

DEVELOPMENTS IN THE APPLICATION OF THE EFFECTIVE POTENTIAL METHOD IN THE STUDY OF SEMICONDUCTOR NANOSTRUCTURES AT THE ATOMIC LEVEL

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ABSTRACT

This paper presents recent developments in the effective potential method for the study of semiconductor nanostructures at the atomic level. By using calculations based on the density functional theory in approaching local density, we demonstrate that the effective potential derivation framework can be extended to different compositions and is not restricted to materials with the same number of anions and cations. We show that this method can be applied to the derivation of atomic impurity potentials. Given the similarity in the results obtained using the effective potential method and the density functional theory, the results allow us to conclude that the new generation of potentials are sufficiently precise to be applied to the study of semiconductor nanostructures in which the number of atoms exceeds the limit for standard calculations made using the density functional theory.

KEYWORDS: Nanoscience, first principles calculations, effective potentials, semi-conductive materials, low-dimensionality systems, atomistic calculations.

AVANCES EN LA APLICACIÓN DE POTENCIALES EFECTIVOS EN EL ESTUDIO DE NANOESTRUCTURAS SEMICONDUCTORAS A NIVEL ATOMÍSTICO

RESUMEN

Se presentan adelantos recientes en el método de potenciales efectivos para el estudio de nanoestructuras semiconductoras a nivel atomístico. Se demuestra que el esquema de derivación de potenciales efectivos, a partir de cálculos basados en la teoría del funcional de la densidad en la aproximación de densidad local, puede ser extendido a diferentes composiciones y no se restringe a materiales con igual número de aniones y cationes. Se muestra que el método puede ser aplicado a la derivación de potenciales atómicos de impurezas. Los resultados permiten concluir, gracias a la similitud de los resultados obtenidos usando potenciales efectivos y usando formalmente la teoría del funcional de la densidad, que la nueva generación de potenciales son lo suficientemente precisos para su aplicación al estudio de nanoestructuras semiconductoras, en donde el número de átomos supera el límite de los cálculos estándar realizados usando la teoría del funcional densidad.

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AVANÇOS NA APLICAÇÃO DE POTENCIAIS EFICAZES NO ESTUDO DE NANOESTRUTURAS SEMICONDUTORAS A NÍVEL ATOMÍSTICO

RESUMO

Se apresentam avanços recentes no método potencial efetivo para o estudo de nanoestruturas semicondutoras ao nível atômico. Mostra-se que o sistema de derivação de potenciais eficazes partindo de cálculos baseados na teoria funcional da densidade na aproximação da densidade local, pode ser estendido a diferentes composições e não se restringe a materiais com um número igual de ânions e cátions. Mostra-se que o método pode ser aplicado para a derivação de potenciais atômicos de impurezas. Os resultados permitem concluir, graças à semelhança dos resultados obtidos usando potenciais efetivos e usando formalmente a teoria do funcional da densidade, que a nova geração de potenciais são o suficientemente precisos para a sua aplicação ao estudo de nanoestruturas semicondutoras, onde o número de átomos excede o limite dos cálculos padrões realizados usando a teoria do funcional da densidade.

PALAVRAS-CHAVE: Nanociência, cálculos de primeiros princípios, potenciais efetivos, materiais semicondutores, sistemas de baixa dimensionalidade, cálculos atômicos.

1. INTRODUCTION

Physics at the nanoscopic scale has been established as a field of work that requires a great understanding of the phenomena of solid state physics. The experimental developments in this area have reached a point at which the effects at the atomic scale have become highly relevant not only in the sphere of growth and fabrication of experimental samples, but also when making measurements of different physical properties. There are, for example, processes such as ionic implantation in materials in which an element of the solid is replaced in order to change its properties. To illustrate this type of experiment, we can cite the case of nitrogen-vacancy centers in diamonds, in which a pair of consecutive carbon atoms in the crystalline material are substituted by a set of one nitrogen atom and a vacancy. This type of configuration shows interesting characteristics in its spin states that can mainly be used in quantum information processing applications. In mesoscopic systems,

such as quantum dots, threads, and wells, fabricated based on a semiconductor, the changes in the atomic structure at the interface level causes changes in the electronic structure of the material's bands, which must be considered when using these nanostructures in modern technological applications. As an additional example, we can consider the case of colloidal dots. These semiconductor nanostructures are dissolved in a solution and used to optically trace the movement of fluids. For efficient applicability of this technique, the quantum dots must be as uniform as possible, both in terms of composition and size, such that their absorption and emission properties are within a narrow range of the visible spectrum. The list of examples extends to all types of systems of modern scientific and technological interest fabricated in the solid state.

In general terms, the science of semiconductor nanostructures has made many achievements and continues to advance. Nanostructures based on semiconductors are currently grown using diverse components and a high degree of control over doping (Kudelski, *et*

al., 2007, Celebi, *et al.*, 2008, Leger, *et al.*, 2005, Besombes, *et al.*, 2004, Leger, *et al.*, 2006, Erwin, *et al.*, 2005). Regarding spectroscopy, this area allows us to study a large number of phenomena related to the interaction of light with the matter and physics of many bodies which result in the creation of quasiparticles with complex behaviors, as is the case of charged excitons and multi-excitons (Warburton, *et al.*, 2000, Urbaszek, *et al.*, 2003, Dekel, *et al.*, 1998) and spin dynamics (Kouwenhoven, Austing, Tarucha, 2001, Loss, DiVincenzo, 1998).

In the theoretical sphere, the demands of defining nanostructures at the atomic scale makes continuous methods, such as the effective mass method and the k.p method (Bastard, 1988), obsolete since they can consider the mesoscopic scale but fail to consider the rapid oscillations of wave functions due to fluctuations at the atomic scale. In their place, we must use first principles techniques such as the Monte Carlo method, density functional theory (DFT), GW, and Bethe-Salpeter, etc., where the atomic identity of the structure is considered, giving maximum limitation of approximations made of the characteristics of each atom in the system and the calculation procedure methodology.

The first principles methods mentioned above are useful to calculate the optical properties of systems that include up to a few hundred atoms. However, the dimensions of the devices which are appropriate for nanotechnology range from a few nanometers to a few hundred nanometers. These dimensions, though they are small, can contain several hundred atoms, making first principles methods less useful in this regime. There are some solutions based, for example, on empirical potentials and tight binding models. These methods can consider a number of atoms that would reach the nanostructure regime, but they contain adjustment parameters that make them lose the first principles identity.

A new methodology has recently been presented which endorses the calculation of structures based on semiconductor materials appropriate for nanotechnology applications, which maintain the first principles identity and are based on density functional theory. The fundamental idea of this method is to extract effective atomic potentials (EAPs) directly from

DFT calculations, which would effectively contain the entire minimization process with regards to the density on which density functional theory is based. In this way, these EAPs can be used to calculate electronic states of nanostructures with several hundred atoms since it will no longer be necessary to perform the self-consistent loops typical of DFT and the calculation of the electronic states of nanostructures can be restricted, thanks to computational algorithms, to the energetic regions relevant for optical properties, which are typically the states near the gamma point of the reciprocal space (Zirkelbach, *et al.*, 2015).

Figure 1 compares some first principles methods and continuous models such as the effective mass model. The figure compares the transferability (a method's capacity to be used in different systems) of the different methods, as well as their applicability in terms of the number of atoms. As was mentioned above, DFT is widely used; however, its applicability is limited to a low number of atoms compared to the nanostructure regime (the grey region in **Figure 1**). On the other hand, we have the continuous methods such as the envelope function. These methods cover a much greater spectrum in terms of the physical dimensions of the nanostructures. They also have high transferability, making them very versatile methods. However, they lose their applicability when we greatly reduce the size of the samples and want to consider the effects of the atomic limit.

Empirical methods offer an intermediate alternative between the two (DFT and effective mass), but their transferability is also limited. The effective atomic potentials method offers an improved alternative since it partly contains the quality of the calculations at the density functional theory level while extending its applicability to structures with a much greater number of atoms and maintaining a high degree of transferability.

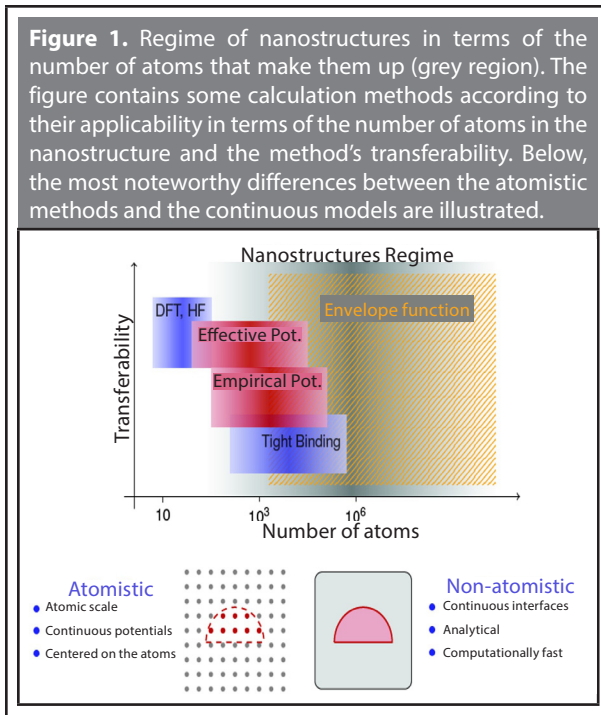
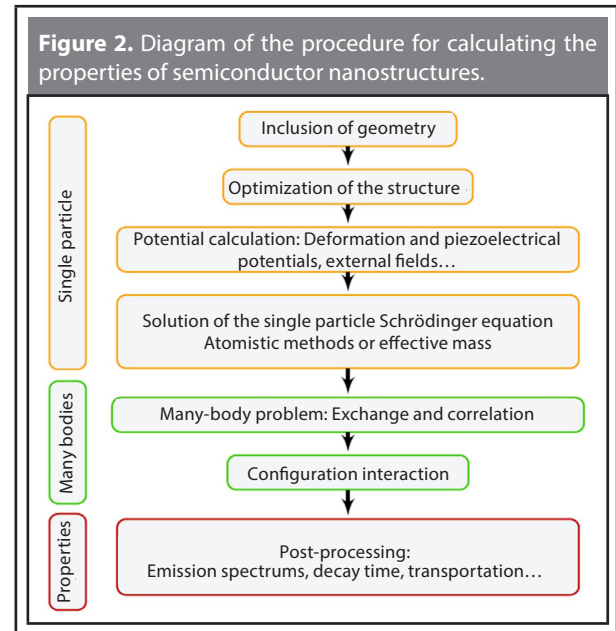


Figure 2 outlines the calculation process for the optical properties of nanostructures fabricated using semiconductors. Generally, solving the single particle Schrödinger equation comes first. To do so, the geometry of the nanostructure being considered must be well defined, that is, whether it is a system in one, two, or three dimensions and what particular orientation the heterostructures have (if they form a pyramidal or spherical quantum dot, for example). We must then calculate the potential energy that will enter into the Schrödinger equation. At this point, we must consider optimization of the structure, which generates piezoelectric and deformation fields. Once the potential is determined, the single particle Schrödinger equation can be solved. At this point, we must choose the calculation method, first principles or continuous methods, according to the type of study to be done. Once the single particle Schrödinger equation has been solved, we must consider the case of having multiple particles confined in the nanostructure, which is related to how the nanostructure is excited. This step is equivalent to solving a many-body problem. With the excited states, we can perform different calculations in a post-processing phase, which characterizes the optical and electronic properties of the nanodevices.

This report presents a review of the procedure to generate effective atomic potentials and shows how this technique can be extended to the generation of potentials for materials with a different number of anions and cations and impurities. The central idea is to clarify the proposed method for generating EAPs and point out possible improvements to the original methodology. Numerical implementation for use of the EAPs is not a part of this report. The considerations herein are useful for increasing the range of applicability of the EAP generation method to new semiconductor structures with dimensions in the nanometer range, which will open the door to new theoretical studies in the field of nanotechnology.



2. METHODOLOGY

In the framework of atomistic calculations, the fundamental purpose is to consider the properties of each atom that makes up the solid-state system being studied. In these conditions, the Hamiltonian defines that the structure's electronic states must be built from the algebraic sum of the potentials of each of the atoms that make up the sample. Once the total local potential $V_{loc}^{eff}(\mathbf{r})$ has been calculated, the single particle Schrödinger equation can be solved.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{loc}^{eff}(r)\right)\Psi_i(r) = \varepsilon_i \Psi_i(r) \quad (1)$$

In DFT, the total effective potential $V_{loc}^{eff}(r)$ describes the interaction of a single electron with the surrounding medium. The effective potential is a density functional and contains terms of Coulombian, Hartree, exchange, and correlation interaction. Details of the method's precise computational and implementation requirements to solve **Equation (1)** can be verified in Zirkelbach (2015) and Cárdenas (2012).

The local effective potential can be expressed as a sum of the potentials centered on the atoms:

$$V_{loc}^{eff}(r) = \sum_{\alpha}^{N_{esp}} \sum_{n}^{N_{\alpha}} v_{\alpha}(r - \tau_{an}) \quad (2)$$

where α represents the type of atomic species, N_{esp} the total number of atomic species, n each of the N_{α} atoms of the species α and τ_{an} the position of each atom.

The construction of the effective atomic potentials is based on **Equation (2)**, which contains the contribution of each of the atoms to the total potential. Note that when any DFT calculation is performed, the local effective potential given after performing the self-consistent loops will contain all of the effects of the density relaxation process and, therefore, each atomic potential $v_{\alpha}(r - \tau_{an})$ will effectively contain the influence of the surrounding medium would have on it.

The total effective local potential as shown in **Equation (2)** is not useful since it corresponds to a single structure, and the atomic potentials are superimposed, making it impossible to identify them and separate them numerically. This issue is solved by representing the potentials in the reciprocal space through a Fourier transform and writing them in terms of the vector that expands in the reciprocal space

$$V_{loc}^{eff}(G) = \frac{1}{\Omega_c} \int_{\Omega_c} V_{loc}^{eff}(r) e^{-iG \cdot r} d^3 r \quad (3)$$

With this transform, we can rewrite the effective potential in the reciprocal space as a Fourier sum

$$V_{loc}^{eff}(G) = \frac{1}{\Omega_c} \sum_{\alpha}^{N_{esp}} \sum_{n}^{N_{\alpha}} e^{-iG \cdot \tau_{an}} v_{\alpha}(G) \quad (4)$$

with

$$v_{\alpha}(G) = \int_{\infty} v_{\alpha}(r) e^{-iG \cdot r} d^3 r \quad (5)$$

In the result shown in **Equation (4)**, we see that all of the atomic potentials are centered on the origin in the reciprocal space, which means this equation can be inverted to write the atomic potentials in terms of the total effective local potential $V_{loc}^{eff}(G)$.

Construction of effective potentials for massive systems

The idea of using an effective potential to calculate the electronic structure of bulk materials was proposed several decades ago. The initial idea was to derive the effective potentials from an adjustment of experimental measurements of the energy levels of bulk materials (Phillips, 1958, Brust, Phillips, Cohen, 1962, Brust, Bassani, Phillips, 1962, Cohen, Bergstresser, 1966, Chelikovsky, Cohen, 1976). This method was useful to determine the optical properties as well as the band structure of various solids using only some three Fourier components of the atomic potentials. Later, a totally theoretical methodology was implemented to determine atomic potentials (Wang, Zunger, 1995, Fu, Zunger, 1997) based on DFT. The central idea of this method was to perform calculations of a bulk material under different conditions, mainly at different network parameter values and using different crystallographic structures. The local effective potential was then transformed to the reciprocal space, and an adjustment to Gaussian functions was performed to obtain a continuous curve for the potentials.

In a more recent proposal made by Cárdenas & Bester (2012), effective atomic potentials are drawn from the expansion in the reciprocal space of the local potential calculated with DFT of two structures with the same binary material. In the original report, the test structure used in this method to calculate the local potential is a block of zinc blende structure material along the crystallographic direction [001]. The block has a unit cell in each direction of the plan and extends along 24 atoms in said direction.

The purpose of using a block of material and not a unit cell of the bulk material is that when performing the Fourier transform, the atomic potentials are described over a dense network of G vectors in the reciprocal space, making the continuous description of the potential

possible through a simple interpolation of data and eliminating the need to adjust the initial generation method to Gaussian functions. In addition, the method allows for having the EAPs evaluated for small G vectors compared to the G_c vector related to the crystal network parameter, which allows us to have EAPs with information about the far-reaching interatomic interactions, not only those with close neighbors, which was one of the great limitations of earlier potentials.

The two calculations mentioned to extract the EAPs are performed on two systems in block form with the same dimension, but where the positions of the anions and cations are exchanged, maintaining the atomic positions. This leads to two local potentials $V_{loc}^{(1)}$ and $V_{loc}^{(2)}$:

$$V_{loc}^{(1)}(r) = \sum_{i=1}^{N_a} v_a(r - \tau_i) + \sum_{j=1}^{N_c} v_c(r - \tau_j), \quad (6)$$

$$V_{loc}^{(2)}(r) = \sum_{j=1}^{N_c} v_c(r - \tau_j) + \sum_{i=1}^{N_a} v_a(r - \tau_i). \quad (7)$$

In expressions (6) and (7), the exchange between the sum indices represents the exchange between the atomic species, $v_a(v_c)$ is the anion potential (cation), and $N_a(N_c)$ is the total number of anions (cations).

The extraction of the EAP is done through the addition and subtraction of the two local potentials

$$V_{loc}^{(1+2)}(r) = V_{loc}^{(1)}(r) + V_{loc}^{(2)}(r) = \sum_{n=1}^{N_{atomos}} v_+(r - \tau_n), \quad (8)$$

$$V_{loc}^{(1-2)}(r) = V_{loc}^{(1)}(r) - V_{loc}^{(2)}(r) = \sum_{n=1}^{N_{atomos}} (-1)^{n+1} v_-(r - \tau_n), \quad (9)$$

where the sum is now for the total number of atoms N_{atomos} . The Fourier transform is applied to relationships (8) and (9), and the result is then given in terms of the following intermediate values

$$v_+ = v_a + v_c, \quad (10)$$

$$v_- = v_a - v_c. \quad (11)$$

Passing through the intermediate variables defined in (10) and (11) restricts the EAP generation method to systems with equal numbers of anions and cations.

Improving the method

The EAP generation method can be improved by suppressing the restrictions imposed by using relationships (10) and (11). Let us note that by limiting the system being considered to the case of having an equal number of anions and cations makes it impossible to apply the method to materials.

The use of v_+ and v_- is unnecessary if we consider the equations from the point of view of linear algebra. When two effective local potentials are calculated, all we are doing is determining two different expressions (**Equations 6 and 7**) in which the two variables we are looking for (v_a and v_c) intervene. Considering this, the system of equations is totally solvable without needing to use v_+ and v_- . We can see this more clearly by making the Fourier transform of $V_{loc}^{(1)}(r)$ and $V_{loc}^{(2)}(r)$ directly:

$$V_{loc}^{(1)}(G) = \frac{1}{\Omega_c} \left[\sum_{i=1}^{N_a(1)} e^{-iG \cdot \tau_i} \right] v_a(G) + \frac{1}{\Omega_c} \left[\sum_{j=1}^{N_c(1)} e^{-iG \cdot \tau_j} \right] v_c(G), \quad (12)$$

$$V_{loc}^{(2)}(G) = \frac{1}{\Omega_c} \left[\sum_{k=1}^{N_a(2)} e^{-iG \cdot \tau_k} \right] v_a(G) + \frac{1}{\Omega_c} \left[\sum_{l=1}^{N_c(2)} e^{-iG \cdot \tau_l} \right] v_c(G), \quad (13)$$

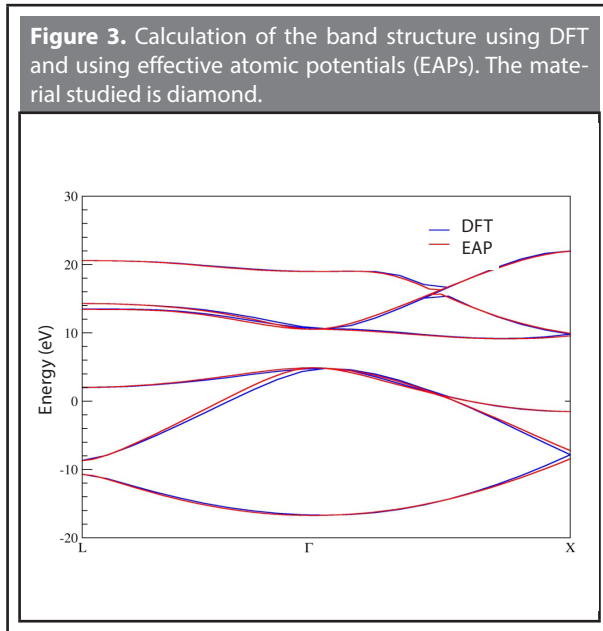
where no restriction has been made regarding the number of anions or cations. The amounts in square brackets depend only on the structure factor. Therefore, for each G vector in the reciprocal space, we can write:

$$V_{loc}^{(1)}(G) = \alpha_1 v_a(G) + \beta_1 v_c(G) \quad (14)$$

$$V_{loc}^{(2)}(G) = \alpha_2 v_a(G) + \beta_2 v_c(G) \quad (15)$$

which we can reverse to find $v_a(G)$ and $v_c(G)$.

Using this new procedure, we have repeated the potentials extraction process performed before by Cárdenas & Bester (2012), obtaining similar results. **Figure 3** shows an example of the calculations done with this type of potentials. The figure shows the band structure of carbon in a zinc blende structure (diamond) calculated with DFT itself, and also calculated with the effective atomic potentials considered here, as was done in Zirkelbach (2015) and Cárdenas & Bester (2012).



Extending the method to generate impurity potentials

Once the effective atomic potentials of the bulk material have been found, we can use them to extract the atomic potentials of impurities. In this case, the task is to rebuild, using the known EAPs, the local effective potential corresponding to the bulk material in order to find the potential that corresponds only to the impurity.

If the system contains an impurity, we are considering a case in which an atom of the bulk material has been substituted by a different species. In these conditions, the system would contain three different types of atoms and the effective local potential would be written as:

$$V_{loc}^{dft}(\mathbf{r}) = \sum_{i=1}^{N_a} v_a(\mathbf{r} - \tau_i) + \sum_{j=1}^{N_c} v_c(\mathbf{r} - \tau_j) + v_{imp}(\mathbf{r} - \tau_{imp}) \quad (15)$$

where $v_{imp}(\mathbf{r} - \tau_{imp})$ refers to the atomic potential of the impurity. From the equation above, if we already know v_a and v_c , we can clarify the impurity potential. If we note v_a^{PAE} and v_c^{PAE} the potentials of the bulk material extracted as was explained above, and we use them to rebuild the local potential in (15), the effective atomic potential of the impurity would be written as:

$$v_{imp}(\mathbf{r} - \tau_{imp}) = V_{loc}^{dft}(\mathbf{r}) - \sum_{i=1}^{N_a} v_a^{PAE}(\mathbf{r} - \tau_i) - \sum_{j=1}^{N_c} v_c^{PAE}(\mathbf{r} - \tau_j) \quad (16)$$

From here, we can continue the procedure explained above for extracting the EAPs in the reciprocal space:

$$v_{imp}(\mathbf{G}) = V_{loc}^{dft}(\mathbf{G}) - \frac{1}{\Omega_c} \left[\sum_{i=1}^{N_a} e^{-i\mathbf{G} \cdot \tau_i} \right] v_a^{PAE}(\mathbf{G}) - \frac{1}{\Omega_c} \left[\sum_{j=1}^{N_c} e^{-i\mathbf{G} \cdot \tau_j} \right] v_c^{PAE}(\mathbf{G}). \quad (17)$$

The amounts in square brackets are again related to the factor of the sample structure and represented totally known amounts.

In extracting the EAPs for impurities, even when the process is fairly simple, it is best in some cases to perform a convergence process. Given the periodic boundary positions in DFT, if we do not consider a unit cell large enough, there will be an interaction between neighboring impurities which will be reflected in the form of the potential. It is therefore necessary to perform test structure calculations increasing the size of the unit cell until we obtain a convergence in the atomic potential obtained.

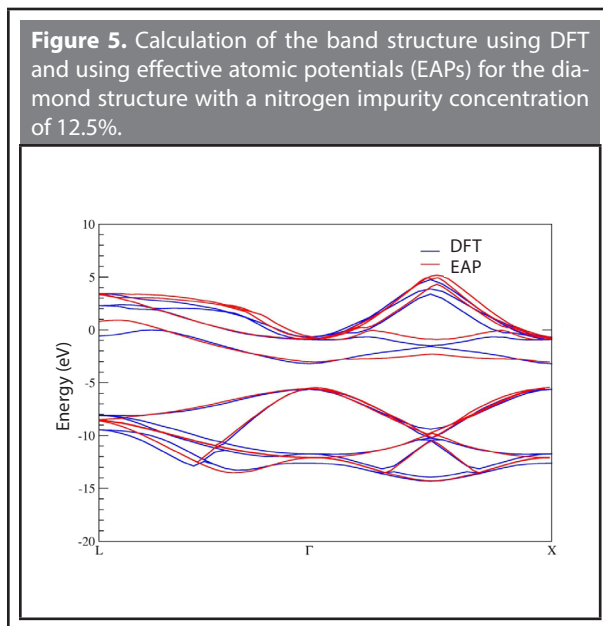
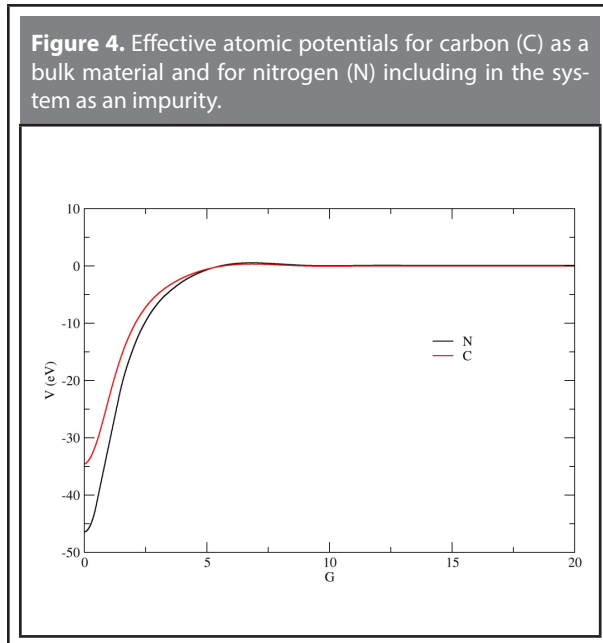
In conclusion, to extract EAPs of impurity atoms, we must follow these steps:

- 1) Generation of the bulk potentials of the material that contains the impurity.
- 2) A DFT calculation for the test structure, that is, of the binary system containing the impurity.
- 3) A convergence test of the test structure.
- 4) Extraction of the effective atomic potential for the impurity through **Equation (17)**

Figure 4 shows an example of the impurity potentials extracted using the method described above. The material chosen for the case of impurities is nitrogen in diamond. The figure shows the effective atomic potential of both the receptor material (C) and the impurity (N). We can see a continuous curve with good behavior for both potentials, which provides confidence in the proposed potential extraction methodology. The calculations shown here of this system's electronic states using the EAPs will be published separately in a rigorous study of this system.

Figure 5, however, shows a simple calculation of the band structure of diamond with a nitrogen impurity.

In this case, we considered a 12.5% nitrogen concentration such that the resulting material is $C_{0.875}N_{0.125}$. The figure shows only the bands close to the material's energy gap. We can see the similarity of the energy bands along the lines of symmetry with special emphasis at the gamma point, which is of relevant importance to the system's optical properties.



3. CONCLUSIONS

In summary, we reviewed the method for generating effective atomic potentials based on density function theory calculations. We showed that the potential generation method for the bulk material is not restricted to binary materials with the same number of anions and cations, but rather that we can extend this method to all types of binary materials. We showed that it is possible to extract the atomic potential of impurities based on effective atomic potentials already obtained and a new DFT calculation, which opens up the possibility of performing atomistic calculations with this technique for systems of interest, such as the case of nitrogen impurities in diamond.

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