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EMPIRICAL MANY-BODY POTENTIAL ENERGY FUNCTIONS USED IN COMPUTER SIMULATIONS OF CONDENSED MATTER PROPERTIES

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Abstract

Empirical many-body potential energy functions (EMBPEFs) are extensively used in atomistic computer simulations, especially in molecular dynamics and Monte-Carlo methods. There are several EMBPEFs used in the literature for different purposes, some of these functions are suitable for bulk and surface properties, and some of them are suitable for cluster properties. In this article the EMBPEFs used in the computer simulation applications for condensed matter properties will be reviewed.

PACS: 34.20.-b

Keywords: Potential energy functions; Empirical potentials; Many-body interactions; Interatomic interactions

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1. Introduction

Many physical properties of matter, in various phases such as solid, liquid and gas, may experimentally be observed and/or determined. It is also possible to theoretically calculate and predict many physical properties of matter again in various phases. Without any doubt calculations done by considering first-principles quantum mechanical methods give accurate results. However, because they require a large computational effort to accurately solve the Schrödinger equation, these methods are currently limited to studies of static properties for systems involving only a few tens of atoms. On the other hand, although they generally lack the accuracy of the former methods, empirical interatomic potentials can handle much larger systems and can be used to study static as well as dynamic properties of such systems [1].

In many areas today, computer simulations are becoming an integral part of many investigative procedures and provide help in understanding various problems at atomistic levels. This information has been used successfully in the interpretation of many experimental results. Many of these simulation techniques, which are called atomistic level simulations, are based on empirical model potentials describing interactions among the atoms in the system.

Atomistic simulation has proved to be a valuable tool for the investigation and understanding of microscopic processes in condensed matter. There are several methods available, molecular dynamics, Monte-Carlo, energy and/or force minimization and lattice dynamics, but they all depend on a knowledge of the interatomic potential. The advantage of computer simulation is that one knows exactly what one is measuring and the disadvantage is that the results one obtains are only as good as the potential that one obtains from them [2].

The concept of model potentials, generally speaking, is based on the Born–Oppenheimer approximation. If it is assumed that in the absence of external forces the total energy of a system of N interacting particles may be expressed as

$$E_N = \phi_1 + \phi_2 + \phi_3 + \dots + \phi_n + \dots, \quad (1)$$

where ϕ_n represents the sum of n -body interaction energies. On the other hand, the total energy of a system of N non-interacting particles may be expressed as

$$E'_N = \phi_1. \quad (2)$$

The difference between these two total energies ($E_N - E'_N$) gives the total interaction energy of a system of N interacting particles as a function of their positions:

$$\Phi = E_N - E'_N = \phi_2 + \phi_3 + \dots + \phi_n + \dots, \quad (3)$$

$$\Phi = \Phi(r_1, r_2, \dots, r_N), \quad (4)$$

$$\phi_2 = \sum_{i < j} U_2(r_i, r_j), \quad (5)$$

$$\phi_3 = \sum_{i < j < k} U_3(r_i, r_j, r_k), \quad (6)$$

⋮

$$\phi_n = \sum_{i < j < \dots < n} U_n(r_i, r_j, \dots, r_n), \quad (7)$$

where U_2 , U_3 , and U_n represent two-, three-, and n -body interactions, respectively.

The quantity Φ is measurable, which describes the total configuration energy (or potential energy) of the system. In this so-called many-body expansion of Φ , it is usually believed that the series has a quick convergence and, therefore, the higher moments may be neglected [3]. Otherwise, this equation cannot be employed for systems containing more than only a few atoms. In practice, it is difficult to handle the n -body expansion in the calculations, on one hand, and it is not easy to define multi-body atomic interactions, on the other hand. For this reason the many-body expansion is usually truncated after the three-body term. The contribution of the truncated terms may be included by inserting various parameters (linear and/or non-linear parameters) to the remaining terms.

In the earlier calculations, in general, the higher terms including even the three-body part were omitted, and the total potential energy Φ was approximated only by the sum of two-body interactions. This approach, which may be regarded as a first-order approximation, not only simplified the statistical mechanical formalisms used in calculating various thermodynamical properties, but, more importantly, it enabled many earlier researchers to run simulation calculations with relatively smaller and less powerful computers. In most of the simulation calculations which are carried out considering this first-order approximation, Lennard–Jones-type functions were employed to mimic two-body interactions. Despite the fact that those so-called Lennard–Jones systems may only represent rare gases where the role of many-body forces is minimal [4], they provided a very useful understanding about many properties and processes in a systematic way that could not be acquired easily by other means.

Studies in the last decade, however, have indicated that, particularly in the case of systems containing atoms other than those with closed-shell structures, this first-order approximation is inappropriate and produces results inconsistent with many experiments due to neglect of many-body interactions [5]. In the last decade in the simulation studies, therefore, in addition to two-body interactions, three-body interactions also are being considered in the calculation of potential energies.

It has been well recognized that the importance of three-body interactions increases with increasing covalent character of the bonding among atoms in the system [6]. While for rare gases the three-body part is negligibly small, for metals and in particular for semiconductors their contribution turns out to be extremely significant.

In addition to providing improved interpretability, interatomic potentials provide computational speed essential for computer simulations of complex materials-science problems. Some such problems, including the direct simulation of fully three-dimensional fracture dynamics, cannot at present be treated reliably even with pair potentials. However, many important problems are simple enough to be treated with interatomic potentials, but too complex to be treated directly with fully quantum mechanical methods [7]. The range of problems treatable by fully quantum mechanical methods will certainly continue to grow with expanding computing capabilities, but in the foreseeable future most materials-science problems will require the use of interatomic potentials or schemes of comparable simplicity.

In this study, we compiled the empirical many-body potential energy functions (EMBPEFs) available in the literature, containing both two- and three-body atomic interactions.

There are around 35 such functions in the literature: different functions proposed for different systems and applied for different properties of the systems. These properties usually include bulk, surface and cluster properties of condensed matter.

This review will describe the explicit forms of the EMBPEFs, their parametrization schemes, their applications, and the parameter set of most of them.

There are a few review articles about the EMBPEFs in the literature, but they focused on certain materials and they did not consider all the EMBPEFs available in the literature [1, 6, 8, 9].

The purpose of this review is to put all the EMBPEFs together and open a wide range of views to the interested researchers.

2. Empirical many-body potential energy functions

The EMBPEFs compiled in this work will be grouped and ordered with respect to the mathematical similarity of the functions. Therefore, a chronological order may not take place. Actually, the EMBPEFs may be classified into two main groups, the first group of functions containing two- and three-body interactions together as a functional form, and the second group of functions containing two- and three-body interactions separately. Therefore, we call the first group of functions as two- and three-body functionals, which we may represent by the notation $\Phi_I = \phi_{2,3}$:

$$\Phi_I \equiv \Phi = \phi_{2,3} = \sum_{i < j < k} U_{ijk}. \quad (8)$$

There are nine PEFs compiled in this group. On the other hand, we call the second group of functions as two- and three-body functions, which we may represent by the notation $\Phi_{II} = \phi_2 + \phi_3$:

$$\Phi_{II} \equiv \Phi = \phi_2 + \phi_3 = \sum_{i < j} U_{ij} + \sum_{i < j < k} W_{ijk}. \quad (9)$$

There are 18 PEFs compiled in this group. There are some functions other than these main groups, such that some of these functions include multi-body interactions, namely four-body interactions. In addition to this type of functions a few of them contain pair interactions only, but they intrinsically contain many-body effects. We may classify all these functions as the third group of functions, which we may represent by the notation Φ_{III} :

$$\Phi_{III} \equiv \Phi = \phi_2 \quad \text{or} \quad \Phi = \phi_1 + \phi_2 + \phi_3 \quad \text{or} \quad \Phi = \phi_2 + \phi_3 + \phi_4. \quad (10)$$

There are 11 PEFs compiled in this group.

Therefore, we will present in this article 38 EMBPEFs in three groups: Group-I functions (Φ_I), Group-II functions (Φ_{II}), and Group-III functions (Φ_{III}). In the following pages we call the PEFs by the name of the authors.

2.1. Group-I EMBPEFs (Φ_I)

2.1.1. Tersoff potential (I) [1]

This PEF was developed for covalent systems [10].

$$\Phi = \phi_{2,3} = \sum_{i < j < k} U_{ijk}, \quad U_{ij,k} = f_c(r_{ij})Ae^{-\lambda_1 r_{ij}} - B_{ij}e^{-\lambda_2 r_{ij}},$$

$$B_{ij} = B_0 e^{-z_{ij}/b}, \quad z_{ij} = \sum_{k \neq i,j} \left[\frac{w(r_{ik})}{w(r_{ij})} \right]^n \times \left[c + e^{-d \cos \theta_{ik}} \right]^{-1}, \quad w(r) = f_c(r)e^{-\lambda_2 r},$$

$$f_c(r) = \begin{cases} 1, & r < R - D, \\ \frac{1}{2} - \frac{1}{2} \sin \left[\frac{1}{2} \pi (r - R)/D \right], & R - D < r < R + D, \\ 0, & r > R + D. \end{cases}$$

The PEF was parameterized for Si which describes bonding and geometry for several structures, including surface and defect properties. The parameters were determined by using the cohesive energy, lattice constant, bulk modulus, the pair energy of Si₂. The parameters of the PEF for Si: $A = 2280$ eV, $B_0 = 171$ eV, $\lambda_1 = 2\lambda_2$, $\lambda_2 = 1.465 \text{ \AA}^{-1}$, $b = 1.324$, $c = 6.5$, $d = 6.02$, $n = 4$, $R = 3.0 \text{ \AA}$, $D = 0.2 \text{ \AA}$.

This PEF does not satisfy the crystal stability of diamond-Si; it gives the BCC structure as most stable.

2.1.2. Dodson potential [2]

This PEF is the modified form of the Tersoff potential (I) [11].

$$\Phi = \phi_{2,3} = \sum_{i < j, k} U_{ij,k}, \quad U_{ij,k} = f_{ij}(Ae^{-2\lambda r_{ij}} - B_{ij}e^{-\lambda r_{ij}}),$$

$$B_{ij} = B_0 e^{-z_{ij}^n/b}, \quad z_{ij} = \sum_{k \neq i, j} \left[\frac{f_{ik}}{f_{ij}} \right]^4 e^{4\lambda(r_{ij} - r_{ik})} \times \left[c + e^{-d \cos \theta_{ijk}} \right]^{-1}.$$

f_{ij} is defined as in Tersoff potential (I). This form of the PEF satisfies the crystal stability of diamond-Si in addition to other properties of diamond-Si predicted by Tersoff potential (I). This PEF can be used for global structural calculations for Si. The parameters of the PEF for Si: $A = 1614.6$ eV, $B_0 = 155.08$ eV, $\lambda_1 = 2.7793 \text{ \AA}^{-1}$, $\lambda_2 = 1.3969 \text{ \AA}^{-1}$, $b = 3.4785$, $c = 0.8543$, $d = 3.9588$, $\eta = 0.6207$.

2.1.3. Tersoff potential (II) [3]

This PEF was developed for covalent systems (silicon, carbon) [12].

$$\Phi = \phi_{2,3} = \sum_{i < j, k} U_{ij,k}, \quad U_{ij,k} = f_c(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})],$$

$$f_R(r) = Ae^{-\lambda_1 r}, \quad f_A(r) = -Be^{-\lambda_2 r}, \quad b_{ij} = (1 + \beta^n \xi_{ij}^n)^{-1/2n},$$

$$\xi_{ij} = \sum_{k \neq i, j} f_c(r_{ik}) g(\theta_{ijk}) \exp[\lambda_3^3 (r_{ij} - r_{ik})^3], \quad g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos \theta)^2}.$$

$f_c(r)$ is defined as in Tersoff potential (I). The PEF satisfies crystal stability and phonon dispersion curve. It was used for the calculation of point defect energies, surface properties, elastic properties, and liquid properties of Si. The PEF was also parameterized for carbon. It describes the structural properties of carbon, including elastic properties, phonons, poly types, and defects. The potential was applied to study amorphous carbon. Parameters of the PEF for Si and C are in Table 1.

2.1.4. Brenner potential (I) [4]

This PEF was developed for carbon [13].

$$\Phi = \phi_{2,3} = \sum_{i < j, k} U_{ij,k}, \quad U_{ij,k} = f_c(r_{ij}) [V_R(r_{ij}) + b_{ij} V_A(r_{ij})],$$

Table 1

Parameter	Si (set 1)	Si (set 2)	C
<i>A</i> (eV)	3264.7	1830.8	1393.6
<i>B</i> (eV)	95.373	471.18	346.74
λ_1 (Å ⁻¹)	3.2394	2.4799	3.4879
λ_2 (Å ⁻¹)	1.3258	1.7322	2.2119
λ_3 (Å ⁻¹)	1.3258	1.7322	0.0
β	0.33675	1.0999×10^{-6}	1.5724×10^{-7}
<i>n</i>	22.956	0.78734	0.72751
<i>h</i>	0.0	-0.59826	-0.57058
<i>c</i>	4.8381	1.0039×10^5	3.8049×10^4
<i>d</i>	2.0417	16.218	4.3484
<i>R</i> (Å)	3.0	2.85	1.95
<i>D</i> (Å)	0.2	0.15	0.15

$$V_R(r_{ij}) = \frac{D_e}{S-1} \exp[-\beta\sqrt{2S}(r_{ij}-r_e)], \quad V_A(r_{ij}) = \frac{SD_e}{S-1} \exp[-\beta\sqrt{2/S}(r_{ij}-r_e)],$$

$$b_{ij} = (1+z_{ij})^{-n}, \quad z_{ij} = \sum_{k \neq i,j} f_c(r_{ik})g(\theta_{ijk})e^{m(r_{ij}-r_{ik})}, \quad g(\theta) = \alpha \left\{ 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h + \cos \theta)^2} \right\}.$$

$f_c(r)$ is defined as in Tersoff potential (I). The PEF was used in the calculation of various properties of diamond and graphite. It was also applied to small carbon clusters. The parameters of the PEF for C (carbon): $D_e = 6.325$ eV, $r_e = 1.28$ Å, $\beta = 1.5$ Å⁻¹, $S = 1.29$, $n = 0.8047$, $\alpha = 0.0113$, $c = 19.0$, $d = 2.5$, $h = 1.0$, $m = 2.25$ Å⁻¹, $R = 2.1$ Å, $D = 0.2$ Å.

2.1.5. Brenner potential (II) [5]

This PEF was developed for hydrocarbons [14].

$$\Phi = \phi_{23} = \sum_{i < j,k} U_{ij,k}, \quad U_{ij,k} = V_R(r_{ij}) - \bar{B}_{ij}V_A(r_{ij})$$

$$V_R(r_{ij}) = f_{ij}(r_{ij}) \frac{D_{ij}}{(S_{ij}-1)} \exp[-\beta_{ij}\sqrt{2S_{ij}}(r_{ij}-r_e)],$$

$$V_A(r_{ij}) = f_{ij}(r_{ij}) \frac{S_{ij}D_{ij}}{(S_{ij}-1)} \exp[-\beta_{ij}\sqrt{2/S_{ij}}(r_{ij}-r_e)]$$

$$f_{ij}(r) = \begin{cases} 1, & r < r_e^{(1)}, \\ \frac{1}{2}[1 + \cos(\pi(r - r_e^{(1)})/(r_e^{(2)} - r_e^{(1)}))], & r_e^{(1)} < r < r_e^{(2)}, \\ 0, & r > r_e^{(2)}, \end{cases}$$

$$\bar{B}_{ij} = \frac{1}{2}(B_{ij} + B_{ji}) + F_{ij}(N_i^{(+)}, N_j^{(+)}, N_{ij}^{con}), \quad B_{ij} = [1 + G_{ij} + H_{ij}(N_i^{(H)}, N_i^{(C)})]^{-\delta_i},$$

$$G_{ij} = \sum_{k \neq i,j} f_{ik}(r_{ik})G_i(\theta_{ijk}) \exp[\alpha_{ijk}[(r_{ij}-r_e) - (r_{ik}-r_e)]],$$

$$N_i^{(H)} = \sum_{j(\text{=hydrogen})} f_{ij}(r_{ij}), \quad N_i^{(C)} = \sum_{j(\text{=carbon})} f_{ij}(r_{ij}), \quad N_i^{(t)} = N_i^{(H)} + N_i^{(C)},$$

$$N_{ij} = 1 + \sum_{k \neq i, j} f_{ik}(x_{ik}) + \sum_{l \neq i, j} f_{jl}(x_{jl}),$$

$$F(x_{ik}) = \begin{cases} 1, & x_{ik} \leq 2, \\ \frac{1}{2}\{1 + \cos(\pi(x_{ik} - 2))\}, & 2 < x_{ik} < 3, \\ 0, & x_{ik} \geq 3, \end{cases}$$

$$x_{ik} = N_k^{\text{tot}} - f_{ik}(r_{ik}), \quad G_c(\theta) = a_0 \left[1 + \frac{c_0^2}{d_0^2} - \frac{c_0^2}{d_0^2 + (1 + \cos \theta)^2} \right].$$

The parameters of the PEF were determined by fitting the function to various properties of hydrocarbon molecules. The PEF gives atomization energy of many hydrocarbon molecules. Adsorption and chemisorption energy of various systems on diamond and graphite surfaces were calculated. The PEF model intramolecular chemical bonding in a variety of small hydrocarbon molecules as well as graphite and diamond lattices. The parameters of the PEF form a long table; they are not given here. One set of parameters include 63 entries and a second set of parameters includes 64 entries.

2.1.6. Chelikowsky–Phillips–Kamal–Strauss potential [6]

This PEF was developed for silicon and carbon [15].

$$\Phi = \phi_{2,3} = \sum_{i < j, k} U_{ij,k}, \quad U_{ij,k} = \frac{A}{r_{ij}^2} \exp[-\beta_1 r_{ij}^2] - \frac{g_{ij}}{r_{ij}} \exp[-\beta_2 r_{ij}^2],$$

$$g_{ij} = g_0 + g_1 S_{ij} S_{ji}, \quad S_{ij} = 1 + \langle \cos(3\theta_{ijk}) \rangle, \quad \langle f(\theta_{ijk}) \rangle = [f]/[1],$$

$$[f(\theta_{ijk})] = \sum_{k \neq i, j} f(\theta_{ijk}) \exp[-(\lambda_1 \theta_{ijk}^4 + \lambda_2 r_{ijk}^4)], \quad r_{ijk} = \frac{1}{2}(r_{ij} + r_{ik}).$$

The PEF was fitted to covalent–metallic phase transitions. It gives energies and structures of silicon clusters. The PEF was also parameterized for carbon and applied to C_{60} . Parameters of the PEF for silicon and carbon are given in Table 2.

2.1.7. Khor–Das Sarma potential (I) [7]

Developed for elemental tetrahedrally bonded semiconductors (C, Si, Ge) [16].

$$\Phi = \phi_{2,3} = \sum_{i < j, k} U_{ij,k}, \quad U_{ij,k} = A f_{ij} [e^{-\theta r_{ij}} - g_{ij}(1 + h_{ij})],$$

$$f_{ij} = e^{-\beta(r_{ij} - R_i)^{\gamma}}, \quad g_{ij} = \frac{B_0}{Z_i^2} e^{-\lambda r_{ij}}, \quad h_{ij} = \sum_{k \neq i, j} [\cos \eta(\theta_{ijk} - \theta_i) - 1].$$

The parameters determined by fitting the PEF to the bulk modulus, the bond–bending force constants of the diamond structure. The PEF gives cohesive energy and equilibrium interatomic distances for various structures. Parameters of the PEF for C, Si, and Ge are given in Table 3.

Table 2

Parameter	Si	C
A (eV Å ²)	182.44	45.59
β_1 (Å ⁻²)	0.550	0.80
β_2 (Å ⁻²)	0.151	0.35
g_0 (eV Å)	7.08	1.33
g_1 (eV Å)	2.644	6.09
λ_1	(2/π) ⁴	(2/π) ⁴
λ_2 (Å ⁻⁴)	0.1773	0.961

Table 3

Parameter	C	Si	Ge
A (eV)	10 237.546	2794.2386	1278.555
B_0	0.938766	0.08251716	0.3481879
θ (Å ⁻¹)	3.20244	3.13269	2.37239
λ (Å ⁻¹)	3.05075	1.34146	1.54775
α	0.08596252	0.6249096	0.381135
β	44.85709	25.44123	17.79861
γ	3.10786	3.38218	3.22877
η	0.1824903	0.90084597	0.6460521

2.1.8. Khor–Das Sarma potential (II) [8]

This PEF was developed to study adatoms on Si(111) surface [17].

$$\Phi = \phi_{2,3} = \sum_{i < j,k} U_{ij,k}, \quad U_{ij,k} = Ae^{-\beta(r_{ij}-R_i)} \left[e^{-\theta r_{ij}} - B_0 e^{-\lambda r_{ij}} G(\theta) F(\theta) / Z_i^x \right],$$

$$Z_i = \sum_j \exp[-\beta(r_{ij} - R_i)^\gamma], \quad G(\theta) = 1 + \sum_{k \neq i,j} [\cos(\eta \Delta\theta_{jik} - 1)],$$

$$\Delta\theta_{jik} = \theta_{jik} - \theta_i, \quad F(\theta_{jik}) = \exp[-\beta_1(\Delta\theta_{jik})^{\gamma_1}] + \exp[\beta_2(\Delta\theta_{jik})^{\gamma_2}] - 1.$$

This PEF is a modification of Khor–Das Sarma potential (I). The additional parameters of the PEF for H₃ on Si(111) system: $\beta_1 = 15.08725154$, $\gamma_1 = 2.04101446$, $\beta_2 = 0.80277415$, $\gamma_2 = 0.90213443$, $\eta = 0.52091562$.

2.1.9. Khor–Das Sarma potential (III) [9]

Developed to study surface reconstruction of Si(111) surface [18].

$$\Phi = \phi_{2,3} = \sum_{i < j,k} U_{ij,k}, \quad U_{ij,k} = Ae^{-\beta(r_{ij}-R_i)} \left[e^{-\theta r_{ij}} - B_0 e^{-\lambda r_{ij}} G(\theta) / Z_i^x \right],$$

$$Z_i = \sum_j \exp[-\beta(r_{ij} - R_i)^\gamma], \quad G(\theta) = F(\theta) \left[1 + \sum_{k \neq i,j} [\cos(\eta \Delta\theta_{jik} - 1)] \right],$$

$$\Delta\theta_{jik} = \theta_{jik} - \theta_i, \quad F(\theta) = \exp[-\beta_1(\Delta\theta_{jik})^{\gamma_1}] - c [1 - \exp[-\beta_2(\Delta\theta_{jik})^{\gamma_2}]].$$

This PEF is a modification of Khor–Das Sarma potential (II). The different and additional parameters of the PEF for Si(111): $\beta_1 = 1.96535918$, $\gamma_1 = 0.74146749$, $\beta_2 = 0.57664720$, $\gamma_2 = 0.30135348$, $c = 0.85$.

2.2. Group-II EMBPEFs (Φ_{II})

2.2.1. Bauer–Maysenholder–Seeger potential [10]

This PEF was developed to investigate point defects in FCC metals [19].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = Ae^{-r_{ij}/\rho} - B/r_{ij}^n, \quad W_{ijk} = C(1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k)/(r_{ij}r_{jk}r_{ki})^m.$$

Parameterized for FCC metals (Cu, Ag, Au), used in point defect properties. The PEF was fitted to lattice constant, elastic constants, and cohesive energy. It was used in the calculation of point defect properties of Cu, Ag, and Au. Various set of parameters were used in the PEF to investigate the parameter dependence of some properties of the FCC metals Cu, Ag, and Au.

2.2.2. Pearson–Takai–Halicioglu–Tiller potential [11]

This PEF was developed for silicon [20].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = \varepsilon \left[\left(\frac{r_0}{r_{ij}} \right)^{12} - 2 \left(\frac{r_0}{r_{ij}} \right)^6 \right], \quad W_{ijk} = Z \frac{(1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k)}{(r_{ij}r_{jk}r_{ki})^3}.$$

The PEF was initially parameterized for silicon. The parameters were fitted to the bond lengths of the dimer and trimer and the lattice parameter and cohesive energy of the diamond structure. This PEF was used to study bulk phase transitions, surface reconstructions, surface point defect formation and diffusion, step reconstruction and interaction. The same potential has been extended to binary and ternary systems, e.g., GaAs, Si–GaAs, Al–GaAs, Au–GaAs [21]. Parameters of the PEF for monoatomic (A), binary (A–B), and ternary (A–B–C) systems are given in Table 4, 5 and 6 respectively.

Table 4

Quantity	Si	Au	Al	Ga	As
ε_{AA} (eV)	2.817	0.976	1.216	1.004	1.164
r_{0AA} (Å)	2.295	2.6685	2.520	2.461	2.491
Z_{AAA} (eV Å ⁹)	3484.0	2009.0	2241.0	1826.4	2151.9

Table 5

Quantity	Ga-As	Al-Ga	Al-As	Au-Ga	Au-As	Si-Ga	Si-As
ϵ_{AB}	1.738	1.121	2.060	0.886	1.750	1.700	2.500
r_{0AB}	2.448	2.490	2.430	2.554	2.535	2.378	2.393
Z_{AAB}	1900.0	2093.3	3000.0	278.7495	6000.0	2809.0	4500.0
Z_{ABB}	4600.0	1955.3	5000.0	1237.6936	5600.0	2265.0	5000.0

Table 6

Quantity	Al-Ga-As	Au-Ga-As	Si-Ga-As
Z_{ABC}	2500.0	3270.0	5000.0

2.2.3. Biswas–Hamann potential (I) [12]

This PEF was developed for silicon [22].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = A_1 e^{-\lambda_1 r_{ij}} + A_2 e^{-\lambda_2 r_{ij}}, \quad W_{ijk} = \sum_{\ell=0}^6 C_\ell \phi_\ell(r_{ij}) \phi_\ell(r_{ik}) P_\ell(\cos \theta_i), \quad \phi_\ell(r) = e^{-\alpha_\ell r}.$$

The PEF was fitted to energies of bulk, surface, layered, and self-interstitial structures. It was applied to structural properties of bulk and clusters of silicon. Parameters of the PEF for Si: $\lambda_1 = 3.946668 \text{ \AA}^{-1}$, $\lambda_2 = 1.191187 \text{ \AA}^{-1}$, $A_1 = 26829.36 \text{ eV}$, $A_2 = -42.59863 \text{ eV}$, $\alpha_0 = 1.246156 \text{ \AA}^{-1}$, $\alpha_1 = 1.901049 \text{ \AA}^{-1}$, $\alpha_2 = \alpha_3 = \alpha_4 = \alpha_5 = \alpha_6 = 1.786959 \text{ \AA}^{-1}$, $C_0 = 91.39775 \text{ eV}$, $C_1 = 16440.13 \text{ eV}$, $C_2 = 9580.299 \text{ eV}$, $C_3 = 6663.147 \text{ eV}$, $C_4 = 3987.710 \text{ eV}$, $C_5 = 2046.722 \text{ eV}$, $C_6 = 701.8867 \text{ eV}$.

2.2.4. Biswas–Hamann potential (II) [13]

This PEF was developed for silicon [23].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = f_c(r_{ij}) \left[A_1 e^{-\lambda_1 r_{ij}^2} + A_2 e^{-\lambda_2 r_{ij}^2} \right], \quad W_{ijk} = V_3(r_{ij}, r_{ik}, \theta) f_c(r_{ij}) f_c(r_{ik}),$$

$$V_3(r_{ij}, r_{ik}, \theta) = B_1 \psi_1(r_{ij}) \psi_1(r_{ik}) (\cos \theta + \frac{1}{3})^2 + B_2 \psi_2(r_{ij}) \psi_2(r_{ik}) (\cos \theta + \frac{1}{3})^3,$$

$$f_c(r) = \left[1 + e^{(r-r_c)/\mu} \right]^{-1}, \quad \psi_i(r) = e^{-\alpha_i r^2}.$$

The PEF was fitted to energies of bulk, surface, layered, and self-interstitial structures. It was applied to structural properties of bulk and clusters of silicon. It is appropriate for properties of the tetrahedral structure. Parameters of the PEF for Si: $\lambda_1 = 0.5200836 \text{ \AA}^{-2}$, $\lambda_2 = 0.4206931 \text{ \AA}^{-2}$, $A_1 = 14229.22 \text{ eV}$, $A_2 = -107.0338 \text{ eV}$, $\alpha_1 = 0.3034373 \text{ \AA}^{-2}$, $\alpha_2 = 0.3191903 \text{ \AA}^{-2}$, $B_1 = 13.02990 \text{ eV}$, $B_2 = 0.6720739 \text{ eV}$, $r_c = 3.9527357 \text{ \AA}$, $\mu = 0.3120580 \text{ \AA}$.

2.2.5. Stillinger–Weber potential [14]

This PEF was developed for silicon [24].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = \varepsilon f_2(r_{ij}/\sigma), \quad W_{ijk} = \varepsilon f_3(r_i/\sigma, r_j/\sigma, r_k/\sigma),$$

$$f_2(r) = \begin{cases} A(Br^{-p} - r^{-q})e^{(r-a)^{-1}}, & r < a, \\ 0, & r \geq a, \end{cases}$$

$$f_3(r_i, r_j, r_k) = h(r_{ij}, r_{ik}, \theta_{jik}) + h(r_{ji}, r_{jk}, \theta_{ijk}) + h(r_{ki}, r_{kj}, \theta_{ikj}),$$

$$h(r_{ij}, r_{ik}, \theta_{jik}) = \lambda e^{[\gamma(r_{ij}-a)^{-1} + \gamma(r_{ik}-a)^{-1}]} \times \left(\frac{1}{3} + \cos \theta_{jik}\right)^2.$$

The PEF was applied to solid and liquid forms of Si. It also gives the structural properties of a-Ge and crystalline Ge. It was used to calculate thermodynamic properties of the crystalline phase and the photon dispersion relations of the crystals.

Parameters of the PEF for Si: $A = 7.049556277$, $B = 0.6022245584$, $p = 4$, $q = 0$, $a = 1.80$, $\lambda = 21.0$, $\gamma = 1.20$, $\sigma = 2.0951 \text{ \AA}$, $\varepsilon = 50 \text{ kcal/mol}$.

Parameters of the PEF for Ge [25]: $A = 7.049556277$, $B = 0.6022245584$, $p = 4$, $q = 0$, $a = 1.80$, $\lambda = 31.0$, $\gamma = 1.20$, $\sigma = 2.181 \text{ \AA}$, $\varepsilon = 1.93 \text{ eV}$.

2.2.6. Gong potential [15]

This PEF was developed for silicon [26].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = A(Br_{ij}^{-p} - r_{ij}^{-q})e^{(r_{ij}-a)^{-1}}, \quad W_{ijk} = h(r_{ji}, r_{ki}) + h(r_{kj}, r_{ij}) + h(r_{ik}, r_{jk}),$$

$$h(r_{ji}, r_{ki}) = \lambda \exp[\gamma(r_{ji}-a)^{-1} + \gamma(r_{ki}-a)^{-1}] \times \lambda_1 [c_1 + (c_0 + \cos \theta_{jik})^2] \left(\frac{1}{3} + \cos \theta_{jik}\right)^2.$$

This PEF is a modified form of the Stillinger–Weber potential. The structural properties of small Si clusters were studied. The parameters of the PEF for Si is the same as the Stillinger–Weber potential, but the numerical values of the additional parameters λ_1 , c_0 , and c_1 are not given in the paper.

2.2.7. Blaisten-Barojas–Khanna potential [16]

This PEF was developed for beryllium [27].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = Ae^{-\alpha r_{ij}} - C \frac{f_B(r_{ij})}{r_{ij}^5}, \quad f_B(r) = \begin{cases} 1, & r > r_0, \\ e^{-B(r_0/r-1)^5}, & r < r_0, \end{cases}$$

$$W_{ijk} = W'_{ijk} (1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k) f_B(r_{ij}) f_B(r_{ik}) f_B(r_{jk}),$$

$$W'_{ijk} = -D(N) e^{-\beta(r_{ij}+r_{ik}+r_{jk})} + \frac{C'}{(r_{ij}r_{ik}r_{jk})^3}, \quad D(N) = \begin{cases} D - G(\frac{1}{4} - 1/N), & N \geq 4, \\ D, & N < 4. \end{cases}$$

The PEF was fitted to small clusters and applied to various clusters of beryllium. It was also used in the simulation of the early stages of crystal growth. Parameters of the PEF for Be (in a.u., hartrees for energy): $A = 77.27716$, $\alpha = 1.71169$, $B = 0.6961$, $C = 87.39774$, $D = 9.65426$, $\beta = 0.495767$, $G = 35.945$, $C' = 673.4099$, $B' = \frac{1}{3}$, $r_0 = 4.04$.

2.2.8. Takai-Lee-Halicioglu-Tiller potential [17]

This PEF was developed for carbon [28].

$$\Phi = \phi_2 + \phi_3 = \sum_{i < j} U_{ij} + \sum_{i < j < k} W_{ijk},$$

$$U_{ij} = e^{(q_1 - q_2 r_{ij})} - q_3 \left[\frac{1}{2} - (1/\pi) \arctan[q_4(r_{ij} - q_5)] \right]^{12},$$

$$W_{ijk} = Z [p + (\cos \theta_i + h)(\cos \theta_j + h)(\cos \theta_k + h)] \exp[-b^2(r_{ij}^2 + r_{ik}^2 + r_{jk}^2)].$$

The parameters were evaluated from fits to various properties of C_2 , graphite, and the diamond crystal. Energy and structure related properties for bulk graphite and diamond were calculated. The PEF was also applied to carbon clusters. Parameters of the PEF for C (carbon): $q_1 = 10.149804$, $q_2 = 7.936986 \text{ \AA}^{-1}$, $q_3 = 261.527033 \text{ eV}$, $q_4 = 0.527263 \text{ \AA}^{-1}$, $q_5 = 3.071221 \text{ \AA}$, $Z = 20.0 \text{ eV}$, $h = 0.205$, $p = 1.340$, $b = 0.588 \text{ \AA}^{-1}$.

2.2.9. Kaxiras-Pandey potential [18]

This PEF was developed for silicon [29].

$$\Phi = \phi_2 + \phi_3 = \sum_{i < j} U_{ij} + \sum_{i < j < k} W_{ijk},$$

$$U_{ij} = A_1 e^{-\alpha_1 r_{ij}^2} - A_2 e^{-\alpha_2 r_{ij}^2}, \quad W_{ijk} = h_{ijk} + h_{jki} + h_{kij},$$

$$h_{ijk} = e^{-\beta(r_{ij}^2 + r_{ik}^2)} [B g^2(\theta_{ijk}) + D g^4(\theta_{ijk})], \quad g(\theta) = \frac{1}{3} + \cos \theta.$$

The PEF was based on quantum mechanical data base. It is used to simulate processes in a diamond lattice of Si, such as atomic exchange, point defects, vacancies, interstitials. Parameters of the PEF for Si (distance in \AA , energy in eV): $A_1 = 57.316072$, $A_2 = 6.4373054$, $\alpha_1 = 0.82335230$, $\alpha_2 = 0.19061589$, $B = 10.188418$, $D = -9.113678$, $\beta = 0.18642554$.

2.2.10. Feuston-Garofalini potential [19]

This PEF was applied to vitreous silica (v-SiO₂) [30].

$$\Phi = \phi_2 + \phi_3 = \sum_{i < j} U_{ij} + \sum_{i < j < k} W_{ijk},$$

$$U_{ij} = A_{ij} e^{-r_{ij}/\rho} + \frac{e^2 Z_i Z_j}{r_{ij}} \operatorname{erfc} \left(\frac{r_{ij}}{\beta_{ij}} \right), \quad A_{ij} = \left(1 + \frac{Z_i}{n_i} + \frac{Z_j}{n_j} \right) b e^{(\sigma_i + \sigma_j)/\rho},$$

$$W_{ijk} = h(r_{ij}, r_{ik}, \theta_{jik}) + h(r_{jk}, r_{ji}, \theta_{kji}) + h(r_{ki}, r_{kj}, \theta_{ikj}),$$

$$h(r_{ij}, r_{ik}, \theta_{jik}) = \begin{cases} \lambda_i e^{\eta_i} \Delta \theta_i, & r_{ij} < r_i^c, r_{ik} < r_i^c \\ 0, & r_{ij} \geq r_i^c, r_{ik} \geq r_i^c \end{cases}$$

$$\eta_i = \gamma_i / (r_{ij} - r_i^c) + \gamma_i / (r_{ik} - r_i^c), \quad \Delta \theta_i = \cos \theta_{jik} - \cos \theta_{jik}^c.$$

The PEF was used to investigate the structural properties of vitreous silica. The RDF and structure factor $S(q)$ were calculated. Parameters of the PEF for vitreous silica (v-SiO₂): $A_{\text{Si-O}} = 3.00 \times 10^{-9}$ erg, $A_{\text{O-O}} = 1.10 \times 10^{-9}$ erg, $A_{\text{Si-Si}} = 1.88 \times 10^{-9}$ erg, $\beta_{\text{Si-O}} = 2.29$ Å, $\beta_{\text{O-O}} = 2.34$ Å, $\beta_{\text{Si-Si}} = 2.34$ Å, $\lambda_{\text{Si}} = 18.0 \times 10^{-11}$ erg, $\gamma_{\text{Si}} = 2.6$ Å, $r_{\text{Si}}^c = 3.0$ Å, $\cos \theta_{\text{O-Si-O}}^c = -\frac{1}{3}$, $\lambda_{\text{O}} = 0.3 \times 10^{-11}$ erg, $\gamma_{\text{O}} = 2.0$ Å, $r_{\text{O}}^c = 2.6$ Å, $\cos \theta_{\text{Si-O-Si}}^c = -\frac{1}{3}$.

2.2.11. Murrell–Mottram potential [20]

This PEF was developed for cubic crystals, and parameterized for silicon [31].

$$\Phi = \phi_2 + \phi_3 = \sum_{i < j} U_{ij} + \sum_{i < j < k} W_{ijk},$$

$$U_{ij} = D[1 + b(r_{ij} - r_e)]e^{-b(r_{ij} - r_e)}, \quad W_{ijk} = P(Q_1, Q_2, Q_3)e^{-aQ_1},$$

$$P(Q_1, Q_2, Q_3) = C_0 + C_1 Q_1 + C_2 Q_1^2 + C_3(Q_2^2 + Q_3^2) + C_4 Q_1^3 + C_5 Q_1(Q_2^2 + Q_3^2) + C_6(Q_3^3 - 3Q_3 Q_2^2),$$

$$\begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{\sqrt{2}}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{bmatrix},$$

$$\rho_1 = \rho_{ij}, \quad \rho_2 = \rho_{ik}, \quad \rho_3 = \rho_{jk}, \quad \rho_{ij} = r_{ij} - r_e.$$

The PEF was tested for different crystalline phases. The parameters were determined by fitting the PEF to the lattice energy, lattice constant, the elastic constants, and the Raman frequency of the diamond lattice of silicon. Parameters of the PEF for Si: $D = 4.007$ eV, $r_e = 2.155$ Å, $C_0 = 0.98$, $C_1 = 0.87$, $C_2 = 6.20$, $C_3 = -2.89$, $C_4 = 6.28$, $C_5 = -6.14$, $C_6 = -10.98$, $a = 5.5$.

2.2.12. Al-Derzi–Johnston–Murrell–Rodríguez–Ruiz potential [21]

This PEF was developed for diamond structure, and parameterized for C (carbon) [32].

$$\Phi = \phi_2 + \phi_3 = \sum_{i < j} U_{ij} + \sum_{i < j < k} W_{ijk},$$

$$U_{ij} = -D(1 + a\rho_{ij})e^{-a\rho_{ij}}, \quad W_{ijk} = DP(Q_1, Q_2, Q_3)e^{-aQ_1}, \quad \rho_{ij} = (r_{ij} - r_e)/r_e$$

$$P(Q_1, Q_2, Q_3) = C_0 + C_1 Q_1 + C_2 Q_1^2 + C_3(Q_2^2 + Q_3^2) + C_4 Q_1^3 + C_5 Q_1(Q_2^2 + Q_3^2) + C_6(Q_3^3 - 3Q_3 Q_2^2) + C_7 Q_1^4 + C_8 Q_1^2(Q_2^2 + Q_3^2) + C_9(Q_2^2 + Q_3^2)^2 + C_{10} Q_1(Q_3^3 - 3Q_3 Q_2^2).$$

The variables Q_i and ρ_i are defined same as in Murrell-Mottram potential. The PEF was parameterized by fitting to the lattice energy, lattice spacings, elastic constants, and the phonon dispersion curves of the diamond carbon. Parameters of the PEF for carbon: $a = 6.70$, $D = 3.258$ eV, $r_e = 1.762$ Å, $C_0 = 0.974$, $C_1 = -0.412$, $C_2 = 22.418$, $C_3 = -9.624$, $C_4 = -20.580$, $C_5 = 14.075$, $C_6 = 9.474$, $C_7 = 12.336$, $C_8 = -42.283$, $C_9 = -0.681$, $C_{10} = -13.435$.

2.2.13. Li-Johnston-Murrell potential [22]

This PEF was developed for silicon [33].

$$\begin{aligned}\Phi &= \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk}, \\ U_{ij} &= -D(1 + a_2\rho_{ij})e^{-a_2\rho_{ij}}, \quad W_{ijk} = DP(Q_1, Q_2, Q_3)e^{-a_3Q_1}, \quad \rho_{ij} = (r_{ij} - r_e)/r_e, \\ P(Q_1, Q_2, Q_3) &= C_0 + C_1Q_1 + C_2Q_1^2 + C_3(Q_2^2 + Q_3^2) + C_4Q_1^3 + C_5Q_1(Q_2^2 + Q_3^2) \\ &\quad + C_6(Q_3^3 - 3Q_3Q_2^2) + C_7Q_1^4 + C_8Q_1^2(Q_2^2 + Q_3^2) + C_9(Q_2^2 + Q_3^2)^2 \\ &\quad + C_{10}Q_1(Q_3^3 - 3Q_3Q_2^2).\end{aligned}$$

The variables Q_i and ρ_i are defined same as in Murrell-Mottram potential. Parameters of the PEF are determined from the properties of solid silicon and it is used to study the structures and energies of silicon microclusters. Parameters of the PEF for Si: $a_2 = a_3 = 6.50$, $D = 2.918$ eV, $r_e = 2.389$ Å, $C_0 = 3.598$, $C_1 = -11.609$, $C_2 = 13.486$, $C_3 = -18.174$, $C_4 = -5.570$, $C_5 = 79.210$, $C_6 = -6.458$, $C_7 = 23.383$, $C_8 = -111.809$, $C_9 = 9.705$, $C_{10} = 38.297$.

2.2.14. Erkoç potential (I) [23]

This PEF was developed for cubic systems, applied to elemental microclusters [34].

$$\begin{aligned}\Phi &= \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk}, \\ U_{ij} &= A \left[\left(\frac{r_0}{r_{ij}} \right)^{2n} \exp[-2\alpha(r_{ij}/r_0)^2] - \left(\frac{r_0}{r_{ij}} \right)^n \exp[-\alpha(r_{ij}/r_0)^2] \right], \\ W_{ijk} &= B(U_{ij}f_{ijk} + U_{ik}f_{ikj} + U_{jk}f_{jki}), \\ A &= -4\epsilon_0, \quad \alpha = \ln(2), \quad n = \sqrt{\frac{r_0^2 k}{2|\epsilon_0|}} - 2\alpha, \quad f_{ijk} = e^{-(r_k^2 + r_j^2)/r_0^2}.\end{aligned}$$

The PEF was parameterized by using the dimer data and bulk cohesive energy of the elements. It is applied to study the structure and energy of the microclusters of the elements. Parameters of the PEF for various elements in different crystalline structures ($\alpha = \ln 2$ for all the elements) are given in Table 7.

2.2.15. Erkoç potential (II) [24]

This PEF was developed for cubic systems, applied to elemental microclusters [35].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

Table 7

Element	Structure	r_0 (Å)	A (eV)	n	B
Ag	FCC	2.48	6.60	2.312351	-1.637860
Al	FCC	2.47	6.20	2.072844	-1.553508
Au	FCC	2.47	9.16	2.806960	-1.605480
Cu	FCC	2.22	8.04	1.801698	-1.619242
Ni	FCC	2.20	8.28	2.892470	-1.290433
Fe	BCC	2.02	3.60	3.195342	-1.061661
Li	BCC	2.67	4.28	0.907914	-1.888711
C	DIA	1.24	24.84	1.680481	-17.293200
Ge	DIA	2.45	10.60	1.417253	-3.344464
Si	DIA	2.25	12.84	1.874024	-4.266564
Cs	BCC	4.47	1.60	1.890859	-2.023773
K	BCC	3.91	2.08	1.608210	-1.979834
Na	BCC	3.08	2.92	1.250439	-2.436817
Ca	FCC	4.28	0.56	3.117158	-0.145373
Pb	FCC	2.93	3.40	3.422940	-1.586818
Pd	FCC	2.57	4.40	6.950465	-0.681378
Pt	FCC	2.34	14.84	2.854446	-1.762003
Cd	HCP	4.82	0.16	4.002629	-0.097190
Mg	HCP	3.89	0.20	2.874987	1.112951
Sc	HCP	2.79	6.60	1.950414	-1.684201
Ti	HCP	1.97	4.92	3.421186	2.287793
Zn	HCP	2.35	0.24	4.566524	3.944883

$$U_{ij} = C_2 A \left[\left(\frac{r_0}{r_{ij}} \right)^{2n} \exp[-2\alpha(r_{ij}/r_0)^2] - \left(\frac{r_0}{r_{ij}} \right)^n \exp[-\alpha(r_{ij}/r_0)^2] \right],$$

$$W_{ijk} = C_3 (U_{ij} f_{ijk} + U_{ik} f_{ikj} + U_{jk} f_{jki}).$$

The quantities A , n , α , and f_{ijk} are defined as in Erkoç potential (I). Parameters of the PEF were determined by using dimer data and bulk cohesive energy of the elements. The bulk stability condition has also been considered. The PEF has been parameterized and applied to FCC [35], BCC [36], DIA (diamond) [37], and RHO (rhombohedral) [38] elemental microclusters. Parameters of the PEF for some FCC, DIA, and BCC structure elements (r_0 , A , n , and α values are the same as in Erkoç potential (I)) are given in Table 8.

Parameters of the PEF for some BCC and RHO structure elements are given in Table 9.

2.2.16. Erkoç potential (III) [25]

This PEF was developed for cubic systems, applied to elemental microclusters [39].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = C_2 \left(\frac{A_1}{r_{ij}^{\lambda_1}} e^{-\alpha_1 r_{ij}^2} - \frac{A_2}{r_{ij}^{\lambda_2}} e^{-\alpha_2 r_{ij}^2} \right), \quad W_{ijk} = C_{31} W_{ijk}^{(1)} + C_{32} W_{ijk}^{(2)},$$

Table 8

Element	Structure	C_2	C_3	Element	Structure	C_2	C_3	
-1.637860	Ag	FCC	0.2338381	-0.1640650	C	DIA	0.4142327	-2.8628860
-1.553508	Al	FCC	0.2635582	-0.1766508	Si	DIA	0.2902184	-0.4736164
-1.605480	Au	FCC	0.2459298	-0.1768174	Ge	DIA	0.2278680	-0.2900124
-1.619242	Cu	FCC	0.1930176	-0.1261549	Li	BCC	0.1375465	-0.0982322
-1.290433	Ni	FCC	0.2860750	-0.1688664	Na	BCC	0.1752010	-0.1633922
-1.061661	Pb	FCC	0.4581129	-0.4052801	K	BCC	0.2106423	-0.1680882
-1.888711	Pd	FCC	0.6671249	-0.3330730	Cs	BCC	0.2651783	-0.2288656
17.293200	Pt	FCC	0.2508586	-0.2004671	Fe	BCC	1.1177254	-1.4442571

Table 9

Element	Structure	r_0 (Å)	A (eV)	n	C_2	C_3	
-0.145373	V	BCC	1.77	9.96	2.739947	1.1128382	-6.6226567
-1.586818	Cr	BCC	1.68	7.12	2.552045	1.1319147	-6.9582166
-0.681378	Nb	BCC	2.10	20.0	2.849568	0.5294501	-1.4977811
-1.762003	As	RHO	2.10	15.84	2.375928	0.2602548	-1.0818833
-0.097190	Sb	RHO	2.34	12.40	2.409013	0.3218016	-1.4833859
1.112951	Bi	RHO	2.6596	8.16	3.071074	0.3438665	-0.8657999
-1.684201							
2.287793							
3.944883							

Table 10

Parameter	Au	Ag	Cu
A_1	345.923364	220.262366	110.766008
A_2	38.9245908	26.0811795	46.1649783
α_1	0.750775965	0.673011507	0.394142248
α_2	0.229377368	0.120620395	0.207225507
λ_1	1.04289230	1.72376253	2.09045946
λ_2	1.05974062	1.81484791	1.49853083
r_0	2.470	2.480	2.220
C_2	0.169729418	0.193714755	0.150036137
C_{31}	0.530820957	0.254330241	0.140549073
C_{32}	1487.33142	784.190491	194.576839

$$W_{ijk}^{(1)} = U_{ij}f_k + U_{ik}f_j + U_{jk}f_i, \quad W_{ijk}^{(2)} = \frac{1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k}{(r_{ij}r_{ik}r_{jk})^3}, \quad f_i = \exp [-(r_{ij}^2 + r_{ik}^2)/r_0^2].$$

The parameters of the PEF were determined by considering the bulk cohesive energy, bulk stability condition, and bulk modulus of the element considered. This PEF satisfies the crystal stability and gives the elastic constants of the elements considered reasonably. Parameters of the PEF for Au, Ag, and Cu (energy in eV, distance in Å) are given in Table 10.

2.2.17. Erkoç potential (IV) [26]

This PEF was developed for cubic systems, applied to copper clusters [40].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = D_{21}U_{ij}^{(21)} + D_{22}U_{ij}^{(22)}, \quad U_{ij}^{(2\ell)} = \frac{A_\ell}{r_{ij}^{2\ell}} \exp[-\alpha_\ell r_{ij}^2], \quad \ell = 1, 2,$$

$$W_{ijk} = D_{31}W_{ijk}^{(31)} + D_{32}W_{ijk}^{(32)}, \quad W_{ijk}^{(3\ell)} = U_{ij}^{(2\ell)}f_k + U_{ik}^{(2\ell)}f_j + U_{jk}^{(2\ell)}f_i, \quad \ell = 1, 2,$$

$$f_i = \exp[-(r_{ij}^2 + r_{ik}^2)/r_{jk}^2]$$

The parameters of the PEF were determined by considering the bulk cohesive energy, bulk stability condition, and elastic constants (C_{11} , C_{12}) of the element considered; therefore it satisfies the bulk modulus of the element considered. This PEF also satisfies the crystal stability of the element considered. Parameters of the PEF for Cu (energy in eV, distance in Å): $A_1 = 110.766008$, $A_2 = -46.1649783$, $\alpha_1 = 0.394142248$, $\alpha_2 = 0.207225507$, $\lambda_1 = 2.09045946$, $\lambda_2 = 1.49853083$, $D_{21} = 0.4683918280$, $D_{22} = 0.2329419830$, $D_{31} = 0.0257056474$, $D_{32} = 0.0156041879$.

2.2.18. Erkoç potential (V) [27]

This PEF was developed for FCC systems [41].

$$\Phi = \phi_2 + \phi_3 = \sum_{i<j} U_{ij} + \sum_{i<j<k} W_{ijk},$$

$$U_{ij} = \varepsilon \left[\frac{n}{m-n} \left(\frac{r_0}{r_{ij}} \right)^m - \frac{m}{m-n} \left(\frac{r_0}{r_{ij}} \right)^n \right] e^{2r^*}$$

$$W_{ijk} = Z_1 G_1(r_{ij}, r_{ik}, r_{jk}) \exp(\alpha r^* + \beta Z_1^*) + Z_2 G_2(r_{ij}, r_{ik}, r_{jk}) \exp(\alpha r^* + \beta Z_2^*),$$

$$G_1(r_{ij}, r_{ik}, r_{jk}) = \frac{1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k}{(r_{ij} r_{ik} r_{jk})^3},$$

$$G_2(r_{ij}, r_{ik}, r_{jk}) = \frac{9 \cos \theta_k - 25 \cos 3\theta_k + 6 \cos(\theta_i - \theta_j)(3 + 5 \cos 2\theta_k)}{r_{ij}^3 r_{ik}^4 r_{jk}^4},$$

$$r^* = \frac{r_0}{R_0}, \quad Z_1^* = \frac{Z_2}{\varepsilon r_0^9}, \quad Z_2^* = \frac{Z_1 R_0}{\varepsilon r_0^{12}}.$$

Here R_0 and r_0 represent the nearest-neighbour distance in the crystal, and equilibrium separation of the dimer, respectively. The effect of many-body interactions on the bulk properties of solids has been investigated for the FCC structure by performing a parametric analysis.

Parameters of the PEF for some FCC elements are given in Table 11.

2.3. Group-III EMBPEFs (Φ_{III})

2.3.1. Bolding–Andersen potential [28]

This PEF was developed for silicon [42].

$$\Phi = \phi_2,$$

Table 11

Element	m	n	Z_1^*	Z_2^*	r^*	α	β
Kr	11	7	0.06	0.0	1.00161	0.0	0.0
Xe	12	6	0.08	0.0	1.00026	0.0	0.0
Al	11	6	0.40	0.06	0.87765	-1.0	-1.0
Cu	10	6	0.35	0.14	0.87143	-1.0	-1.0
Pb	10	6	0.25	0.05	0.92256	-1.0	-1.0
Pd	12	5	0.03	0.22	0.93932	-1.0	-1.0

$$\phi_2 = \sum_{i < j} f_c(r_{ij}) \left[V_R(r_{ij}) + I_{ij}^\pi V_\pi(r_{ij}) + I_{ij}^\sigma V_\sigma(r_{ij}) \right],$$

$$f_c(r) = \begin{cases} 1, & r < R - D, \\ \frac{1}{2} - \frac{1}{2} \sin\left[\frac{1}{2}\pi(r - R)/D\right], & R - D < r < R + D, \\ 0, & r > R + D, \end{cases}$$

$$V_R(r) = \frac{1}{2}(V^{\text{bond}}(r) + V^{\text{anti}}(r)), \quad V_\pi(r) = a_1 \{ \tanh[a_2(r - a_3)] - 1 \},$$

$$V_\sigma(r) = \frac{1}{2}(V^{\text{bond}}(r) - V^{\text{anti}}(r)) - V_\pi(r), \quad V^{\text{bond}}(r) = -D_c \left(1 + \sum_{i=1}^6 b_i \rho^i \right) e^{-b_1 \rho},$$

$$V^{\text{anti}}(r) = (b_8 + b_9 \rho + b_{10} \rho^2) e^{-b_7 \rho}, \quad \rho = r - r_c,$$

$$I_{ij}^\sigma = \frac{1}{I_1} \cdot \frac{1}{I_2}, \quad I_1 = 1 + Z_{ij}^{a_0} \left(\sum_{k \neq i, j} a_4 S_{ik} S_{jk} + \sum_{k < \ell \neq i, j} a_5 S_{ik} S_{i\ell} S_{jk} S_{j\ell} S_{k\ell} \right),$$

$$I_2 = 1 + Z_{ij}^{a_7} \left(\sum_{k \neq i, j} [S_{ik} P(\theta_{jik}) + S_{jk} P(\theta_{ijk})] \right), \quad Z_{ij} = \sum_{k \neq i, j} (S_{ik} + S_{jk}),$$

$$P(0) = \sum_{n=0}^6 d_n \cos^n(0); \quad S_{ik} = S(r_{ik}) = S(r) = \begin{cases} 1, & r < r_c, \\ f_c(r) \frac{V_R(r) + V_\sigma(r)}{V_R(r_c) + V_\sigma(r_c)}, & r \geq r_c, \end{cases}$$

$$I_{ij}^\pi = S(Z_i^j) S(Z_j^i) e^{-I_3}; \quad I_3 = \sum_{k \neq i, j} F_3 + \sum_{k, \ell \neq i, j} F_4 + \sum_{k, \ell, m \neq i, j} F_5,$$

$$S(Z) = \begin{cases} 1, & Z < 2, \\ c_1 + c_2 Z + c_3 Z^2 + c_4 Z^3, & 2 \leq Z \leq 2.5, \\ 0, & Z > 2.5, \end{cases} \quad Z_i^j = \sum_{k \neq i, j} S_{ik},$$

$$F_3 = a_8 S_{ik} S_{jk} + \frac{a_9}{1 + Z_{ij}} \left[S_{ik} (1 - S_{jk}^4) + S_{jk} (1 - S_{ik}^4) \right],$$

$$F_4 = a_{10} (S_{ik} S_{i\ell} S_{jk} S_{j\ell}) + \frac{a_{11}}{1 + Z_{ij}^2} \left[S_{ik} S_{j\ell} (1 - S_{i\ell}) (1 - S_{jk}) + S_{i\ell} S_{jk} (1 - S_{ik}) (1 - S_{j\ell}) \right]$$

$$+ a_{12} \frac{v_{ijk\ell}^2}{r_{ij}^2} \left(\frac{S_{ik} S_{j\ell}}{r_{ik}^2 r_{j\ell}^2} + \frac{S_{i\ell} S_{jk}}{r_{i\ell}^2 r_{jk}^2} + \frac{S_{ik} S_{i\ell}}{r_{ik}^2 r_{i\ell}^2} + \frac{S_{jk} S_{j\ell}}{r_{jk}^2 r_{j\ell}^2} \right),$$

$$F_5 = a_{13}(S_{ik}S_{jk}S_{i'l}S_{jm}S_{k'l}S_{km} + S_{ik}S_{jk}S_{im}S_{j'l}S_{k'l}S_{km} + S_{i'l}S_{j'l}S_{ik}S_{jm}S_{k'l}S_{l'm}) \\ + a_{13}(S_{i'l}S_{j'l}S_{im}S_{jk}S_{k'l}S_{l'm}S_{im}S_{jm}S_{ik}S_{j'l}S_{km}S_{l'm} + S_{im}S_{jm}S_{i'l}S_{jk}S_{km}S_{l'm}),$$

$$v_{ijk'l} = \mathbf{r}_{ij} \cdot \mathbf{r}_{j'l} \times \mathbf{r}_{ik}.$$

The parameters were chosen to fit a variety of data on silicon, including the structure and energy of small clusters, the crystal structures, the elastic constants, and the surface properties. The PEF was used to model small clusters, crystal phases, point defects, and surface reconstructions. Parameter set of the PEF contains 36 entries; they are not given here.

2.3.2. Brenner–Garrison potential [29]

This PEF was developed for silicon (covalent solids) [43].

$$\Phi = \phi_2 + \phi_3,$$

$$\phi_2 = \sum_i^4 \left[3(a_1 + a_2) \left(\lambda_{ii}^2 - \frac{D_1^2}{4a^2} \right) + Ae^{-BR_i^2} \right],$$

$$\lambda_{ii} = \begin{cases} \frac{D_1}{2a}(1 - e^{\gamma\delta_i}), & R_i < R_{\max}, \\ \frac{D_1}{2a}, & R_i \geq R_{\max}, \end{cases} \quad \gamma = \frac{R_{\max}^2 - 3a^2}{D_1}, \quad \delta_i = \frac{\gamma(R_i^2 - 3a^2)}{R_i^2 - R_{\max}^2},$$

$$\phi_3 = \sum_{i,j}^6 \left[a_2 \lambda_{ij}(\lambda_{ij} + \lambda_{ii} + \lambda_{jj}) + a_1(\lambda_{ii}\lambda_{jj} - \frac{D_2^2}{4a^2}) \right],$$

$$\lambda_{ii} = \begin{cases} \frac{D_2}{2a}(1 - e^{\gamma\eta_i}), & Q_{ii} < Q_{\max}, \\ \frac{D_2}{2a}, & Q_{ii} \geq Q_{\max}, \end{cases} \quad Q_{ii} = R_i^2 - 3a^2 + \frac{(R_i^2 - 3a^2)^4}{Q_{\max}^3},$$

$$\gamma = \frac{Q_{\max}}{D_2}, \quad \eta_i = \frac{\gamma Q_{ii}}{Q_{ii} - Q_{\max}}, \quad \lambda_{ij} = \frac{3a}{2} \left(\frac{R_i \cdot R_j}{R_i R_j} + \frac{1}{3} \right) D(R_i)D(R_j),$$

$$D(R_i) = \begin{cases} e^{\xi_i}, & R_i < R_{\max}, \\ 0, & R_i \geq R_{\max}, \end{cases} \quad \xi_i = \frac{(R_i^2 - 3a^2)^2}{R_i^4 - R_{\max}^4}.$$

The PEF was developed for covalent solids, applied to Si. The PEF is based on valence force field. The PEF predicts the phonon dispersion relations, cohesive energy, room-temperature Debye–Waller factor, and stabilization energy of the {100} symmetric dimer reconstruction. Parameters of the PEF for Si: $a = 1.357 \text{ \AA}$, $D_1 = 3.0034 \text{ \AA}^2$, $D_2 = 1.2877 \text{ \AA}^2$, $R_{\max} = 3.65 \text{ \AA}$, $A = 97013 \text{ eV}$, $B = 3.33 \text{ \AA}^{-2}$, $Q_{\max} = 6.73 \text{ \AA}^2$, $a_1 = 0.399 \text{ eV/\AA}^2$, $a_2 = 0.157 \text{ eV/\AA}^2$.

2.3.3. Cieplak–Kollman potential [30]

This PEF was developed for aqueous solutions of Li^+ and Na^+ ions [44].

$$\Phi = \phi_2 + \phi_3, \quad \phi_2 = E_{w-w} + E_{w-i} + E_{\text{pol}}, \quad \phi_3 = E_{i-w-w},$$

$$E_{w-w} = \sum_{i < j} \frac{q_i q_j}{r_{ij}} + \sum_{i < j}^{O,O} A_{ij} e^{-B_{ij} r_{ij}} - \sum_{i < j}^{O-O} F \left[C_6 \left(\frac{g_6}{R_{\text{sc}}} \right)^6 \right] \\ + \sum_{i < j}^{O,H} A_{ij} e^{-B_{ij}(r_{ij}-r_{\text{min}})} (e^{-B_{ij}(r_{ij}-r_{\text{min}})} - 2),$$

$$g_n = 1 - \exp \left(-\frac{2.1}{n} R_{\text{au}} - \frac{0.109}{n^{1/2}} R_{\text{au}}^2 \right), \quad F = 1 - R_{\text{au}}^{2.326} e^{-R_{\text{au}}}$$

$$R_{\text{au}} = R_{\text{sc}}/0.529177, \quad R_{\text{sc}} = 0.94834673 \times R_{\text{OO}},$$

$$E_{w-i} = \sum_{i=w, j=\text{ion}} \left[\frac{q_i q_j}{r_{ij}} + \frac{\sqrt{A_i A_j}}{r_{ij}^{12}} - \frac{\sqrt{C_i C_j}}{r_{ij}^6} \right], \quad A_i = \varepsilon_i (r_i^* + r_j^*)^{12}, \quad C_i = 2\varepsilon_i (r_i^* + r_j^*)^6,$$

$$E_{\text{pol}} = -\frac{1}{2} \sum_j \alpha_j (E_j E_j^0), \quad E_{i-w-w} = D e^{-\beta(r_{ij} + r_{ik})} e^{-\gamma r_{jk}}.$$

The PEF was developed for the systems containing H_2O molecules and Li^+ or Na^+ ions. Ion solvation enthalpies are calculated. The relative free energy of hydration of Li^+ and Na^+ is calculated. The parameter set of this PEF contains 30 entries; they are not given here.

2.3.4. Mistriotis–Flytzanis–Farantos potential [31]

This PEF was developed for silicon clusters [45].

$$\Phi = \phi_2 + \phi_3 + \phi_4,$$

$$\phi_2 = \sum_{i < j} A (B r_{ij}^4 - 1) e^{z(r_{ij}-R)}, \quad r_{ij} < R, \quad \phi_3 = \sum_{i < j < k} (h_{jik} + h_{ijk} + h_{ikj}),$$

$$h_{jik} = \lambda_3 f_{ij} f_{ik} (1 - e^{-Q(\cos \theta_{jik} + 1/3)^2}), \quad f_{ij} = e^{z/(r_{ij}-R)},$$

$$\phi_4 = \sum_{i < j < k < l} (g_{ijkl} + g_{jikl} + g_{kijl} + g_{lijk}), \quad g_{ijkl} = \lambda_4 f_{ij} f_{ik} f_{il} (1 - e^{-Q\Delta_{ijkl}}),$$

$$\Delta_{ijkl} = (\cos \theta_{jik} + \frac{1}{3})^2 + (\cos \theta_{jil} + \frac{1}{3})^2 + (\cos \theta_{kil} + \frac{1}{3})^2.$$

This was applied to silicon clusters, Si_n , $n > 6$. The PEF was fit to lattice constant, cohesive energy, and the melting properties. Parameters of the PEF for Si: $A = 16.30076 \text{ eV}$, $B = 11.58113 \text{ \AA}^4$, $\alpha = 2.0951 \text{ \AA}$, $R = 3.77118 \text{ \AA}$, $\lambda_3 = 4.0$, $\lambda_4 = 47.0$, $\gamma = 2.4$, $Q = 5.0$.

2.3.5. Mistriotis–Froudakis–Vendras–Flytzanis potential [32]

This PEF was developed for silicon clusters and surfaces [46].

$$\Phi = \phi_2 + \phi_3 + \phi_4,$$

$$\begin{aligned}\phi_2 &= \sum_{i<j} A(Br_{ij}^4 - 1)f_{ij}, \quad f_{ij} = e^{\alpha(r_{ij}-R)}, \\ \phi_3 &= \sum_{i<j<k} (h_{jik} + h_{ijk} + h_{ikj}), \quad h_{jik} = \lambda_3 f_{ij} f_{ik} (1 - e^{-Q(\cos \theta_{jk} + 1/3)^2}), \\ \phi_4 &= \sum_{i<j<k<l} (g_{ijkl} + g_{jikl} + g_{kijl} + g_{lijk}), \quad g_{ijkl} = \lambda_4 f_{ij} f_{jk} f_{kl} (1 - e^{-Q\Delta_{ijkl}}), \\ \Delta_{ijkl} &= (\cos \theta_{ijk} + \frac{1}{3})^2 + (\cos \theta_{ijkl} - \frac{1}{3})^2 (\cos \theta_{ijkl} + 1)^2 + (\cos \theta_{jkl} + \frac{1}{3})^2.\end{aligned}$$

The PEF simulates silicon cluster properties and Si(111) and Si(100) surface reconstructions. This PEF is the modified form of the previous PEF. Parameters of the PEF for Si: $A = 16.3$ eV, $B = 11.581 \text{ \AA}^4$, $\alpha = 2.095 \text{ \AA}$, $R = 3.77 \text{ \AA}$, $\lambda_3 = 4.0$, $\lambda_4 = 17.0$, $\gamma = 2.4$, $Q = 5.0$.

2.3.6. Daw-Baskes potential [33]

This PEF was developed for metals [47].

$$\begin{aligned}\Phi &= \sum_i F_i(\rho_{hi}) + \sum_{i<j} \phi_{ij}(r_{ij}), \quad \rho_{hi} = \sum_{j \neq i} \rho_j^a(r_{ij}), \\ \rho_j^a(r) &= n_1 \rho_{j_1}(r) + n_2 \rho_{j_2}(r), \quad \phi_{ij}(r) = \frac{Z_i(r)Z_j(r)}{r}, \quad Z(r) = Z_0(1 + \beta r^\nu)e^{-\alpha r}.\end{aligned}$$

This PEF is called embedded-atom method (EAM). EAM based on density functional theory, to calculate the ground-state properties of metal systems, such as total energy, lattice constant, elastic constants, sublimation energy, and vacancy formation energy, surface energy and surface relaxation of various surfaces of metals. Properties of H in bulk metal, binding site and adsorption energy of H on metal surfaces were also studied. Parameter set of this PEF contains many variables; they are not given here.

2.3.7. Price-Parker-Leslie potential [34]

This PEF was developed for silicates (Mg_2SiO_4) [48].

$$\begin{aligned}\Phi &= \phi_1 + \phi_2 + \phi_3, \\ \phi_1 &= \frac{1}{2} \sum_i k_i r_i^2, \quad \phi_2 = \sum_{i<j} \left[A_{ij} e^{-r_{ij}/B_{ij}} - \frac{C_{ij}}{r_{ij}^6} + \frac{e^2 q_i q_j}{r_{ij}} \right], \quad \phi_3 = \sum_{i<j<k} k_{ijk} (\theta_{ijk} - \theta_0)^2.\end{aligned}$$

The PEF was derived empirically using data from simple binary oxides. The lattice dynamical and thermodynamic properties of the Mg_2SiO_4 polymorphs were predicted. The PEF was used to model the infrared and Raman behaviour of forsterite (Mg_2SiO_4). The phonon dispersion relationships of the Mg_2SiO_4 polymorphs predicted by the PEF were used to calculate the heat capacities, entropies, thermal expansion coefficients and Gruneisen parameters of these phases. The phase diagram of this system was constructed. Parameters of the PEF for Mg_2SiO_4 system: $q_{\text{Mg}} = +2.0$, $q_{\text{Si}} = +4.0$, $q_{\text{O}} = +0.848$, $A_{\text{Mg-O}} = 1428.5$ eV, $A_{\text{Si-O}} = 1283.9$ eV, $A_{\text{O-O}} = 22764.3$ eV, $B_{\text{Mg-O}} = 0.2945 \text{ \AA}$, $B_{\text{Si-O}} = 0.3205 \text{ \AA}$, $B_{\text{O-O}} = 0.1490 \text{ \AA}$, $C_{\text{Si-O}} = 10.7 \text{ eV \AA}^6$, $C_{\text{O-O}} = 27.88 \text{ eV \AA}^6$, $k_{\text{O-Si-O}} = 2.09 \text{ eV/rad}^2$, $k_{\text{O-Shell}} = 74.9 \text{ eV/\AA}^2$.

2.3.8. Price–Wall–Parker potential [35]

This PEF was developed for silicates [49].

$$\Phi = \phi_1 + \phi_2 + \phi_3,$$

$$\phi_1 = \frac{1}{2} \sum_i k_i r_i^2, \quad \phi_2 = \sum_{i<j} \left[A_{ij} e^{-r_{ij}/B_{ij}} - \frac{C_{ij}}{r_{ij}^6} + \frac{e^2 q_i q_j}{r_{ij}} \right],$$

$$\phi_3 = \sum_{i<j<k} \left[k_{ijk} (\theta_{ijk} - \theta_0)^2 + D_{ijk} \frac{(1 + 3 \cos \theta_i \cos \theta_j \cos \theta_k)}{(r_{ij} r_{jk} r_{ik})^3} \right].$$

The PEF was used to investigate the properties of perfect high-density silicate crystals, including their elastic and spectroscopic characteristics. The simulation of phase relations and defect properties were investigated. The activation energies for diffusion in forsterite and perovskite were calculated. The high-temperature superionic conductivity of magnesium silicate perovskite was calculated. Parameters of the PEF for Mg_2SiO_4 system: $q_{\text{Mg}} = +2.0$, $q_{\text{Si}} = +4.0$, $q_{\text{O}} = +0.848$, $A_{\text{Mg-O}} = 875.0 \text{ eV}$, $A_{\text{Si-O}} = 1283.9 \text{ eV}$, $A_{\text{O-O}} = 22764.3 \text{ eV}$, $B_{\text{Mg-O}} = 0.3225 \text{ \AA}$, $B_{\text{Si-O}} = 0.3205 \text{ \AA}$, $B_{\text{O-O}} = 0.1490 \text{ \AA}$, $C_{\text{Si-O}} = 10.7 \text{ eV \AA}^6$, $C_{\text{O-O}} = 27.88 \text{ eV \AA}^6$, $k_{\text{O-Si-O}} = 2.09 \text{ eV/rad}^2$, $k_{\text{O-Shell}} = 74.9 \text{ eV/\AA}^2$, $D_{\text{O-Mg-O}} = 120.0 \text{ eV \AA}^9$.

2.3.9. Erkoç potential (VI) [36]

This PEF was developed for cubic systems. Applied to FCC metal microclusters (Cu, Ag, Au) [50].

$$\Phi = D_{21} \phi_{21} + D_{22} \phi_{22}, \quad \phi_{2\ell} = \sum_{i<j} U_{ij}^{(2\ell)}, \quad U_{ij}^{(2\ell)} = \frac{A_\ell}{r_{ij}^{2\ell}} \exp[-\lambda_\ell r_{ij}^2], \quad \ell = 1, 2$$

The parameters of the PEF were determined by considering the bulk cohesive energy and bulk stability condition. The PEF satisfies the crystal stability, and gives elastic constants and bulk modulus reasonably for the elements considered. Energy and structure of microclusters of the elements have also been studied. The parameters of the PEF for Cu, Ag, and Au (energy in eV, distance in \AA) are given in Table 12.

Table 12

Parameter	Cu	Ag	Au
A_1	110.766008	220.262366	345.923364
λ_1	2.09045946	1.72376253	1.04289230
α_1	0.394142248	0.673011507	0.750775965
A_2	-46.1649783	-26.0811795	-38.9245908
λ_2	1.49853083	1.81484791	1.05974062
α_2	0.2072255507	0.120620395	0.229377368
D_{21}	0.436092895	1.00610152	0.888911352
D_{22}	0.245082238	0.221234242	0.254280292

Table 13

Element	d (Å)	A (eV)	β	c (Å)	c_0	c_1	c_2
V	3.692767	2.010637	0.0	3.80	-0.8816318	1.4907756	-0.3976370
Nb	3.915354	3.013789	0.0	4.20	-1.5640104	2.0055779	-0.4663764
Ta	4.076980	2.591061	0.0	4.20	1.2157373	0.0271471	-0.1217350
Cr	3.915720	1.453418	1.8	2.90	29.1429813	-23.3975027	4.7578297
Mo	4.114825	1.887117	0.0	3.25	43.4475218	-31.9332978	6.0804249
W	4.400224	1.896373	0.0	3.25	47.1346499	-33.7665655	6.2541999
Fe	3.699579	1.889846	1.8	3.40	1.2110601	-0.7510840	0.1380773

2.3.10. Ackland potential [37]

This PEF was developed for covalently bonded systems, particularly for silicon. This was applied to crystal, point defect, and surface properties of silicon [51].

$$\Phi = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N A e^{-\alpha r_{ij}} - \frac{1}{2} \sum_{i=1}^N \sum_{n=1}^4 B r_{ik_n} e^{-\beta r_{ik_n}}$$

The parameters of the PEF were determined by considering the cohesive energy, lattice parameter, and bulk modulus of diamond silicon. Parameters of the PEF for Si: $A = 208442.8$, $B = 16.63588$, $\alpha = 5.673585$, $\beta = 1.144811$.

2.3.11. Finnis–Sinclair potential [38]

This PEF was developed for transition metals, and was applied to vacancy and surface properties of BCC transition metal elements [52].

$$\Phi = U_N + U_P, \quad U_N = -A f(\rho), \quad U_P = \frac{1}{2} \sum_{i \neq 0} V(r_i)$$

$$f(\rho) = \sqrt{\rho}, \quad \rho = \sum_{i \neq 0} \phi(r_i),$$

$$\begin{aligned} \phi(r) &= (r-d)^2 + \beta(r-d)^3/d, & r \leq d, \\ &= 0, & r > d, \end{aligned}$$

$$\begin{aligned} V(r) &= (r-c)^2(c_0 + c_1 r + c_2 r^2), & r \leq c, \\ &= 0, & r > c. \end{aligned}$$

The parameters of the PEF were determined by considering the lattice constant, cohesive energy, elastic constants, shear modulus, and Cauchy pressure of the elements considered. Parameters of the PEF for some BCC elements are given in Table 13.

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Appendix A

List of the EMBPEFs parameterized for the element(s) and/or systems

Potential	#	Element(s) and/or system
Φ_I		
Tersoff (I)	1	Si
Dodson	2	Si
Tersoff (II)	3	Si, C
Brenner (I)	4	C
Brenner (II)	5	Hydrocarbons
Chelikowsky et al.	6	Si, C
Khor–Das Sarma (I)	7	C, Si, Ge
Khor–Das Sarma (II)	8	H ₃ -Si(1 1 1)
Khor–Das Sarma (III)	9	Si(1 1 1)
Φ_{II}		
Bauer et al.	10	Cu, Ag, Au
Pearson et al.	11	Si, GaAs, Si–GaAs, Al–GaAs, Au–GaAs
Biswas–Hamann (I)	12	Si
Biswas–Hamann (II)	13	Si
Stillinger–Weber	14	Si, Ge
Gong	15	Si
Blaisten–Barojas–Khanna	16	Be
Takai et al.	17	C
Kaxiras–Pandey	18	Si
Feuston–Garofalini	19	v-SiO ₂
Murrell–Mottram	20	Si
Al-Derzi et al.	21	C
Li et al.	22	Si
Erkoç (I)	23	Ag, Al, Au, Cu, Ni; Fe, Li; C, Ge, Si; Cs, K, Na; Ca, Pb, Pd, Pt; Cd, Mg, Sc, Ti, Zn
Erkoç (II)	24	Ag, Al, Au, Cu, Ni, Pb, Pd, Pt; C, Si, Ge; Li, Na, K, Cs, Fe; V, Cr, Nb; As, Sb, Bi
Erkoç (III)	25	Au, Ag, Cu
Erkoç (IV)	26	Cu
Erkoç (V)	27	Kr, Xe, Al, Cu, Pb, Pd
Φ_{III}		
Bolding–Anderson	28	Si
Brenner–Garrison	29	Si
Cieplak–Kollman	30	Aqueous solutions of Li ⁺ , Na ⁺
Mistriotis et al.	31	Si _n

Potential	#	Element(s) and/or system
Mistriotis et al.	32	Si
Daw–Baskes	33	Metals
Price et al.	34	MgSiO ₄
Price et al.	35	MgSiO ₄
Erkoç (VI)	36	Cu, Ag, Au
Ackland	37	Si
Finnis–Sinclair	38	V, Nb, Ta, Cr, Mo, W, Fe

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