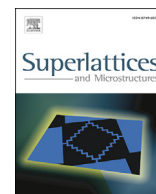


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Effective passivant pseudopotentials for semiconductors: Beyond the spherical approximation

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ABSTRACT

A new type of atomic pseudopotential for passivation of semiconductor surfaces is presented. These pseudopotentials are intended to be used with empirical or effective pseudopotentials methods, where the main goal is to address nanostructures composed of thousands of atoms, but at low computational costs in comparison to density functional theory (DFT). It is shown that the spherical approximation, which is currently used for these potentials, is not suitable for describing passivants and that, instead, they have to be regarded as complex quantities in reciprocal space. A methodology to extract and implement the new pseudopotentials are described here based on an analytic formulation. Passivants for six different semiconductor compounds (GaAs, AlAs, Si, Ge, CdSe and ZnO) are generated, and their accuracy and high transferability are demonstrated by the calculation of the electronic states of different kinds of surfaces and structures and comparison to DFT calculations. The results show that the DFT results can be reproduced with high fidelity with the passivant potentials here presented.

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1. Introduction

The fabrication of semiconductor nanostructures is nowadays controlled at the atomic scale. At the same time, new experimental ideas make evident the relevance of the atomic identity of the experimental samples [1–7]. In this sense, to be able to theoretically study low dimensional semiconductor structures, it is equally required to apply modern atomistic methods, capable of considering characteristics such as precise composition, shape and size of the structures [8–13].

One of the major difficulties of going to the atomic limit with theoretical methods, as far as semiconductor nanostructures are concerned, are the number of atoms conforming the samples. When we talk about semiconductor quantum wells, wires or dots, we are talking about systems composed of several thousands atoms. These sizes, still in the nanometer regime, are far beyond the limit of several *ab initio* techniques in terms of computational costs.

Different ways to try to overcome this numerical inconvenient have been proposed. Specialized basis sets, for example, have been effectively used to calculate band structures and total energies of solids [14,15]. Other alternative is the use of optimized atomic pseudopotentials (PSPs), where the general idea is to soften the innermost part of the potentials and all-electron wavefunctions by well behaved functions leading to a faster plane-wave convergence [16–23].

Based on a fitting procedure, the empirical pseudopotential method (EPM) was first used to construct atomic pseudopotentials with spherical symmetry, where the PSPs were adjusted empirically until reproducing the experimentally determined energy levels of bulk crystals [19,20]. This idea has been reviewed different times [24], until arriving to the atomic

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effective pseudopotentials (AEPs) [22,11]. These spherical PSPs have been successfully used in bulk semiconductor physics since many years ago [20,23,25,26].

An extra difficulty arises in the study of semiconductor nanostructures where, besides having a considerably high number of atoms, the sample surfaces play a significant role. This area of research is currently very active and empirical spherical PSPs have been used so far [13,27–30], but their accuracy has not been formally demonstrated. DFT methods, even though accurate, are difficult to apply due to the number of atoms present in the samples, as mentioned before. The spherical PSPs and the EPM reproduce the scattering due to all the electrons of bulk systems, saving computational costs, but must behave quite different to the surface potentials because the charge transfer phenomena considerably change.

In this paper, a new type of effective passivant pseudopotential (EPP) is presented. It is shown that in order to effectively passivate semiconductor surfaces, it is mandatory to go beyond the spherical approximation and consider passivant potentials as complex quantities in reciprocal space. A way to extract both, the imaginary and real components of the EPPs, is introduced, based on analytic expressions that relate the PSPs and the effective crystal potential from DFT of two carefully chosen semiconductor slabs in zincblende structure. In this way, if the bulk PSPs are previously known [22], the crystal potential can be reconstructed and, hence, extract the effective passivant potentials.

It has to be mentioned that the methodology introduced here is completely general, and that the use of non-spherical pseudopotentials for the correct description of semiconductor surfaces holds for any atomistic method following the philosophy of the EPM or the AEPs, but they are described here mostly in terms of AEPs [22], meaning that the pseudopotentials are in the form of tabulated data. On the other hand, the aim of the method is not to compete with DFT or other *ab-initio* method, but to offer an alternative where the computational capabilities don't allow for the application of more accurate methods. To the contrary, the reliability of the EPPs is supported on comparisons to DFT calculations of electronic states of different systems.

The new PSPs will therefore allow for the theoretical study of the optoelectronic properties of semiconductor systems where surfaces are expected to play a significant role, keeping the atomistic identity of the system, but overcoming the current problems of the computational limitations that modern atomistic methods have, since the self-consistent routines will be skipped, making the calculations less demanding computationally speaking.

2. Methodology

In order to study the optical and electronic properties of semiconductor low dimensional systems, we need to solve the Schrödinger equation for the states near the band gap of the nanostructure

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(\mathbf{r}) \right) \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r}), \quad (1)$$

where the effective potential $V_{\text{eff}}(\mathbf{r})$ carries the information of the interaction of the single electron with its surrounding: the external Coulomb interaction with the atomic nuclei (V_{ext}), the Hartree (V_{Hartree}) and exchange-correlation (V_{xc}) terms.

$$V_{\text{eff}}(\mathbf{r}) = V_{\text{ext}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{xc}}(\mathbf{r}). \quad (2)$$

In DFT, the Coulomb potential is commonly introduced in the frozen-core approximation, by replacing the true potential by pseudopotentials, where the core electrons are frozen in their atomic configuration. At the same time, the pseudopotentials are divided into a local and a nonlocal part, where the nonlocal part is written as a sum of angular momentum projectors [11,22,31].

$$V_{\text{ext}} \rightarrow V_{\text{psp,loc}} + V_{\text{psp,nloc}}, \quad (3)$$

where nonlocal part of the pseudopotentials can be implemented using the separable form of the Kleinman and Bylander projectors [31].

The advantage of the AEPs and EPM over DFT relays, first of all, on the fact that in DFT the effective crystal potential $V_{\text{eff}}(\mathbf{r})$, being a functional of the electronic density, is defined only after a minimization procedure through a self-consistent routine, while the empirical or effective PSPs contain the all electron scattering, and the effective potential needs therefore to be computed only once. On the other hand, since the crystal potential is immediately know with effective potentials, the solution of Eq. (1) can be limited to the states near the band gap, without any need of calculating the full band spectrum [22,11].

In the case of the AEPs, the atomic pseudopotentials are extracted from the local part of the effective potential

$$V_{\text{loc}}(\mathbf{r}) = V_{\text{psp,loc}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{xc}}(\mathbf{r}), \quad (4)$$

delivered by a DFT calculation as explained in previous reports [22,11], and then used together with the Kleinman and Bylander projectors to immediately construct the effective potentials in Eq. (1) of any semiconductor nanostructure, via the addition of the atomic PSPs as done in the EPM.

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