C2/m$ phase remains unreported to date. In particular, no reports are available on the seismic velocities of the high-pressure MgCO_3 – $C2/m$ phase. Current theoretical data (Marcondes et al., 2016; Yao C et al., 2018; Li Z and Stackhouse, 2020), which are derived from first-principles calculations, do not consider the influence of temperature. Owing to its remarkable stability at high temperatures and pressures, magnesite plays a crucial role in the deep carbon cycle within the Earth's interior. Nevertheless, substantial uncertainties persist regarding the comprehensive mechanisms of the deep carbon cycle, the pressure–temperature (P – T) phase diagram, and the stability of magnesite under extreme conditions.

Modeling the MgCO_3 system under the extreme conditions of the Earth's deep interior poses multiple challenges: the energy differences between various phases are subtle, the bonding characteristics are complex (predominantly ionic, with contributions from covalent and metallic interactions), and the crystal structures of these phases are highly similar. Such factors may underlie the inconsistencies reported in earlier melting simulations utilizing empirical potential functions. Density functional theory (DFT; Perdew et al., 1996) is currently recognized as an accurate approach for describing the energy of a system without making any *a priori* assumptions regarding bonding characteristics. Nevertheless, DFT calculations are associated with high computational costs, and melting events are infrequent in conventional molecular dynamics simulations. Consequently, a self-consistent determination of the melting temperature has not yet been realized. For a wide range of structurally simple materials, simulations utilizing the coexistence of solid and liquid phases have proven to provide reliable determinations of melting points (Alfè et al., 2002; Vočadlo et al., 2004; Alfè, 2005). However, this approach relies on a sufficiently large system size to ensure the stability of the solid–liquid interface, and the simulations are typically time-consuming. As a result, it imposes significant demands on computational resources and is often challenging to realize within the framework of DFT-based calculations.

Machine learning potentials (MLPs) represent a novel approach in atomic simulations, which, in principle, offer the accuracy of *ab initio* calculations while enabling the simulation of large-scale systems and long time-scale processes (Behler and Parrinello,

2007; Zhang LF et al., 2018). Consequently, MLPs are particularly suitable for conducting solid–liquid coexistence simulations and investigating melting phenomena. Nevertheless, constructing an MLP that exhibits robust performance over a broad pressure and temperature range for the MgCO_3 system remains a significant challenge. To the best of our knowledge, no such efforts have been reported thus far. Machine learning potentials are typically trained on DFT data obtained from a limited configuration space, such as those generated by *ab initio* molecular dynamics (AIMD) simulations. However, this process faces three main challenges. First, the range of thermodynamic conditions sampled in molecular dynamics simulations is limited, and multiple runs are often required to cover the target pressure–temperature region. Second, because phase transitions are rare events, individual simulations usually sample only a single phase, resulting in phase bias in the trained MLPs. Third, transition states are critical for accurately describing solid–liquid interfacial properties, but their transient nature makes them difficult to capture with conventional sampling approaches.

In this study, we investigate the MgCO_3 system across the entire range of mantle pressures and temperatures, extending up to the uppermost region of the Earth's outer core, with pressures reaching as high as 140 GPa and temperatures up to 3600 K. We develop a set of magnesite potential models with AIMD accuracy. By combining these models with classical molecular dynamics, we simulate the behavior of large-scale magnesite systems over extended timescales under high-temperature and high-pressure conditions. Through the application of two-phase molecular dynamics simulations, we derive the equation of state and the P – T phase diagram for magnesite within the pressure and temperature conditions characteristic of the lower mantle.

2. Materials and Methods

2.1 DeePMD Approach

Machine learning has demonstrated significant potential in simulating the Born–Oppenheimer potential energy surface. As a nonparametric approach, it can approximate the potential energy surface to any desired level of accuracy. Therefore, in this work, we developed a deep potential (DP) for MgCO_3 by fitting the potential energy surface using machine learning methods.

The training of the DP was carried out using the DeePMD-kit (Wang H et al., 2018; Zhang LF et al., 2018). In DeePMD, the total energy is expressed as the sum of the energies of all atoms, namely

$$E = \sum_{i=1}^N E_i = \sum_{i=1}^N \varepsilon(D_i),$$

where N is the total number of atoms and E_i is the contribution of the i th atom to the total energy. The descriptor D_i represents the local atomic environment and is a function of the coordinates of atoms surrounding atom i . This approach ensures that the potential energy surface preserves the translational, rotational, and permutation symmetries of the structure. In our work, three hidden layers are used. The embedding network consists of [25, 50, 100] neurons, whereas the fitting network consists of [240, 240, 240]

neurons. In the local environment, the descriptor components decay smoothly to zero between 0.5 and 6 Å, with a cutoff radius of 6 Å. The initial learning rate, final learning rate, and decay steps were set to 0.001, 3.51×10^{-8} , and 5000, respectively. The model underwent a training process for 2,000,000 steps and was developed without the incorporation of virtual data throughout the training phase. During training, the loss function (Wang H et al., 2018) was defined as

$$L(P_\varepsilon, P_f, P_\xi) = \frac{P_\varepsilon}{N} \Delta E^2 + \frac{P_f}{3N} \sum |\Delta F_i|^2 + \frac{P_\xi}{9N} \|\Delta \Xi\|^2. \quad (1)$$

In the equation, P_ε , P_f , and P_ξ are the respective weights during the learning process. Because virtual data are not included in the training, $P_\xi = 0$. Weight P_ε gradually increases from 0.02 to 1, whereas P_f decreases from 1000 to 1, indicating that the force term is dominant at the beginning, whereas the energy and virtual terms become more important toward the end. The terms containing ΔE and ΔF represent the root mean square errors (RMSEs) of energy and force, respectively, which are defined as follows:

$$\text{RMSE} = \sqrt{\frac{1}{m} \sum_{i=1}^m (x_i - \hat{x}_i)^2}, \quad (2)$$

In the equation, m is the number of samples, x_i represents the DFT data, and $\hat{x}_i$ represents the data predicted by the DP.

2.2 Ab Initio Calculations

The training set for the DP was constructed from a multi-temperature, multi-pressure dataset generated during AIMD simulations (Table S1). During the structural optimization process, the pseudopotentials utilized were based on the PBE_sol functional within the generalized gradient approximation. Previous studies have demonstrated the accuracy of PBE_sol in describing the properties of magnesite (Liu ZJ et al., 2022b). To address the limitations of single short-time AIMD simulations in sampling solid–liquid interfaces, metastable phase transition pathways, and the diversity of liquid configurations within the broad phase space spanning 0–140 GPa and 300–5000 K, in this study we implement a systematic integrated sampling strategy. Specifically, this strategy performs multiple independent and sufficiently long (6–20 ps) AIMD simulations at key P – T points—including stable solid phase regions, high-pressure liquid regions, and two-phase coexistence regions. This approach efficiently constructs a representative configuration library that covers solid, liquid, and interfacial regions. The final training set was meticulously designed to balance the proportions of solid and liquid phase structures, with special inclusion of interfacial configurations. This process ensures that the trained DP can accurately describe the complex physico-chemical processes involved in the transition from solid to liquid states.

For the specific simulation parameters, the plane-wave cutoff energy is set to 900 eV, the energy convergence criterion is set to 1×10^{-4} eV, and Brillouin zone k-point sampling is restricted to the Γ -point only. The simulation system consists of 120 atoms and is subjected to heating simulations in the NPT ensemble, with a time step of 1 fs and a total simulation time of 10 ps. To ensure the

completeness of the dataset, 10,000 steps of AIMD simulations were performed for each of the two structures within the lower mantle pressure range, resulting in a comprehensive dataset. Subsequently, 80% of the entire dataset is used as the training set, whereas the remaining 20% is designated as the validation set. This approach empowers the trained DP model to comprehensively learn high-precision data features, encompassing critical information such as forces, energies, and bond angles. The construction of the dataset was carried out using the Vienna *ab initio* Simulation Package (VASP; Kresse and Furthmüller, 1996; Kresse and Joubert, 1999).

2.3 Two-Phase Simulations

The two-phase method is a simulation technique designed to determine the melting point of materials, grounded in the principle of thermodynamic equilibrium. The core mechanism involves constructing a microscopic model in which solid and liquid phases coexist; by observing the energy exchange between these two phases under constant pressure, the system ultimately reaches thermodynamic equilibrium at the melting temperature. In this work, a model with a solid-to-liquid ratio of 1:1 was constructed using a Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS; Plimpton, 1995). The sizes of the supercells are $5 \times 5 \times 6$ ($R\bar{3}c$) and $4 \times 4 \times 6$ ($C2/m$), respectively. In the system, half of the atoms are immobilized, whereas the remaining atoms are heated at high temperatures for an extended period to ensure that all unfixed atoms are thoroughly melted. Subsequently, the heated atoms are rapidly cooled to a temperature slightly above the melting point and maintained at this level for a certain duration. Finally, the initially fixed atoms are released, whereas the remaining half are immobilized, and the temperature is gradually raised to the predicted melting point (T_m) so that the system achieves an initial configuration with solid–liquid coexistence. The heating and cooling steps are conducted under the NPT ensemble (Zhang Y and Maginn, 2012; Hong QJ and Van De Walle, 2013), and the final relaxation occurs in the NPH ensemble (Dang K et al., 2023), with the entire process simulated over 600 ps. By observing the final morphology of the system, the phase transition temperature can be determined: if the system ultimately appears molten, it indicates that the simulation temperature exceeds the melting point of the crystal; if it remains crystalline, the temperature is below the melting point. Additionally, analyzing the system's radial distribution function quantitatively characterizes the degree of atomic order, providing further confirmation of the phase state. By using this dual assessment method and systematically adjusting simulation temperature parameters, the thermodynamic upper limit of the $MgCO_3$ melting curve—that is, its solid–liquid phase transition temperature—is determined. The boundary between phase I and phase II is determined by Gibbs free energy. The calculation of the Gibbs free energy is realized by the Phonopy software of the QHA (Togo and Tanaka, 2015) and its LAMMPS interface software PhonoLAMMPS (Carreras, 2020).

2.4 Seismic Wave Velocity

Within the framework of finite-temperature molecular dynamics

simulations, the single-crystal elastic constants C_{ij} were determined by means of fitting the time-averaged stress response to a series of applied finite strains over long equilibrated trajectories. On the basis of symmetries of phase I and II of $MgCO_3$, we then calculated the Voigt upper bound assuming uniform strain and the Reuss lower bound assuming uniform stress. Finally, we used the Voigt–Reuss–Hill (VRH) averaging scheme (Reuss, 1929; Hill, 1952; Voigt, 1966) to determine the bulk and shear moduli. The elastic wave propagation properties of minerals, including compressional wave velocity (V_p) and shear wave velocity (V_s), can be accurately determined from the elastic constants of their single crystals (Anderson, 1963). According to crystal elasticity theory, these two wave velocities reflect the mechanical response capabilities of minerals in different directions. Specifically, V_p corresponds to the propagation velocity of longitudinal waves in the crystal, whereas V_s characterizes the propagation of transverse waves:

$$V_p = \sqrt{\frac{3B + 4G}{3\rho}}, V_s = \sqrt{\frac{G}{\rho}}. \quad (3)$$

Here, ρ is the density, B is the Bulk Modulus, and G is the Shear Modulus.

3. Results and discussion

3.1 Benchmarks of the MLP

We then compare the energies and atomic forces predicted by the MLP with those obtained from DFT simulations for the validation set. Predicted energies and forces align precisely with the DFT reference data (Figure 1). The model achieves RMSEs of 4.694 meV/atom for energy and 0.209 eV/Å for forces, confirming high training fidelity.

Within the lower mantle, $MgCO_3$ mainly exists in two structures, as illustrated in Figure 2, with space groups $R\bar{3}c$ ($Z = 6$, hereafter referred to as phase I; Z is number of formula units per unit cell) and $C2/m$ ($Z = 12$, hereafter referred to as phase II). At 0 GPa, the lattice parameters of phase I are $a = b = 4.651$ Å and $c = 14.976$ Å. In this structure, the CO_3^{2-} groups adopt a planar triangular configuration, with the carbon atom located at the center of the triangle and bonded to three oxygen atoms. Each Mg^{2+} ion is coordinated by six O^{2-} ions to form an octahedral structure, and the CO_3^{2-} groups are connected to Mg^{2+} ions through their oxygen atoms. At 90 GPa, the lattice parameters of phase II are $a = 8.219$ Å, $b = 6.163$ Å, $c = 7.113$ Å, and $\beta = 102.903^\circ$. Four oxygen atoms are closely arranged around the carbon atom, collectively forming a regular tetrahedral geometry. Furthermore, the coordination environment in this structure is unique: the coordination number of Mg can be either 8 or 10, resulting in the formation of chemical bonds. All lattice parameters are listed in Table S2, and they are in complete agreement with previous theoretical and experimental results. This result demonstrates the accuracy of our fitted DP, which can be reliably used for subsequent calculations.

The phonon dispersion relation characterizes the evolution of phonon energies with respect to the wave vector. As a quantum manifestation of lattice vibrations, the form of the dispersion directly reflects the interatomic interactions and structural features of the crystal lattice. By analyzing this relationship, one

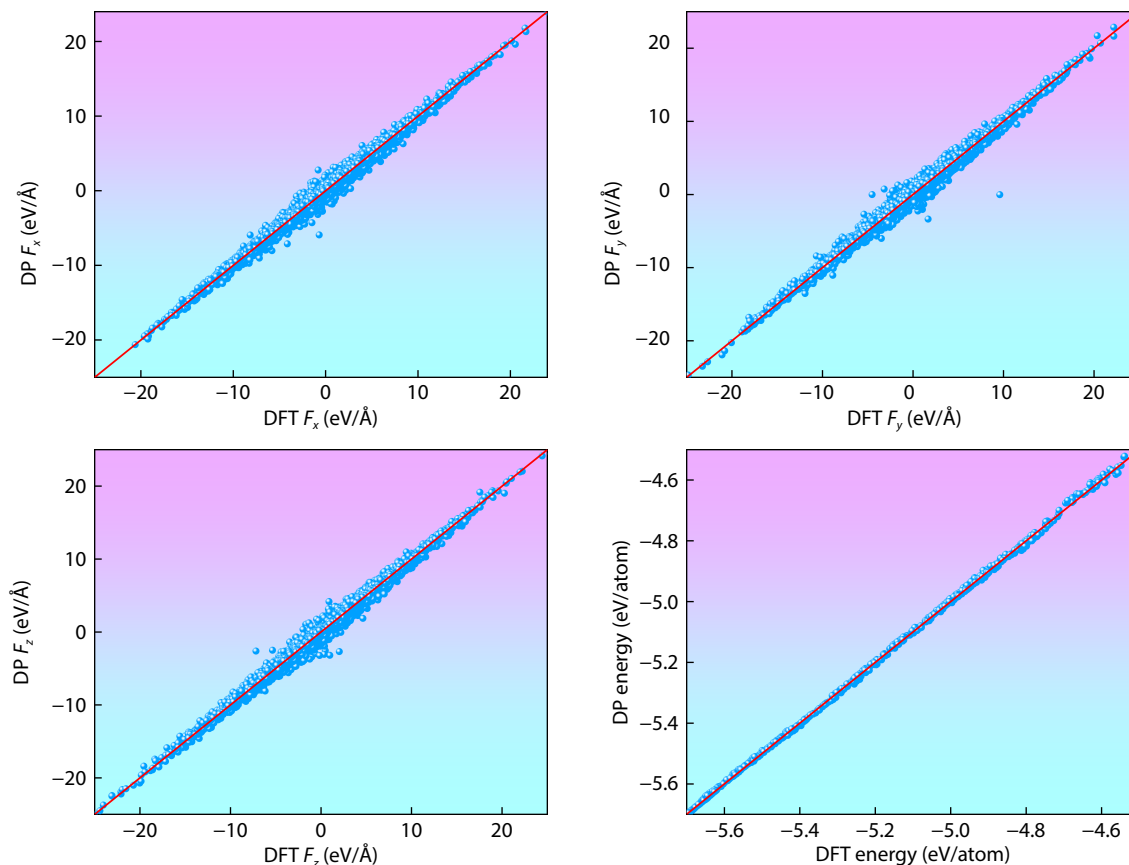


Figure 1. Comparison of energies and atomic forces predicted by the DP with DFT reference data for the validation set.

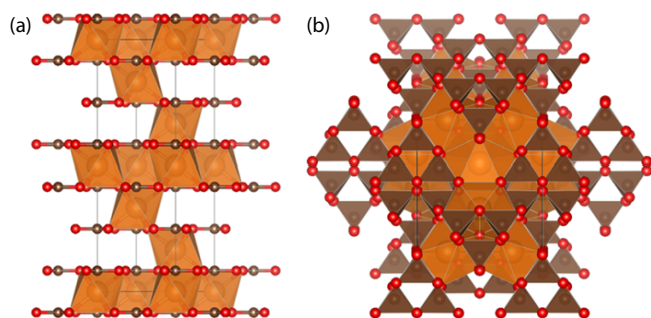


Figure 2. Magnesite crystal structure. (a) $R\bar{3}c$ structure, (b) $C2/m$ structure. C = brown, Mg = yellow, and O = red.

can uncover key physical properties, such as phonon scattering mechanisms, thermal transport behavior, and electron–phonon coupling. Figure S1 shows the phonon dispersion curves of $\text{MgCO}_3\text{-I}$ at 0 GPa and 0 K. The DeePMD and DFT calculation results are in good agreement, and no imaginary frequencies are observed throughout the Brillouin zone. This finding indicates that the structure is dynamically stable under the DP, further confirming the reliability of the DP.

3.2 Equations of State

Figure 3a presents the equation of state of MgCO_3 over the pressure range of 0–80 GPa. In the 0–70 GPa interval, the volume of phase I at 300 K decreases linearly with increasing pressure,

consistent with previously reported experimental data. Importantly, the simulations successfully reproduce the stability of phase I within this pressure range, providing preliminary validation for the applicability of the utilized potential under high-pressure conditions. To further assess the properties of the high-pressure phase, we conduct equation of state simulations for phase II at 300 K (Figure 3b). The results indicate that the volume of phase II decreases monotonically with increasing pressure, and the slope of its P – V (Pressure–Volume) curve is much smaller than that of phase I, suggesting a significantly higher bulk modulus and thus greater incompressibility. This enhanced rigidity arises from the more compact coordination environment under high pressures, revealing the superior structural stability of phase II. Consequently, in high-pressure subduction environments, magnesite is more likely to exist in this rigid phase II form, which could markedly delay the decarbonation reaction of carbonates and provide critical constraints on deep carbon flux.

3.3 High-Pressure Melting Curve

Two-phase molecular dynamics simulations can accurately determine the melting temperature. In this method, a perfect crystal with a 50% solid–liquid ratio is used, and variations in the solid–liquid ratio within the supercell have only a minimal effect on the melting point (Wang XW et al., 2024). The identification of solid and liquid phases is mainly based on the radial distribution function (RDF) $g(r)$. As shown in Figure 4a, we present the RDFs of

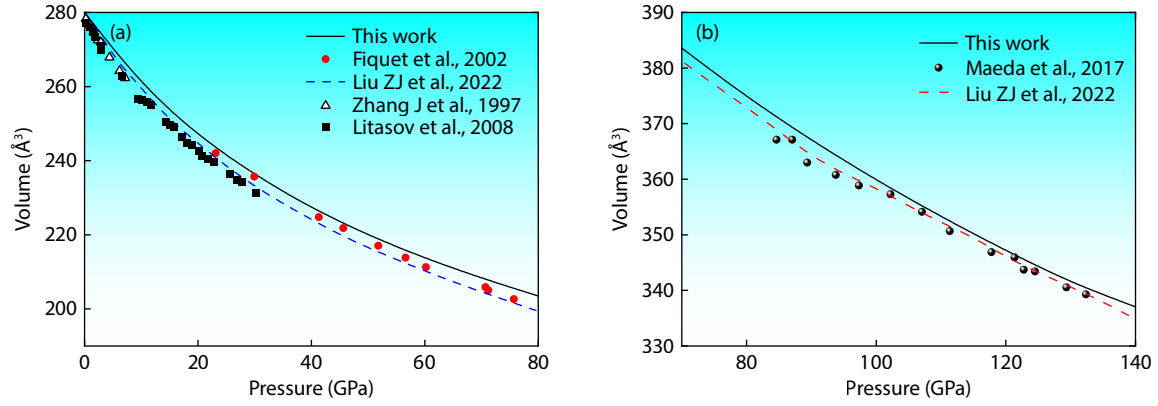


Figure 3. Equation of state for MgCO_3 with available results. (a) $R\bar{3}c$ structure; (b) $C2/m$ structure, where the solid black lines are the present work; the circles are the work of Fiquet et al. (2002), or Maeda et al. (2017); the dashed lines are the work of Liu ZJ et al. (2022a, b); the hollow triangles are the work of Zhang J et al. (1997); and the solid black squares are the work of Litasov et al. (2008).

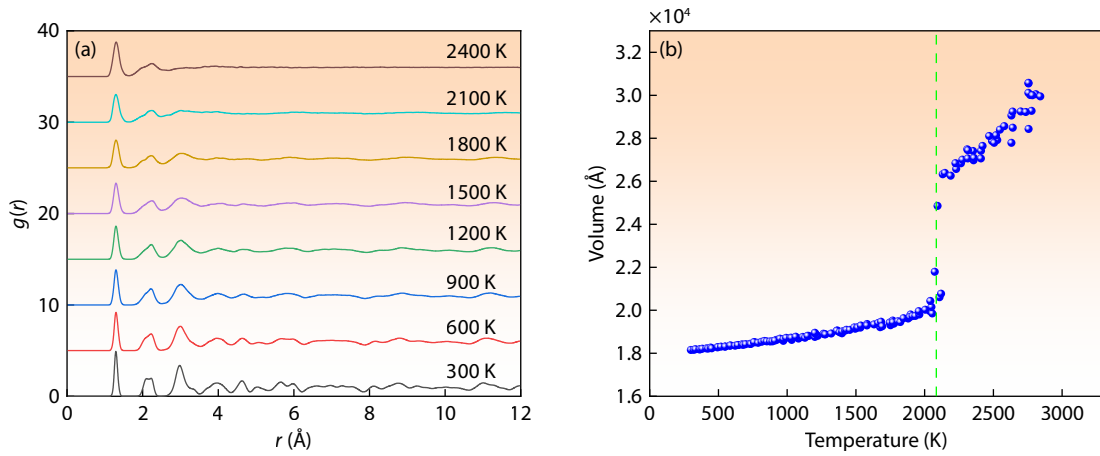


Figure 4. (a) Variations in the RDF of the $R\bar{3}c$ structure with temperature at 0 GPa. (b) Volume following temperature changes during single-phase method melting.

MgCO_3 at various temperatures under ambient pressure. For ease of comparison, the RDF curves at all temperatures except 300 K are vertically shifted along the y-axis. At 300 K, the $g(r)$ of MgCO_3 exhibits multiple peaks within the range of 0–12 Å, such as the Mg–O coordination peak at 1.3 Å (with a peak height of approximately 6.82) and the O–O coordination peak at 3.03 Å (with a peak height of approximately 3.1). Overall, the $g(r)$ displays the long-range order characteristic of a crystalline structure, indicating that MgCO_3 is in the solid state at 300 K. As the temperature increases, the peaks in the medium-range (4–12 Å) region become significantly weaker. For example, at 1200 K, the heights of the minor peaks beyond 6 Å decrease by more than 10%, indicating a gradual loss of long-range order. When the temperature rises to 2100 K, $g(r)$ displays prominent peaks only at short-range distances: the first coordination peak (Mg–O, around 1.3 Å) has a height of approximately 4.15, and the second coordination peak (O–O, around 2.25 Å) has a height of approximately 1.45. Beyond 4 Å, $g(r)$ quickly converges to 1 (with fluctuations less than ± 0.1), which is characteristic of the short-range order and long-range disorder typical of liquid states, indicating that MgCO_3 is fully molten.

During single-phase simulations, the melting process of the material is mainly characterized by the weakening of interatomic interactions and increased structural disorder. This process is also accompanied by abrupt changes in thermodynamic parameters such as volume, entropy, and enthalpy. Figure 4b shows the abrupt change in volume as a function of temperature.

On the basis of the aforementioned melting criteria, we systematically scan the temperature–pressure space for MgCO_3 within the range of 0–140 GPa and 300–5500 K. The melting process is illustrated in Figure 5, and a complete melting phase diagram is obtained, as shown in Figure 7. The results show that, within the broad parameter space simulating mantle conditions, MgCO_3 melt consistently exhibits excellent liquid stability, with its melting boundary significantly higher than previously predicted by theoretical models. Specifically, in the low-pressure range (0–70 GPa), the melting curve exhibits a relatively gentle slope. For example, at 30 GPa, the melting point is approximately 2329 K, which is consistent with the results reported by Solopova et al. (2015) but significantly lower than the steep increase reported by Katsura and Ito (1990). Additionally, it is approximately 100–500 K lower than the decomposition line of MgCO_3 . In the high-pressure range

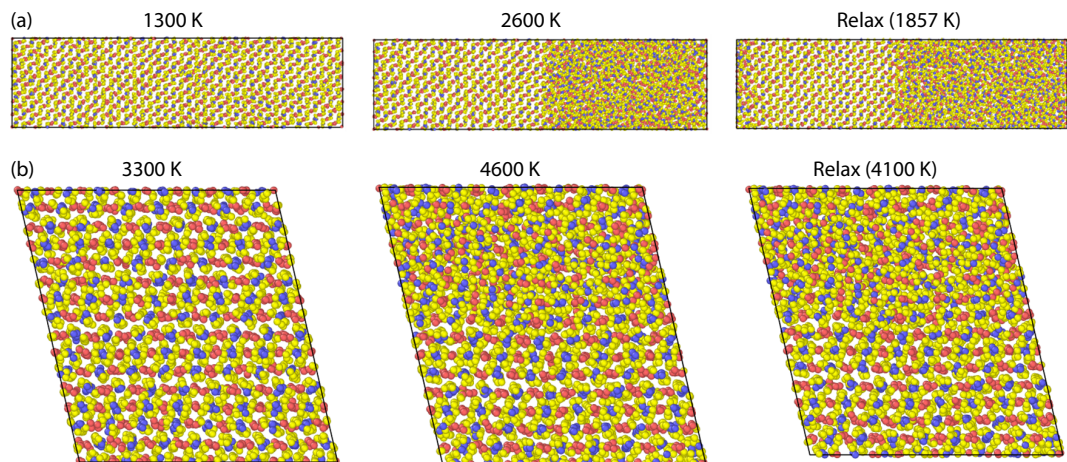


Figure 5. Snapshots of the melting process at varying temperatures for MgCO_3 . (a) Phase I at 0 GPa and (b) phase II at 80 GPa.

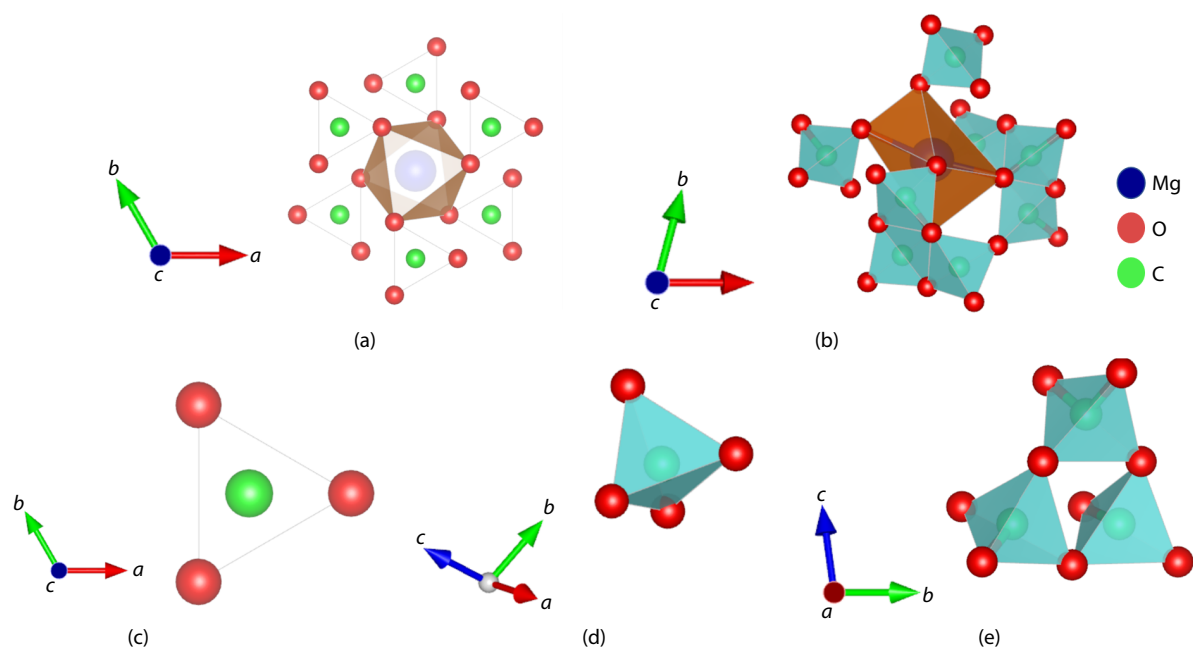


Figure 6. Refined characterization of the two structures of MgCO_3 , with phase I on the left and phase II on the right. The blue polygons indicate Mg atoms, the green balls indicate C atoms, and the red balls indicate O atoms.

of 80–140 GPa, MgCO_3 remains stable in the $C2/m$ structure. Its melting curve exhibits a continuously increasing positive gradient, with $dT_m/dP = 19.3 \text{ K GPa}^{-1}$, and the melting point reaches 5079 K at 140 GPa.

At the triple point where the melting curve intersects the phase I–phase II boundary, the abrupt increase in melting point and the pronounced changes in the slope and shape of the curve indicate that the material undergoes significant transformations in its physical properties between these two phases. Phase I and phase II correspond to two distinct crystal structures or atomic arrangements, as illustrated in Figures 6a and 6b.

As shown in Figure 6, in phase I, the carbon atoms adopt sp^2 hybridization and form planar triangular CO_3^{2-} groups (as illustrated in Figure 6c). The C–O bond length is approximately 1.28 Å, exhibiting a clear double-bond character. Upon entering phase II,

the carbon atoms switch to sp^3 hybridization, with each carbon atom tetrahedrally coordinated to four oxygen atoms. The C–O bond length increases to approximately 1.43 Å and the bond order decreases, but the number of bonds increases. The most revolutionary feature of the $C2/m$ structure is that the CO_4^{4-} tetrahedra (as shown in Figure 6d) are connected by sharing vertex oxygen atoms, forming trimeric ring-shaped $\text{C}_3\text{O}_9^{6-}$ polymeric units (as illustrated in Figure 6e). Such structures manifest crystallographically as two-dimensional corrugated layers, which are coupled by Mg^{2+} ions between the layers. Unlike the isolated groups in phase I, the fragmentation of the $\text{C}_3\text{O}_9^{6-}$ rings requires the simultaneous breaking of at least three C–O covalent bonds. This transformation alters the manner of atomic interactions, resulting in a more stable structure in phase II. Consequently, a higher temperature is required for melting, which is manifested as a sudden increase in the melting point. Additionally, the change

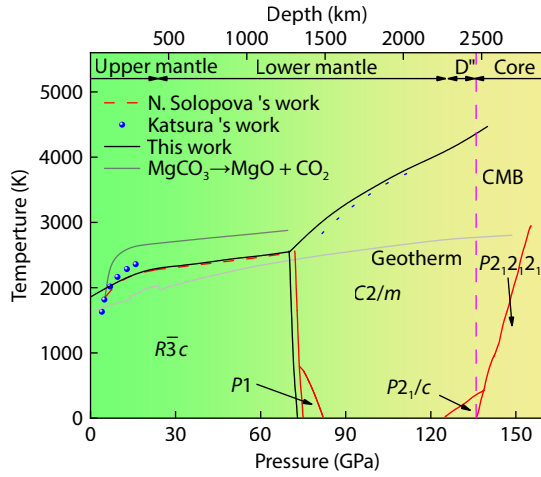


Figure 7. Phase stability of MgCO_3 in the depth range from the mantle to the outermost core and its correspondence with the internal structure of the Earth, where the solid black line is this work, the circle is the work of Katsura and Ito (1990), the dashed red line is the work of Solopova et al. (2015), the thin solid gray line is the decomposition of MgCO_3 into MgO and CO_2 (Fiquet et al., 2002), the solid red line indicates the phase boundary of MgCO_3 (Li Z and Stackhouse, 2020), and the wide solid gray line is the geothermal gradient (Katsura et al., 2010), with no decomposition of MgCO_3 observed above the dashed blue line (Binck et al., 2020). CMB, core–mantle boundary.

in the slope of the melting curve reflects the different sensitivity to pressure during the melting process.

By integrating previous data and incorporating the melting behavior of the C2/m phase, this study constructs an accurate melting phase diagram from the transition zone to the core–mantle boundary. Further analysis shows that, throughout the pressure–temperature range of the lower mantle (23–136 GPa, ~1900–4000 K), the melting curve of MgCO_3 consistently lies approximately 800–2000 K above the geotherm. This thermal

gradient suggests that the crystal lattice of MgCO_3 remains rigid under deep mantle conditions. In a simplified pure- MgCO_3 system, the stable solid phase zone could theoretically impede large-scale percolation of carbonate melts in the deep lower mantle. However, under realistic mantle conditions, the actual mobility of carbon is strongly modulated by Fe/Mg partitioning, the Ca solid solution, H_2O content, oxygen fugacity, and silicate–carbonate eutectic melting, all of which significantly lower the solidus temperature relative to our pure-system calculations.

3.4 Seismic Wave Velocity

To further investigate the seismic wave velocity, we calculate the elastic constants C_{ij} , as well as the bulk modulus and shear modulus of magnesite for phase I and II at 300 K, as shown in Tables 1 and 2. To enhance the robustness and transportability of the DP model, we augment the training set by incorporating stress-strain configurations. Features of the resulting elastic constants fit well with the previously available experimental velocities (Chen PF et al., 2006; Sanchez-Valle et al., 2011) and static DFT, and the maximum numerical difference among these methods does not exceed 6%. In particular, throughout the elastic constants in this study, no essential change occurs in the relative differences. In addition, we emphasize that using finite-temperature molecular dynamics simulations has allowed us to derive the elastic constants by fitting time-averaged stress responses to applied finite strains, which, in combination with the VRH averaging scheme, provides a robust framework for simulating the elastic properties of MgCO_3 under finite temperature and pressure. These results are in close agreement with the available experimental data (Tables 1 and 2) as well as with the static DFT calculations, proving the reliability of the method for determining the elastic properties of MgCO_3 under high-temperature and high-pressure conditions. We then calculated the seismic wave velocities of phase I and phase II of MgCO_3 at 1500 K (in the solid state) and compared them with the Preliminary Reference Earth Model (PREM; Dziewonski and Anderson, 1981). The detailed results are

Table 1. Calculated elastic constants C_{ij} , bulk modulus, shear modulus, and seismic wave velocities for phase I of MgCO_3 at 0 GPa and 300 K, and comparison with prior experimental results at room temperature conditions.

$R3c$	This study (DeePMD)	DFT (Liu ZJ et al., 2022b)	Yao C et al. (2018)	Yang J et al. (2014)	Sanchez-Valle et al. (2011)	Chen PF et al. (2006)
C_{11} (GPa)	249.68	260.38	266	260.7 (± 1.0)	262.0 (± 2.0)	260.3 (± 2.6)
C_{33} (GPa)	143.27	150.85	151.6	157.6 (± 2.6)	157.0 (± 2.0)	153.7 (± 4.1)
C_{44} (GPa)	58.11	56.81	58.6	57.8 (± 0.4)	58.4 (± 0.5)	59.7 (± 1.4)
C_{12} (GPa)	75.33	77.45	78.8	74.3 (± 1.5)	75.5 (± 2.0)	82.9 (± 4.5)
C_{13} (GPa)	57.47	61.55	64.6	59.7 (± 2.1)	61.0 (± 1.0)	59.6 (± 3.1)
C_{14} (GPa)	22.07	20.21	22.3	19.7 (± 0.2)	19.8 (± 0.3)	20.1 (± 1.3)
B (GPa)	112.95	—	117.5	114.7 (± 1.3)	115.7 (± 1.0)	115.3
G (GPa)	72.53	—	69.1	69.9 (± 0.6)	70.1 (± 0.8)	69.3
V_p (km/s)	8.36	—	8.31	8.28 (± 0.04)	8.30 (± 0.07)	8.32
V_s (km/s)	4.92	—	4.77	4.82 (± 0.02)	4.81 (± 0.03)	4.81
V_p/V_s	1.7	—	1.742	1.725	1.726	1.73

Table 2. Calculated elastic constants C_{ij} , bulk modulus, shear modulus, and seismic wave velocities for phase II of MgCO_3 at 80 GPa and 300 K, and comparison with DFT results at 80 GPa and 0 K.

$C2/m$	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}
DP	647.19	606.04	690.62	138.07	137.23	187.46
DFT	651.22	610.19	696.37	141.45	140.08	191.53
C_{12}	C_{13}	C_{15}	C_{23}	C_{25}	C_{35}	C_{46}
347.38	278.05	272.81	−14.07	24.84	11.37	35.96
349.67	282.61	273.16	−17.37	27.48	13.68	37.54

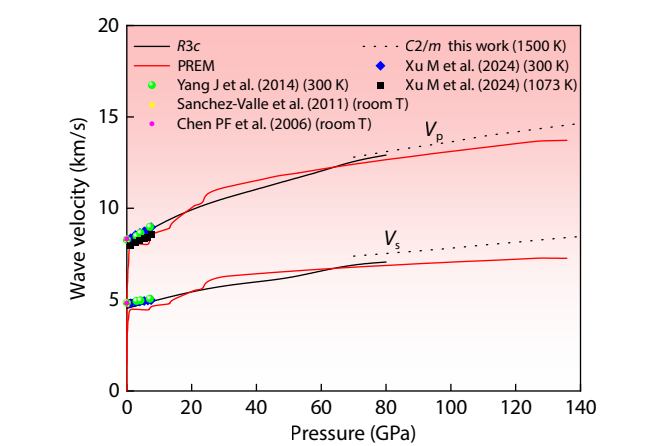


Figure 8. Calculated seismic wave velocity at 1500 K for MgCO_3 as a function of pressure, and comparison with prior experimental results and PREM.

shown in Figure 8. Across the entire pressure range, the elastic wave velocities derived from theoretical calculations show excellent agreement with the experimental data reported in references (Yang J et al., 2014; Xu M et al., 2024), with relative deviations consistently remaining below 2%. This result further demonstrates the reliability of the DeePMD method. Specifically, as pressure increases, V_p gradually rises, reaching approximately 9.79 km/s at 20 GPa (corresponding to a depth of approximately 500 km), which is consistent with trends reported in related literature. At 0 GPa, $V_s = 4.80$ km/s, increasing to 5.32 km/s at 20 GPa. Within this pressure range, the wave velocities of MgCO_3 are significantly higher than those of the PREM reference curve, exhibiting a distinct high-velocity anomaly.

The seismic velocities of MgCO_3 were calculated using DeePMD simulations at 1500 K. This approach explicitly incorporates intrinsic anharmonic phonon–phonon interactions, providing a more physically realistic description of thermal softening at high temperatures. These results are in close agreement with those reported by Yao C et al. (2018) under comparable isothermal conditions. In the pressure range of 20–70 GPa, V_p increases gradually from 9.79 km/s to 12.14 km/s, whereas V_s rises to 6.01 km/s. This change in wave velocities corresponds to the region from the base of the mantle transition zone to the top of the lower mantle (approximately 600–1500 km in depth). Within this interval, MgCO_3 remains in phase I but exhibits pretransition softening, with wave velocities falling below the PREM values even before transforming into the $C2/m$ structure. At these depths, subducted

carbon is transitioning from upper mantle mineral phases to lower mantle phase states, which may represent an important geochemical “gateway”. Within the pressure range of 80–140 GPa (>1500 km), MgCO_3 ultimately transforms into the $C2/m$ structure, which possesses a higher density and elastic modulus. The V_p increases from approximately 12.5 km/s and reaches 14.5 km/s at 140 GPa (about 2900 km depth), whereas V_s also rises from approximately 6.1 km/s to greater than 7.0 km/s, both significantly exceeding the PREM reference values.

The wave velocities of MgCO_3 again surpass those of PREM, indicating that carbon can not only be transported to the core–mantle boundary, but also may participate in the deep mantle’s chemical and dynamic processes in the form of high-velocity phases. Throughout this range, V_p remains higher than V_s , with a V_p/V_s ratio of approximately 1.7, in excellent agreement with the experimentally observed value of 1.742. Notably, our results for V_p and V_s of MgCO_3 (phase I) at 1500 K within the pressure range of 0–80 GPa are comparable to the PREM profile. Our results provide new data support for how these anharmonic interactions refine the predicted behavior of magnesite under deep-mantle conditions.

4. Conclusions

By combining *ab initio* data, a DP machine learning model, and two-phase coexistence molecular dynamics simulations, we have systematically investigated the phase stability, melting behavior, and elastic properties of MgCO_3 over pressures of 0–140 GPa and temperatures up to 5000 K. The DP accurately reproduces key benchmark properties of magnesite, including its ambient-pressure melting temperature, equation of state, and phonon stability, providing confidence in its transferability across a wide pressure–temperature range. Our simulations establish melting curves for both the low-pressure magnesite structure and the high-pressure $C2/m$ phase. The $C2/m$ phase exhibits a markedly higher melting temperature and a larger positive Clapeyron slope, which we attribute to pressure-induced changes in carbon coordination and polymerization of CO_4 tetrahedra. Under the assumptions of a pure MgCO_3 system, the melting boundary remains well above typical lower mantle geotherms, implying that crystalline MgCO_3 could persist to great depths without melting or decomposing. Elastic wave velocity calculations indicate a pressure-dependent high–low–high anomaly pattern relative to PREM, associated with elastic softening near structural transitions and stiffening in the high-pressure phase. We emphasize that these comparisons are qualitative, as the Earth’s mantle is a multiphase

aggregate; nevertheless, the results provide mineral-physics constraints that can be incorporated into seismic and geodynamic models. The present study neglects compositional complexity, including Fe and Ca substitution, volatile components, and redox effects, all of which are expected to lower melting temperatures and modify stability fields under realistic mantle conditions. Future work should extend the DP framework to multicomponent carbonate systems and integrate thermodynamic results with geodynamic modeling to better quantify the fate of carbon in Earth's deep interior.

Acknowledgments

First, this work was supported by the Talent Innovation and Entrepreneurship Project of Lanzhou City (Grant No. 2023-3-103), the Innovation Fund Project for College Teachers under the Gansu Provincial Department of Education (Grant No. 2024A-138), and the Foundation of Key Laboratory of Cloud Computing of Gansu Province and the Young Scholars Science Foundation of Lanzhou Jiaotong University (Grant No. 2024026).

Second, I would like to express my heartfelt thanks to my supervisor, ZiJiang Liu, for his valuable guidance and enlightened perspective on this paper and toward myself. Professor Liu unfortunately passed away on May 1, 2025, due to illness. I would like to dedicate this article to my mentor. May his soul rest in peace.

CRedit Authorship Contribution Statement

ZhongShan He: Writing–review and editing, Writing–original draft, Visualization, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. XiLong Dou: Writing–review and editing, Validation, Supervision. RunFu Liu: Software, Formal analysis, Data curation. ZiJiang Liu: Software, Formal analysis, Data curation. Yuan Guo: Project administration, Funding acquisition, Conceptualization. XiaoWei Sun: Software, Formal analysis, Data curation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

All data used in this study are authentic and available upon reasonable request. Data and codes can be obtained by contacting the corresponding author by e-mail (xilongdou369@163.com).

References

- Alfè, D., Gillan, M. J., and Price, G. D. (2002). Complementary approaches to the *ab initio* calculation of melting properties. *J. Chem. Phys.*, 116(14), 6170–6177. <https://doi.org/10.1063/1.1460865>
- Alfè, D. (2005). Melting curve of MgO from first-principles simulations. *Phys. Rev. Lett.*, 94(23), 235701. <https://doi.org/10.1103/PhysRevLett.94.235701>
- Anderson, O. L. (1963). A simplified method for calculating the Debye temperature from elastic constants. *J. Phys. Chem. Solids*, 24(7), 909–917. [https://doi.org/10.1016/0022-3697\(63\)90067-2](https://doi.org/10.1016/0022-3697(63)90067-2)
- Bayarjargal, L., Fruhner, C. J., Schrod, N., and Winkler, B. (2018). CaCO₃ phase diagram studied with Raman spectroscopy at pressures up to 50 GPa and high temperatures and DFT modeling. *Phys. Earth Planet. Inter.*, 281, 31–45. <https://doi.org/10.1016/j.pepi.2018.05.002>
- Behler, J., and Parrinello, M. (2007). Generalized neural-network representation of high-dimensional potential-energy surfaces. *Phys. Rev. Lett.*, 98(14), 146401. <https://doi.org/10.1103/PhysRevLett.98.146401>
- Binck, J., Bayarjargal, L., Lobanov, S. S., Morgenroth, W., Luchitskaia, R., Pickard, C. J., Milman, V., Refson, K., Jochym, D. B., ... Winkler, B. (2020). Phase stabilities of MgCO₃ and MgCO₃-II studied by Raman spectroscopy, x-ray diffraction, and density functional theory calculations. *Phys. Rev. Mater.*, 4(5), 055001. <https://doi.org/10.1103/physrevmaterials.4.055001>
- Boulard, E., Gloter, A., Corgne, A., Antonangeli, D., Auzende, A. L., Perrillat, J. P., Guyot, F., and Fiquet, G. (2011). New host for carbon in the deep Earth. *Proc. Natl. Acad. Sci. USA*, 108(13), 5184–5187. <https://doi.org/10.1073/pnas.1016934108>
- Carreras, A. (2020). phonolAMMPS: A python interface for LAMMPS phonon calculations using phonopy. *Zenodo*. <https://ui.adsabs.harvard.edu/abs/2020zndo...3940626C>
- Cerantola, V., Bykova, E., Kuppenko, I., Merlini, M., Ismailova, L., McCammon, C., Bykov, M., Chumakov, A. I., Petitgirard, S., ... Dubrovinsky, L. (2017). Stability of iron-bearing carbonates in the deep Earth's interior. *Nat. Commun.*, 8(1), 15960. <https://doi.org/10.1038/ncomms15960>
- Chen, P. F., Chiao, L. Y., Huang, P. H., Yang, Y. J., and Liu, L. G. (2006). Elasticity of magnesite and dolomite from a genetic algorithm for inverting Brillouin spectroscopy measurements. *Phys. Earth Planet. Inter.*, 155(1-2), 73–86. <https://doi.org/10.1016/j.pepi.2005.10.004>
- Dang, K., Chen, J., Rodgers, B., and Fensin, S. (2023). LAVA 1.0: A general-purpose python toolkit for calculation of material properties with LAMMPS and VASP. *Comput. Phys. Commun.*, 286, 108667. <https://doi.org/10.1016/j.cpc.2023.108667>
- Dziewonski, A. M., and Anderson, D. L. (1981). Preliminary reference Earth model. *Phys. Earth Planet. Inter.*, 25(4), 297–356. [https://doi.org/10.1016/0031-9201\(81\)90046-7](https://doi.org/10.1016/0031-9201(81)90046-7)
- Fiquet, G., and Reynard, B. (1999). High-pressure equation of state of magnesite: New data and a reappraisal. *Am. Mineral.*, 84(5-6), 856–860. <https://doi.org/10.2138/am-1999-5-619>
- Fiquet, G., Guyot, F. O., Kunz, M., Matas, J., Andrault, D., and Hanfland, M. (2002). Structural refinements of magnesite at very high pressure. *Am. Mineral.*, 87(8-9), 1261–1265. <https://doi.org/10.2138/am-2002-8-927>
- Hill, R. (1952). The elastic behaviour of a crystalline aggregate. *Proc. Phys. Soc. Sect. A*, 65(5), 349. <https://doi.org/10.1088/0370-1298/65/5/307>
- Hong, Q. J., and Van De Walle, A. (2013). Solid-liquid coexistence in small systems: A statistical method to calculate melting temperatures. *J. Chem. Phys.*, 139(9), 094114. <https://doi.org/10.1063/1.4819792>
- Isshiki, M., Irifune, T., Hirose, K., Ono, S., Ohishi, Y., Watanuki, T., Nishibori, E., Takata, M., and Sakata, M. (2004). Stability of magnesite and its high-pressure form in the lowermost mantle. *Nature*, 427(6969), 60–63. <https://doi.org/10.1038/nature02181>
- Katsura, T., and Ito, E. (1990). Melting and subsolidus phase relations in the MgSiO₃-MgCO₃ system at high pressures: Implications to evolution of the Earth's atmosphere. *Earth Planet. Sci. Lett.*, 99(1-2), 110–117. [https://doi.org/10.1016/0012-821X\(90\)90074-8](https://doi.org/10.1016/0012-821X(90)90074-8)
- Katsura, T., Yoneda, A., Yamazaki, D., Yoshino, T., and Ito, E. (2010). Adiabatic temperature profile in the mantle. *Phys. Earth Planet. Inter.*, 183(1-2), 212–218. <https://doi.org/10.1016/j.pepi.2010.07.001>
- Kresse, G., and Furthmüller, J. (1996). Efficiency of *ab-initio* total energy calculations for metals and semiconductors using a plane-wave basis set. *Comp. Mater. Sci.*, 6(1), 15–50. [https://doi.org/10.1016/0927-0256\(96\)00008-0](https://doi.org/10.1016/0927-0256(96)00008-0)
- Kresse, G., and Joubert, D. (1999). From ultrasoft pseudopotentials to the projector augmented-wave method. *Phys. Rev. B*, 59(3), 1758–1775. <https://doi.org/10.1103/physrevb.59.1758>
- Li, Z., and Stackhouse, S. (2020). Iron-rich carbonates stabilized by magnetic entropy at lower mantle conditions. *Earth Planet. Sci. Lett.*, 531, 115959. <https://doi.org/10.1016/j.epsl.2019.115959>
- Litasov, K. D., Fei, Y. W., Ohtani, E., Kuribayashi, T., and Funakoshi, K. (2008).

- Thermal equation of state of magnesite to 32GPa and 2073K. *Phys. Earth Planet. Inter.*, 168(3–4), 191–203. <https://doi.org/10.1016/j.pepi.2008.06.018>
- Liu, Z. J., Li, T., Sun, X. W., Zhang, C. R., and Ju, J. Q. (2022a). Comparative study on high-pressure physical properties of monoclinic MgCO_3 and Mg_2CO_4 . *Sci. Rep.*, 12(1), 19485. <https://doi.org/10.1038/s41598-022-24033-8>
- Liu, Z. J., Sun, X. W., Zhang, C. R., Zhang, S. J., Zhang, Z. R., and Jin, N. Z. (2022b). First-principles calculations of high-pressure physical properties anisotropy for magnesite. *Sci. Rep.*, 12(1), 3691. <https://doi.org/10.1038/s41598-022-07705-3>
- Maeda, F., Ohtani, E., Kamada, S., Sakamaki, T., Hirao, N., and Ohishi, Y. (2017). Diamond formation in the deep lower mantle: A high-pressure reaction of MgCO_3 and SiO_2 . *Sci. Rep.*, 7(1), 40602. <https://doi.org/10.1038/srep40602>
- Marcondes, M. L., Justo, J. F., and Assali, L. V. C. (2016). Carbonates at high pressures: Possible carriers for deep carbon reservoirs in the Earth's lower mantle. *Phys. Rev. B*, 94(10), 104112. <https://doi.org/10.1103/physrevb.94.104112>
- Oganov, A. R., Ono, S., Ma, Y. M., Glass, C. W., and Garcia, A. (2008). Novel high-pressure structures of MgCO_3 , CaCO_3 and CO_2 and their role in Earth's lower mantle. *Earth Planet. Sci. Lett.*, 273(1–2), 38–47. <https://doi.org/10.1016/j.epsl.2008.06.005>
- Perdew, J. P., Burke, K., and Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Phys. Rev. Lett.*, 77(18), 3865–3868. <https://doi.org/10.1103/physrevlett.77.3865>
- Pickard, C. J., and Needs, R. J. (2015). Structures and stability of calcium and magnesium carbonates at mantle pressures. *Phys. Rev. B*, 91(10), 104101. <https://doi.org/10.1103/physrevb.91.104101>
- Plank, T., and Manning, C. E. (2019). Subducting carbon. *Nature*, 574(7778), 343–352. <https://doi.org/10.1038/s41586-019-1643-z>
- Plimpton, S. (1995). Fast parallel algorithms for short-range molecular dynamics. *J. Comput. Phys.*, 117(1), 1–19. <https://doi.org/10.1006/jcph.1995.1039>
- Reuss, A. (1929). Berechnung der fließgrenze von mischkristallen auf grund der plastizitätsbedingung für einkristalle. *ZAMM - J. Appl. Mathem. Mechan.*, 9(1), 49–58. <https://doi.org/10.1002/zamm.19290090104>
- Rohrbach, A., and Schmidt, M. W. (2011). Redox freezing and melting in the Earth's deep mantle resulting from carbon–iron redox coupling. *Nature*, 472(7342), 209–212. <https://doi.org/10.1038/nature09899>
- Sanchez-Valle, C., Ghosh, S., and Rosa, A. D. (2011). Sound velocities of ferromagnesian carbonates and the seismic detection of carbonates in eclogites and the mantle. *Geophys. Res. Lett.*, 38(24), L24315. <https://doi.org/10.1029/2011GL049981>
- Santos, S. S. M., Marcondes, M. L., Justo, J. F., and Assali, L. V. C. (2019). Stability of calcium and magnesium carbonates at Earth's lower mantle thermodynamic conditions. *Earth Planet. Sci. Lett.*, 506, 1–7. <https://doi.org/10.1016/j.epsl.2018.10.030>
- Solopova, N. A., Dubrovinsky, L., Spivak, A. V., Litvin, Y. A., and Dubrovinskaya, N. (2015). Melting and decomposition of MgCO_3 at pressures up to 84 GPa. *Phys. Chem. Miner.*, 42(1), 73–81. <https://doi.org/10.1007/s00269-014-0701-1>
- Sun, W. D., Hawkesworth, C. J., Yao, C., Zhang, C. C., Huang, R. F., Liu, X., Sun, X. L., Ireland, T., Song, M. S., ... Wu, Z. Q. (2018). Carbonated mantle domains at the base of the Earth's transition zone. *Chem. Geol.*, 478, 69–75. <https://doi.org/10.1016/j.chemgeo.2017.08.001>
- Togo, A., and Tanaka, I. (2015). First principles phonon calculations in materials science. *Scr. Mater.*, 108, 1–5. <https://doi.org/10.1016/j.scriptamat.2015.07.021>
- Tsuchiya, J., Nishida, R., and Tsuchiya, T. (2020). First principles calculation of the stability of iron bearing carbonates at high pressure conditions. *Minerals*, 10(1), 54. <https://doi.org/10.3390/min10010054>
- Vočadlo, L., Alfè, D., Price, G. D., and Gillan, M. J. (2004). *Ab initio* melting curve of copper by the phase coexistence approach. *J. Chem. Phys.*, 120(6), 2872–2878. <https://doi.org/10.1063/1.1640344>
- Voigt, W. (1966). Wechselbeziehungen zwischen zwei Tensortripeln. (Elastizität und innere Reibung.). In W. Voigt (Ed.), *Lehrbuch der Kristallphysik: Mit Ausschluß der Kristalloptik* (pp. 560–800). Wiesbaden: Vieweg+Teubner Verlag. https://doi.org/10.1007/978-3-663-15884-4_8
- Wang, H., Zhang, L. F., Han, J. Q., and E, W. N. (2018). DeePMD-kit: A deep learning package for many-body potential energy representation and molecular dynamics. *Comput. Phys. Commun.*, 228, 178–184. <https://doi.org/10.1016/j.cpc.2018.03.016>
- Wang, X. W., Yang, M. X., Gai, X. Q., Sun, Y. B., Cao, B. H., Chen, J. J., Liang, M., Tian, F. B., and Li, L. (2024). A comprehensive investigation on the accuracy and efficiency of methods for melting temperature calculation using molecular dynamics simulations. *J. Mol. Liq.*, 395, 123924. <https://doi.org/10.1016/j.molliq.2023.123924>
- Xu, M., Jing, Z. C., Van Orman, J. A., Yu, T., and Wang, Y. B. (2024). In situ determination of thermoelastic properties of magnesite at high pressure and temperature with implications to seismic detectability of moderately carbonated lithologies in the Earth's mantle. *J. Geophys. Res.: Solid Earth*, 129(5), e2023JB028455. <https://doi.org/10.1029/2023JB028455>
- Yang, J., Mao, Z., Lin, J. F., and Prakapenka, V. B. (2014). Single-crystal elasticity of the deep-mantle magnesite at high pressure and temperature. *Earth Planet. Sci. Lett.*, 392, 292–299. <https://doi.org/10.1016/j.epsl.2014.01.027>
- Yao, C., Wu, Z. Q., Zou, F., and Sun, W. D. (2018). Thermodynamic and elastic properties of magnesite at mantle conditions: First-principles calculations. *Geochim. Geophys. Geosyst.*, 19(8), 2719–2731. <https://doi.org/10.1029/2017GC007396>
- Yao, X., Xie, C. W., Dong, X., Oganov, A. R., and Zeng, Q. F. (2018). Novel high-pressure calcium carbonates. *Phys. Rev. B*, 98(1), 014108. <https://doi.org/10.1103/PhysRevB.98.014108>
- Zhang, J., Martinez, I., Guyot, F., Gillet, P., and Saxena, S. K. (1997). X-ray diffraction study of magnesite at high pressure and high temperature. *Phys. Chem. Miner.*, 24(2), 122–130. <https://doi.org/10.1007/s002690050025>
- Zhang, L. F., Han, J. Q., Wang, H., Car, R., and E, W. N. (2018). Deep potential molecular dynamics: A scalable model with the accuracy of quantum mechanics. *Phys. Rev. Lett.*, 120(14), 143001. <https://doi.org/10.1103/physrevlett.120.143001>
- Zhang, Y., and Maginn, E. J. (2012). A comparison of methods for melting point calculation using molecular dynamics simulations. *J. Chem. Phys.*, 136(14), 144116. <https://doi.org/10.1063/1.3702587>
- Zhang, Z. G., Mao, Z., Liu, X., Zhang, Y. G., and Brodholt, J. (2018). Stability and reactions of CaCO_3 polymorphs in the Earth's deep mantle. *J. Geophys. Res.: Solid Earth*, 123(8), 6491–6500. <https://doi.org/10.1029/2018JB015654>
- Zhou, S. Y., Liu, D. H., Zhang, C. Y., Wang, X. B., and Song, L. (2025). *Ab initio* molecular dynamics investigation of the proton conductivity and dynamics behavior of hydrous ringwoodite under high temperatures and pressure. *Earth Planet. Phys.*, 9(4), 842–852. <https://doi.org/10.26464/epp2025049>