DFT-Based Optimization of Morse Potential Parameters for Selected Metallic and Non-Metallic Materials

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Abstract.
The accurate description of interatomic interactions is essential for understanding the structural, mechanical, and thermal properties of metals at the atomic scale. The Morse potential is a widely used empirical model due to its simple analytical form and ability to capture basic bonding characteristics. However, its accuracy strongly depends on the choice of potential parameters, which are often obtained from experimental data or semi-empirical approaches and may not reliably represent non-ideal conditions such as defects, high stress, or phase transitions. In this work, we develop, optimize, and validate Morse potential parameters for several materials, including C, B, Ti, Al, Ni, and Fe, using reference data from DFT calculations. DFT simulations are performed using the open-source Quantum ESPRESSO package to obtain total energy data for isolated atomic pairs at various interatomic separation distances. The Morse potential parameters, namely the potential well depth (D), equilibrium distance (r_e), and stiffness parameter (α), are determined by fitting the DFT total energy curves over a wide range of interatomic distances, including regions below and above the equilibrium separation up to the asymptotic limit. The fitted parameters are validated by comparing the resulting Morse potential energy profiles with the corresponding DFT reference data. This approach ensures that the optimized parameters accurately reproduce the underlying ab initio energy landscape while retaining the computational efficiency of empirical potentials. The resulting Morse parameters are intended for use in large-scale molecular dynamics simulations, particularly for modeling ballistic impact and armor systems involving materials such as B_4C, Ti-based alloys, and polymer–metal composites. This study provides a systematic framework for deriving DFT-consistent Morse potential parameters, enabling more reliable atomistic simulations of metallic and composite materials under extreme loading conditions.
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Keywords: Morse Potential, DFT, Total Energy, Separation Energy, Data Fitting

Introduction

Studies on the properties of metals at the atomic scale are one of the main focuses in the fields of materials physics and computation. Modeling interatomic interactions has long been used to understand the structural, mechanical, and thermal behavior of various types of metals [1]. One well-known potential model is the Morse potential, developed by Philip M. Morse to describe the binding energy in diatomic molecules, which has since been widely applied to simple metal systems [2-3]. This model is relatively simple but capable of representing basic bonding behavior, making it frequently used in molecular dynamics simulations and material property studies [4].

However, the accuracy of the Morse potential is highly dependent on the parameters used, namely the potential well depth, equilibrium distance, and stiffness constant [5]. Many previous studies have used parameters obtained from experimental data or semi-empirical approaches [6]. These parameters are not always able to capture variations in metal electronic properties or non-ideal conditions, such as high stress, crystal defects, or phase changes. Therefore, validation and optimization of Morse parameters are important to ensure that this simple model remains consistent with more accurate quantitative data [7].

In recent decades, the Density Functional Theory (DFT) method has become one of the most widely used ab initio approaches for studying the electronic properties and total energy of solid systems [8]. DFT allows for relatively efficient calculations with high accuracy in describing the basic structure of metals, bond energies, and mechanical properties [9]. Quantum Espresso software is one of the open-source DFT computing packages widely used for materials research [9–11]. However, the direct application of DFT to systems with a large number of atoms requires significant computational costs, making it difficult to use for long-term or large-scale simulations [13].

This limitation has led to the need for a hybrid strategy using DFT as a benchmark to optimize simple potential models such as Morse. Several previous studies have examined efforts to calibrate interatomic potential parameters using DFT calculation results, both in transition metals and simple metals [13,14]. However, studies that specifically focus on optimizing Morse potential parameters for specific metals with direct validation against DFT calculation results are still limited. This opens up opportunities for research to produce more representative potential parameters, while maintaining the computational efficiency that is the advantage of simple models [16].

This study aims to optimize and validate Morse potential parameters for specific metals by utilizing DFT calculation results through Quantum Espresso. To obtain Morse potential parameters (D_e, α, r_e) for specific metals, DFT simulation results for these metals will be fitted to a two-atom metal system at a specific distance. The fitting refers to the total separation energy data for a number of separation distances r against the Morse potential model. By fitting the total energy data of several separation distance data points below the equilibrium distance and several separation distance data points above the equilibrium distance up to the asymptotic distance, we will obtain three Morse potential parameters for this metal. In this way, the research is expected to produce potential parameters that are not only more accurate and consistent with quantum theory, but can also be applied in large-scale material simulations with lower computational costs. The contribution of this research lies in providing theoretically validated Morse parameter data, which can be used as a basis for developing material simulations for engineering applications and further research [17].

Theoretical Background

In this study, a DFT-consistent description of interatomic interactions is required to capture the physical behavior of the system. The Morse potential is an effective model for describing anharmonic interatomic interactions in diatomic systems. The parameter values of this potential are determined using first-principles calculations based on DFT calculation. Quantum ESPRESSO Code is used to initiate the total energy as a function of interatomic distance, which will be fitted to the Morse Potential in order to obtain parameters that have physical meaning.

Morse Potential and Parameters

The Morse potential, introduced by Philip M. Morse in 1929, was originally developed to describe the vibrational energy of diatomic molecules [18]. Due to its mathematical simplicity and low computational cost, it has been widely applied to metallic systems [19]. For cubic metals, parameterization based on experimental lattice energy, lattice constants, and compressibility has shown good agreement with elastic properties [20]. In molecular dynamics simulations, Morse-type two-body potentials remain attractive for metal–nonmetal and metal–impurity systems because of their computational efficiency in force evaluation [19].

Although the Morse potential was initially designed for covalent bonding in non-metallic systems [18], its two-body formulation inherently neglects bond-angle dependence and many-body effects. As a result, more complex covalent structures are typically modeled using many-body potentials such as Tersoff, Stillinger–Weber, or REBO. Nevertheless, recent parameterizations based on dispersion-corrected density functional theory have demonstrated that the Morse potential can successfully describe metal–surface interactions, such as Ni or Ag on graphene and silicene, reproducing binding energies and equilibrium bond lengths [21]. These studies indicate that, despite its simplicity, the Morse potential can capture essential features of both covalent and metallic bonding in selected model systems.

The determination of Morse potential parameters D_e, α, and r_e is commonly based on experimental data reported in the literature or on quantum-mechanical simulations, including density functional theory (DFT) calculations performed using Quantum ESPRESSO. A classical approach for metallic systems was introduced by Girifalco and Weizer (1959), in which Morse parameters are derived from macroscopic experimental properties such as sublimation energy, lattice constant, and bulk modulus [20]. For face-centered cubic (FCC) and body-centered cubic (BCC) metals, fitting the Morse equation of state to experimental data has been shown to yield good agreement with elastic constants and lattice energies [20].

More recent studies have demonstrated that Morse parameters can also be extracted from first-principles calculations. In particular, dispersion-corrected DFT (DFT-D) has been successfully applied to metal–graphene and metal–silicene systems, producing Morse parameters that reproduce binding energies, equilibrium bond lengths, and vibrational frequencies of adsorbed metal atoms [21]. Other theoretical approaches, such as Extended X-ray Absorption Fine Structure (EXAFS) analysis, have also been proposed for evaluating Morse parameters from thermal disorder effects using sublimation energy and crystal compressibility data. Overall, Morse potential parameters may be obtained from macroscopic experimental measurements, existing parameterizations in the literature, or fitting procedures applied to DFT-derived potential energy surfaces [22]. Equation (1) is a general form of Morse potential:

$$V(r) = E_0 + D_e\left(1 - e^{-\alpha(r-r_e)}\right)^2 \qquad (1)$$

with the following definitions:
- $V(r)$: potential energy as a function of interatomic distance r,
- E_0 : minimum energy of the system,
- D_e : dissociation energy (depth of the potential well),
- r_e : equilibrium interatomic distance,
- α : constant related to bond stiffness.

Density Functional Theory

Density Functional Theory (DFT) is an ab initio approach for evaluating the electronic properties of materials based on the electron density formalism [23, 24]. Its theoretical foundation is provided by the Hohenberg–Kohn theorems and the Kohn–Sham formulation, in which a many-electron system is mapped onto an equivalent system of non-interacting electrons moving in an effective potential [24]. Within this framework, the total energy of the system is expressed as a functional of the electron density,

$$E[n(\mathbf{r})] = T_s[n] + \int V_{\text{ext}}(\mathbf{r})\, n(\mathbf{r})\, d\mathbf{r} + \frac{1}{2}\int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}d\mathbf{r}' + E_{\text{xc}}[n], \qquad (2)$$

where $T_s[n]$ is the kinetic energy of non-interacting electrons, V_{ext} is the external potential, and E_{xc} denotes the exchange–correlation functional.

A key advantage of DFT is its ability to predict structural and energetic properties without the use of empirical parameters, thereby providing a first-principles basis for determining binding energies and interatomic forces. Limitations of DFT primarily arise from the choice of exchange–correlation functional and the computational cost associated with large-scale systems. Nevertheless, DFT calculations provide a systematic and transferable reference dataset that is often more comprehensive than experimentally available data [25]. Consequently, DFT-derived energies and forces are widely employed as optimization targets for simplified interatomic potentials, including the Morse potential, enabling reliable validation and parameter optimization within atomistic modeling frameworks.

In the present study, the focus is not on the theoretical development of DFT itself. Instead, DFT is employed as a reliable first-principles tool to generate total energy data of atomic systems. Specifically, DFT calculations are used to compute the total energy of a metal dimer as a function of interatomic separation, from which the separation energy curve is obtained. These DFT-derived energy–distance data serve as the reference dataset for fitting the Morse potential parameters. In this context, DFT provides a consistent *ab initio* energy landscape that enables the determination and validation of physically meaningful Morse potential parameters.

Quantum ESPRESSO

Quantum ESPRESSO represents a widely adopted computational platform for density functional theory (DFT) calculations in solid-state materials studies. The package consists of a free and open-source collection of codes dedicated to electronic structure calculations and materials modeling within the DFT framework, employing plane-wave basis sets together with norm-conserving, ultrasoft, and projector augmented-wave (PAW) pseudopotentials [24]. Its modular design and advanced parallelization capabilities support efficient simulations of large and complex material systems. Continuous development by an international research community under the GNU General Public License has contributed to its broad acceptance in computational materials science. First-principles evaluation of quantities such as total energy, crystal lattice parameters, and elastic constants using Quantum ESPRESSO provides essential reference data for Morse potential parameter optimization.

DFT-Based Optimization of Morse Potential Parameters

A variety of optimization methodologies have been proposed for determining Morse potential parameters using DFT-derived reference data. A classical approach is the Girifalco–Weizer method, which exploits crystalline symmetry in parameter estimation. Within this framework, the equilibrium distance r_e is obtained from DFT-optimized lattice constants, while the potential well depth D is calibrated to reproduce DFT cohesive or lattice energies. The stiffness parameter α is subsequently determined using bulk modulus values calculated from DFT [19]. This combined adjustment of lattice constant, bulk modulus, and sublimation energy enables a consistent reproduction of the structural and elastic properties of metallic systems [19].

An alternative approach involves direct numerical fitting of interatomic energy–distance relationships obtained from DFT calculations. In this procedure, a series of DFT simulations is performed at different interatomic separations to construct a reference potential energy curve, which is then fitted using the Morse functional form. The initial parameter set is refined through numerical optimization techniques that minimize the deviation between the Morse potential and the DFT energy profile over selected configurations. Through this fitting process, Morse potential parameters can be systematically aligned with ab initio reference data. The effectiveness of this strategy has been demonstrated in dispersion-corrected DFT (DFT-D) studies, such as the work of Galashev et al., which reported accurate reproduction of binding energies and vibrational characteristics using optimized Morse parameters [21].

Previous studies have reported extensive fitting and validation of Morse potential parameters against both DFT and experimental datasets. Galashev *et al.* (2019) derived Morse parameters for interactions between metal atoms (Ni, Ag, and Li) and graphene or silicene substrates using dispersion-corrected DFT calculations, achieving good agreement in binding energies, equilibrium atomic distances, and vibrational frequencies [21]. Poletaev *et al.* (2017) applied the Morse potential to face-centered cubic (FCC) metals while explicitly accounting for interatomic interactions up to the fifth coordination shell [26]. Although their study focused on elemental metals, the proposed methodology provides a relevant reference for materials such as Fe, including austenitic phases and higher-order elastic properties.

In molecular dynamics (MD) simulations, Morse and modified Morse potentials are widely used to model metals and complex materials [27]. Their validity is commonly assessed by comparing elastic constants, melting temperatures, and defect formation energies with results from DFT calculations and experimental data. Recent developments, including density functional theory with van der Waals corrections (DFT+vdW) and delta-machine-learning-assisted fitting strategies, have further improved the consistency of interatomic potential parameters with high-level DFT energy surfaces [25–27]. Nevertheless, studies explicitly reporting Morse parameterization for heavy transition metals (e.g., W and V) or electropositive p-block elements (e.g., Ti) remain limited, as embedded-atom method (EAM) and modified embedded-atom method (MEAM) potentials are more commonly employed for these systems.

The lattice constant is a fundamental parameter that defines the unit cell dimensions of crystalline materials [31]. It corresponds to the characteristic spacing between lattice points along crystallographic directions, such as the cubic lattice parameter *a* in cubic crystal systems. The lattice constant directly determines the unit cell volume and atomic packing density, and even small deviations in its value can lead to significant changes in material properties, including elastic

moduli, binding energies, and electronic band structures. Consequently, convergence of lattice constants is commonly used as a primary validation criterion in DFT-based materials modeling to ensure consistency between optimized structures and experimental reference data [31].

Within DFT, lattice constants are evaluated through total energy minimization with respect to variations in the unit cell geometry. Structural optimization procedures, such as variable-cell relaxation (vc-relax), allow simultaneous optimization of lattice parameters and cell shape until the macroscopic stress tensor is minimized. Alternatively, total energies $E(V)$ may be calculated for a series of unit cell volumes, followed by equation-of-state fitting to determine the equilibrium volume V_0 corresponding to the minimum energy. The resulting lattice parameters are sensitive to the choice of exchange–correlation (XC) functional employed in the DFT calculations [28].

Materials and Methods

Studied Elements

The selected elements are representative of materials commonly employed in high-strength structural components, protective systems, and metal–ceramic composites. Transition metals such as Fe, Ni, Ti, and W form the basis of steel and alloy systems used in armor and high-load applications, while non-metallic elements such as B and C are key constituents of ultra-hard ceramic materials, including boron carbide and carbon-based coatings. Silicon and oxygen are included to represent semiconductor and oxide bonding environments frequently encountered at material interfaces. Together, these elements provide a physically meaningful test set for evaluating the transferability of Morse potential parameters across metallic, covalent, and mixed bonding regimes.

Computational and Fitting Procedure

First-principles calculations were performed using the Quantum ESPRESSO package within the density functional theory (DFT) framework. The Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional was employed, along with norm-conserving pseudopotentials from the Quantum ESPRESSO library. Initial atomic configurations for bulk structures were based on literature lattice parameters, followed by full DFT structural relaxation.

To parameterize the Morse potential, total energies (or more precisely the separation energy) and interatomic forces were computed for isolated diatomic systems via self-consistent field (SCF) calculations, with interatomic distances systematically varied around the equilibrium value. The resulting energy–distance curves served as reference data for fitting the Morse potential parameters. Forces were obtained directly using the built-in stress tensor calculation in Quantum ESPRESSO (activated via the tprnfor option). The DFT-derived data were tabulated with columns for interatomic distance (in Å), total energy (in eV), and force (in eV/Å).

Parameter optimization was achieved through nonlinear least-squares regression to minimize deviations between the ab initio energies and the Morse potential function [Eq. (1)]. The goodness of fit was quantified using the coefficient of determination (R^2). The optimized Morse parameters were further validated by comparison with available experimental or literature values, ensuring a physically reasonable description of interatomic bonding.

Validation of the fitted potentials was performed in LAMMPS via isotropic structural relaxation using the conjugate-gradient algorithm. Key outputs included total energy (indicating system stability), cohesive energy per atom (reflecting bond strength), relaxed lattice parameters (for comparison with reference data), and system pressure (monitored to confirm convergence to equilibrium). These results were compiled in tables listing lattice parameters, total energy, cohesive energy, and pressure. **Figure 1** shows the flowchart of fitting procedure of potential parameters based on the separation energy.
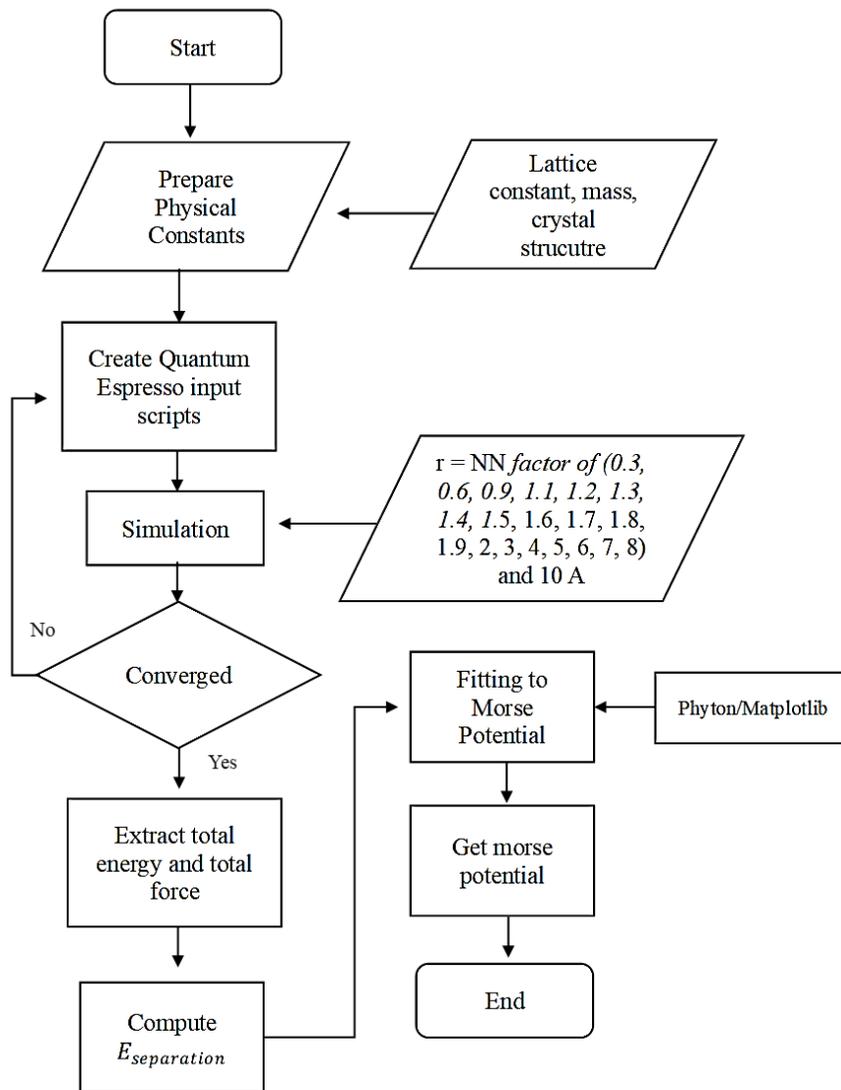
Figure 1. Fitting procedure

Fitting is very easy and can be done with a Python program that has tools for fitting data.

Dimer Separation Energy from DFT Calculations

The separation energy of a dimer is evaluated using first-principles total energy calculations within the framework of Density Functional Theory (DFT). In this approach, the total energy of a two-atom system is computed as a function of the interatomic distance r, allowing direct assessment of the bonding interaction between the atoms.

For a given atomic species, three total energies are required: (i) the total energy of the dimer system $E_{dimer}(r)$ at a specific interatomic separation, (ii) the total energy of a single isolated atom E_{atom}, and (iii) the reference energy corresponding to two non-interacting atoms. The dimer separation energy $E_{sep}(r)$ is defined as

$$E_{sep}(r) = E_{dimer}(r) - 2E_{atom}. \tag{3}$$

A negative value of E_{sep} indicates an energetically favorable bonded state, while values approaching zero correspond to the dissociation limit where the atoms become non-interacting. By varying the interatomic distance r over a sufficiently wide range, a complete energy–distance curve is obtained, from which the equilibrium bond length, binding energy, and curvature of the potential energy well can be determined.

This DFT-derived separation energy curve serves as the reference dataset for fitting the Morse potential parameters, ensuring that the empirical potential accurately reproduces the fundamental features of the *ab initio* interatomic interaction, including bond strength and equilibrium separation.

Results and Discussion

Total energy and distance profiles for eight elements which is Fe, Ti, Al, W, C, B, Si, O, and Ni are obtained from Density Functional Theory (DFT) calculations using Quantum ESPRESSO. These data are subsequently fitted using the Morse potential formulation, yielding three fundamental parameters: the potential well depth (D_e), stiffness constant (α), and equilibrium distance (r_e). The resulting parameter sets reflect element-specific bonding characteristics related to interatomic bond strength and structural stability.

1. Iron (Fe)
The nearest-neighbor distance provides an important reference for selecting physically meaningful interatomic separation ranges in DFT simulations. For body-centered cubic (BCC) iron, the nearest-neighbor distance obtained from the DFT-optimized lattice constant is approximately 2.53 Å. This value is used only as an initial guideline for constructing the Fe–Fe separation distances in the dimer calculations and should not be confused with the equilibrium bond distance of the Morse potential.

Table S1 (see Tables in the supplementary material) presents the separation energy of the Fe dimer obtained from DFT calculations using the Quantum ESPRESSO package, evaluated according to Eq. (3). The DFT energy–distance data were fitted to the Morse potential function, yielding optimized parameters of $D_e = 3.3061\,eV$, $\alpha = 2.1687\,Å^{-1}$, and $r_e = 1.8662\,Å$. The high coefficient of determination ($R^2 = 0.999997$) indicates an excellent agreement between the Morse potential and the DFT reference data. The resulting fitted energy curve is shown in **Figure 2**.

2. Titanium (Ti)

Titanium (Ti) has a nearest-neighbor distance of approximately 2.90 Å, obtained from the DFT-optimized crystal structure and used as a reference for selecting the interatomic separation range in the dimer calculations. **Table S2** presents the separation energy of the Ti dimer obtained from Density Functional Theory (DFT) calculations using the Quantum ESPRESSO package, evaluated according to Eq. (3). Fitting the DFT energy–distance data to the Morse potential yields optimized parameters of $D_e = 16.9443$ eV, $\alpha = 1.2202 \text{Å}^{-1}$, and $r_e = 2.0516$ Å. The high coefficient of determination ($R^2 = 0.999901$) indicates excellent agreement between the Morse potential and the DFT reference data. Compared to Fe, titanium exhibits a significantly larger potential well depth, reflecting stronger effective bonding in the Ti–Ti dimer. The equilibrium distance r_e is also larger, consistent with the larger atomic size of Ti. The relatively smaller stiffness parameter α indicates a broader potential well, corresponding to increased bond flexibility. These features are consistent with the partially directional bonding character of transition metals with mixed metallic and covalent contributions.

3. Aluminium (Al)

For face-centered cubic (FCC) aluminum, the nearest-neighbor distance derived from the DFT-optimized lattice constant is approximately 2.86 Å. This value is used only as an initial guideline for constructing the Al–Al dimer separation range and should not be directly identified with the equilibrium distance of the Morse potential. **Table S3** presents the separation energy of the Al dimer obtained from Density Functional Theory (DFT) calculations using the Quantum ESPRESSO package, evaluated according to Eq. (3). Fitting the DFT energy–distance data to the Morse potential yields parameters of $D_e = 15.4098$ eV, $\alpha = 0.56 \text{Å}^{-1}$, and $r_e = 2.75 \text{Å}$. The coefficient of determination for the fit is $R^2 = 0.987$, indicating good agreement between the Morse potential and the DFT reference data. Compared to transition metals such as Fe and Ti, aluminum exhibits a broader and shallower effective potential well, as reflected by the smaller stiffness parameter α. This behavior is consistent with the relatively lower elastic modulus and higher ductility of aluminum. The equilibrium distance r_e is close to the bulk nearest-neighbor distance, reflecting the predominantly metallic and weakly directional bonding character of Al.

4. Tungsten (W)

The nearest-neighbor distance serves as a reference for selecting physically meaningful interatomic separations in the DFT simulations. For body-centered cubic (BCC) tungsten, the nearest-neighbor distance derived from the DFT-optimized lattice constant is approximately 2.74 Å. This value is used only as a guideline for constructing the W–W dimer separation range and should not be directly associated with the equilibrium distance of the Morse potential.

Table S4 presents the separation energy of the W dimer obtained from Density Functional Theory (DFT) calculations using the Quantum ESPRESSO package, evaluated according to Eq. (3). Fitting the DFT energy–distance data to the Morse potential yields optimized parameters of $D_e = 10.6879$ eV, $\alpha = 1.7456 \text{Å}^{-1}$, and $r_e = 2.0184 \text{Å}$. The coefficient of determination of the fit is $R^2 = 0.999$, indicating excellent agreement between the Morse potential and the DFT reference data. Compared to lighter metals, tungsten exhibits a relatively deep and narrow effective potential well, as reflected by the large stiffness parameter α. This behavior indicates strong resistance to bond stretching and is qualitatively consistent with the known mechanical rigidity and high thermal stability of tungsten. While the fitted Morse parameters are derived from dimer calculations, they capture key trends associated with the strong bonding character of W.

5. Nickel (Ni)

For Ni structure, NN distant is obtained as 2.65 Å. **Table S9** is the separation energy for Si from DFT Quantum Espresso simulation, that can be computed using Eq.(3). From data fitting we found that the potential parameter for Ni are D_e = 3.0471 eV, α = 1.9651 Å^{-1} and r_e = 1.9855 Å. The regression coefficient of fitting for this Ni is R^2 = 0.999999.

For non-metallic elements such as carbon (C) and boron (B), the obtained well depths of D_e=5.786 eV for C, and 2.9223 eV for B, together with short equilibrium distances of r_e =1.3015 Å for C and 1.65551 Å for B, indicate strong covalent bonding. Also, α = 2.1407 Å^{-1} for C and α = 1.595 Å^{-1} for B. The comparatively lower well depths relative to heavy metals suggest that overall cohesion in these systems is predominantly governed by orbital hybridization rather than metallic bonding contributions.

Silicon (Si) and oxygen (O) display consistent bonding trends. Silicon exhibits intermediate bonding strength with D_e =3.5403 eV, α = 1.2809 Å^{-1} for and r_e = 2.2057 Å, characteristic of semiconducting materials with partial covalent character. Oxygen shows a higher potential depth of D_e = 7.1494 eV, α = 2.5806 Å^{-1} and a shorter equilibrium distance of r_e = 1.2157 Å, indicative of strong polar covalent bonding.

Figure 2 is a plotting of the Morse potential parameters for the 9 elements studied.
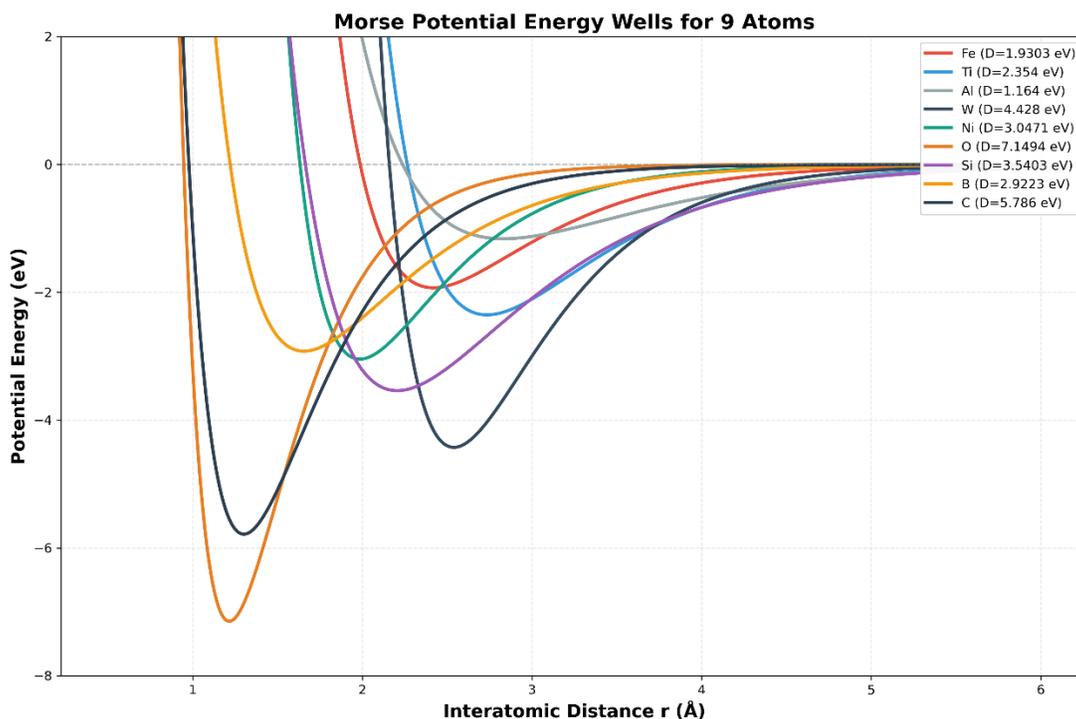

Figure 2. Morse Potential Graph of 9 Elements.

Conclusions

In this study, Morse potential parameters (D_e, α, and r_e) were extracted for eight elements, namely Fe, Ti, Al, W, C, B, Si, O, and Ni, through fitting of dimer separation energy profiles obtained from Density Functional Theory (DFT) calculations performed using the Quantum ESPRESSO package. The resulting parameters show a high level of consistency with the ab initio reference data, as indicated by coefficients of determination (R^2) close to unity for all investigated elements. These results demonstrate that the Morse potential provides a reliable representation of DFT-derived interatomic energy–distance relationships at the dimer level for both transition metals and selected non-metallic elements. The Morse potential parameters in this study are:

Fe: D = 1.9303 eV, α = 1.6082 Å^{-1}, r_e = 2.4185 Å
Ti: D = 2.354 eV, α = 1.475 Å^{-1}, r_e = 2.735 Å
Al: D = 1.164 eV, α = 1.164 Å^{-1}, r_e = 2.833 Å
W: D = 4.428 eV, α = 1.822 Å^{-1}, r_e = 2.540 Å
Ni: D = 3.0471 eV, α = 1.9651 Å^{-1}, r_e = 1.9855 Å
O: D = 7.1494 eV, α = 2.5806 Å^{-1}, r_e = 1.2157 Å
Si: D = 3.5403 eV, α = 1.2809 Å^{-1}, r_e = 2.2057 Å
B: D = 2.9223 eV, α = 1.595 Å^{-1}, r_e = 1.6555 Å
C: D = 5.786 eV, α = 2.1407 Å^{-1}, r_e = 1.3015 Å

Systematic trends in the fitted parameters are observed across the studied elements. Heavier transition metals such as W and Ti exhibit larger effective potential depths and stiffness parameters, reflecting stronger resistance to bond deformation, while elements such as Al and Si display broader and more compliant effective bonding characteristics. Although the present parameterization is based on dimer-level DFT data and has not yet been fully validated in large-scale molecular dynamics simulations, the obtained Morse parameters provide a physically consistent and transferable starting point for subsequent MD studies. Future work will focus on validating these parameters through simulations of bulk properties, defect energetics, and thermomechanical behavior in metallic and composite systems.

Acknowledgements

References

[1] J. Hafner, "Atomic-scale computational materials science," *Acta Materialia*, vol. 48, no. 1, pp. 71–92, 2000, doi: https://doi.org/10.1016/S1359-6454(99)00288-8.
[2] E. Yazdankish, "Analytical Bound-State solution of the Schrodinger equation for the morse potential within the Nikiforov-Uvarov method," *Mathematics and Computational Sciences*, vol. 2, no. 1, pp. 61–70, 2021, doi: 10.30511/mcs.2021.522714.1016.

[3]   H. Karimah, A. Arkundato, R. D. Syarifah, A. K. Rivai, and F. Monado, "Lennard-Jones and Morse potential comparison for studying the liquid lead corrosion," *AIP Conference Proceedings*, vol. 2663, no. 1, p. 30002, Sep. 2022, doi: 10.1063/5.0108088.

[4]   B. I. Costescu, I. B. Baldus, and F. Gräter, "Graphene mechanics: I. Efficient first principles based Morse potential.," *Physical chemistry chemical physics : PCCP*, vol. 16, no. 24, pp. 12591–12598, Jun. 2014, doi: 10.1039/c3cp55340j.

[5]   M. Al-Raeei, "Morse potential specific bond volume: a simple formula with applications to dimers and soft–hard slab slider," *Journal of Physics: Condensed Matter*, vol. 34, no. 28, p. 284001, 2022, doi: 10.1088/1361-648X/ac6a9b.

[6]   M. Ou *et al.*, "A novel approach based on semi-empirical model for degradation prediction of fuel cells," *Journal of Power Sources*, vol. 488, p. 229435, 2021, [Online]. Available: https://api.semanticscholar.org/CorpusID:233663669.

[7]   C. A. Onate *et al.*, "Theoretic measure and thermal properties of a standard Morse potential model.," *Journal of molecular modeling*, vol. 29, no. 2, p. 34, Jan. 2023, doi: 10.1007/s00894-022-05441-z.

[8]   P. J. Hasnip, K. Refson, M. I. J. Probert, J. R. Yates, S. J. Clark, and C. J. Pickard, "Density functional theory in the solid state," *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 372, no. 2011, 2014, doi: 10.1098/rsta.2013.0270.

[9]   P. Barua, M. M. Hossain, M. A. Ali, M. M. Uddin, S. H. Naqib, and A. K. M. A. Islam, "Effects of transition metals on physical properties of M2BC (M = V, Nb, Mo and Ta): A DFT calculation," *Journal of Alloys and Compounds*, vol. 770, pp. 523–534, 2019, doi: https://doi.org/10.1016/j.jallcom.2018.08.155.

[10]   E. Purwandari, R. Asih, R. Arifin, A. Subekti, and D. Darminto, "The study on structure and electronic property of amorphous carbon using density functional theory," *AIP Conference Proceedings*, vol. 2604, no. 1, p. 20031, May 2023, doi: 10.1063/5.0117052.

[11]   F. A. Putra, E. Purwandari, and B. S. Nugroho, "Study of Electronic Properties of GaAs Semiconductor Using Density Functional Theory," *Computational And Experimental Research In Materials And Renewable Energy*, vol. 4, no. 2, p. 94, 2021, doi: 10.19184/cerimre.v4i2.28375.

[12]   M. Abu Radia and S. A. Saafan, "An Overview for Beginners on Density Functional Theory in Computational Materials Science and Some of the Related Software Packages," *Egyptian Journal of Solids*, vol. 47, no. 1, pp. 110–138, 2025, doi: 10.21608/ejs.2025.366425.1061.

[13]   A. V Akimov and O. V Prezhdo, "Large-Scale Computations in Chemistry: A Bird's Eye View of a Vibrant Field.," *Chemical reviews*, vol. 115, no. 12, pp. 5797–5890, Jun. 2015, doi: 10.1021/cr500524c.

[14]   J. A. Moriarty and M. Widom, "First-principles interatomic potentials for transition-metal aluminides: Theory and trends across the $3d$ series," *Physical Review B*, vol. 56, no. 13, pp. 7905–7917, Oct. 1997, doi: 10.1103/PhysRevB.56.7905.

[15]   J. A. Moriarty, "Density-functional formulation of the generalized pseudopotential theory. III. Transition-metal interatomic potentials," *Physical Review B*, vol. 38, no. 5, pp. 3199–3231, Aug. 1988, doi: 10.1103/PhysRevB.38.3199.

[16]   J. Hestness, N. Ardalani, and G. Diamos, "Beyond human-level accuracy: computational challenges in deep learning," in *Proceedings of the 24th Symposium on Principles and Practice of Parallel Programming*, 2019, pp. 1–14, doi: 10.1145/3293883.3295710.

[17]   S. Nickabadi, P. Aghdasi, and R. Ansari, "Synergistic DFT and FEM study of stanene nanosheet mechanics: Morse potential coefficients and beyond," *Applied Physics A*, vol.

130, 2024, [Online]. Available: https://api.semanticscholar.org/CorpusID:269571957.

[18] P. M. Morse, "Diatomic Molecules According to the Wave Mechanics. II. Vibrational Levels," *Physical Review*, vol. 34, no. 1, pp. 57–64, Jul. 1929, doi: 10.1103/PhysRev.34.57.

[19] Y. Wang, X. Ruan, and A. K. Roy, "Two-temperature nonequilibrium molecular dynamics simulation of thermal transport across metal-nonmetal interfaces," *Physical Review B*, vol. 85, no. 20, p. 205311, May 2012, doi: 10.1103/PhysRevB.85.205311.

[20] L. A. Girifalco and V. G. Weizer, "Application of the Morse Potential Function to Cubic Metals," *Physical Review*, vol. 114, no. 3, pp. 687–690, May 1959, doi: 10.1103/PhysRev.114.687.

[21] A. Y. Galashev, K. P. Katin, and M. M. Maslov, "Morse parameters for the interaction of metals with graphene and silicene," *Physics Letters A*, vol. 383, no. 2, pp. 252–258, 2019, doi: https://doi.org/10.1016/j.physleta.2018.10.025.

[22] T. A. Sipkens *et al.*, "In situ nanoparticle size measurements of gas-borne silicon nanoparticles by time-resolved laser-induced incandescence," *Applied Physics B*, vol. 116, no. 3, pp. 623–636, 2014, doi: 10.1007/s00340-013-5745-2.

[23] A. Arkundato, A. Agung, I. Ratnadewi, and K. A. Syah, "Hybrid DFT-ML-MD Approach for Derivation of Lennard-Jones Interatomic Potential Parameters of Al," vol. 6, no. 2, 2025.

[24] P. Giannozzi *et al.*, "QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials," *Journal of physics: Condensed matter*, vol. 21, no. 39, p. 395502, 2009, doi: 10.1088/0953-8984/21/39/395502.

[25] H. Ö. Pamuk and T. Halicioğlu, "Evaluation of morse parameters for metals," *physica status solidi (a)*, vol. 37, no. 2, pp. 695–699, Oct. 1976, doi: https://doi.org/10.1002/pssa.2210370242.

[26] K. F. Garrity, J. W. Bennett, K. M. Rabe, and D. Vanderbilt, "Pseudopotentials for high-throughput DFT calculations," *Computational Materials Science*, vol. 81, pp. 446–452, 2014, doi: https://doi.org/10.1016/j.commatsci.2013.08.053.

[27] M. Abdul, B. Imanullah, and A. Arkundato, "Density of Liquid Lead as Function of Temperature and Pressure Based on the Molecular Dynamics Method," vol. 1, no. 1, pp. 1–6, 2018.

[28] J. P. Perdew, K. Burke, and M. Ernzerhof, "Generalized Gradient Approximation Made Simple," *Physical Review Letters*, vol. 77, no. 18, pp. 3865–3868, Oct. 1996, doi: 10.1103/PhysRevLett.77.3865.

[29] T. Urbańczyk, J. Koperski, G. Kaszewski, M. Synak, J. Swenda, and M. Krośnicki, "Genetic algorithm for obtaining potential energy curve of diatomic molecules based on dispersed fluorescence spectra.," *Scientific reports*, vol. 13, no. 1, p. 17413, Oct. 2023, doi: 10.1038/s41598-023-44488-7.

[30] T. Urbańczyk and J. Koperski, "Genetic Algorithm for quick finding of diatomic molecule potential parameters," *Molecular Simulation*, vol. 46, no. 14, pp. 1073–1083, Sep. 2020, doi: 10.1080/08927022.2020.1803493.

[31] R. S. McEntire and Y.-L. Shen, "Parametric variations of the interatomic potential in atomistic analysis of nano-scale metal plasticity," *International Journal of Mechanics and Materials in Design*, vol. 4, no. 4, pp. 361–374, 2008, doi: 10.1007/s10999-008-9060-8.

Additional information

Supplementary Information Supplementary material associated with this article is available online *here*.

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