

Electronic Structure of Heterogeneous Materials

Application to optical properties

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Abstract

The objective of this work is to find a description of the group IV elements Silicon, Carbon and Germanium and calculate the electronic structure and optical properties of materials containing those elements. To calculate the band structure we will use pseudopotentials. We will use an Empirical Pseudopotential Method to find the better fitting to the pseudopotentials to the experimental known data about the band structure to each of this elements. We start by fitting the pseudopotentials to an *ab initio* LDA pseudopotential generator, to find the first acceptable set of pseudopotentials' parameters. From that we further adjust the potentials to the experiment, and find a better fit. After that the optical properties of the bulk Si, C and Ge are calculated. The purpose is to generate a pseudopotential to each of this elements that simulates correctly the properties and can be transferable to supercells of Si-Ge-C. We want to predict the behaviour of Si-Ge-C nanostructures.

Keywords: Nanotechnologies, Simulation of Materials, Condensed Matter Physics, Solid State Applications, Pseudopotentials

1. Introduction

In micro and nanotechnologies of today, there is an high interest in semiconductor materials that have a direct gap that can be grown in silicon, since it is the material that is widely used in integrated circuits. We are ultimately interested in the study of materials based in super-lattices of Si-Ge with C impurities, and to simulate its optical properties.

We are interested in simulating cells with many atoms. There are already quite a few methods to do so, each one with its positive and negative points. The “reference” method for electronic structure calculations are done uses the Kohn-Sham equations [KS65] with the local-density approximation (LDA) [PW92, KS65] for the exchange-correlation energy and potential (as we will describe later on). However this calculations can lead to results with very bad agreement with experiment for the band gap of semiconductors and insulators. For example, in Si, with LDA, the band-gap is predicted to be one half of its value, while in Ge the band gap is very small or even disappears.

There are more recent exchange and correlations potentials, like the Tran-Blaha functions [TB09], which gives improved band gaps for a variety of insulators and semiconductors.

In a condensed matter system an excited electron and the hole it left behind, referred to collectively as an exciton, move through a sea of all the other electrons and a background of the much heavier ions. The Bethe-Salpeter equation approach [SB51] describes the time evolution of that electron-hole pair. The GW approximation (GWA) is used to calculate the self-energy of a many-body system of electrons [AG00]. The approximation to be made is that the expansion of the self-energy ϵ in terms of the single particle Green's function G and the screened Coulomb interaction W can be approximated to the lowest order term. Both the Bethe-Salpeter equation approach and the GW method

can yield very accurate band gaps, but require very heavy calculations.

The Empirical Pseudopotential Method (EPM) relies on the experimental results to fit a set of parameters used to describe the potentials that act on the electrons. This has the advantage that, if the programming is efficient, the calculations can be made very quickly, and therefore a very large number of atoms can be included in the simulation cell. There are although “dangers” in this method, since it is very tempting to use a model with a big number of parameters that fit very well to the experience but don't have any physical meaning, since with a large number of parameters we can fit anything.

The method we are going to use is the an EPM with only a few parameters with physical meaning, to be fit to experiment. It is possible for the band gap to be adjusted very precisely.

There is no black box in this work! This means that everything is rederived from the beginning, since this is a research project with pedagogical purposes. For this reason, the software used is written MATHEMATICA, since the programs are closer to the mathematical equations.

2. Background

2.1. The pseudopotential method

The pseudopotential model describes a solid as a sea of valence electrons moving in a periodic background of cores. The space can be divided into two regions: the region near the nuclei, the “core”, composed primarily of tightly bound core electrons which are not very affected by the neighbour atoms, and the valence electron region which is involved in bonding the atoms together. This results that the atoms in the same group - such as Carbon, Silicon and Germanium (group IV, for ex.) are treated in mostly the same way - apart from a few “details”. The focus of the calculation is only on the accuracy of the valence electron wavefunction away from the core. The potential in the ion core is strongly

attractive for the valence electrons, but the requirement for the valence wavefunctions to be orthogonal to those of the core contributes to an effective repulsive potential for valence states. This results in a net weakly attractive potential that affects the valence electrons.

2.2. Empirical Pseudopotential method

The Empirical Pseudopotential Method (EPM) relies on experimental results for the construction of the pseudopotential and the predictions made with the pseudopotentials should converge as best as possible with experience.

Lets assume first that the pseudopotential is local, i.e., independent of ℓ . The Schrödinger equation for an electron in an effective potential $V(\vec{r})$ is [Che96]

$$\left(-\frac{1}{2}\nabla^2 + V(\vec{r})\right)\psi_{\vec{k}}(\vec{r}) = E(\vec{k})\psi_{\vec{k}}(\vec{r}). \quad (1)$$

In a crystal, the potential $V(\vec{r})$ is periodic in the lattice and has a Fourier expansion

$$V(\vec{r}) = \sum_{\vec{G}} V(\vec{G}) S(\vec{G}) e^{i\vec{G} \cdot \vec{r}}, \quad (2)$$

where \vec{G} is a reciprocal lattice vector, $V(\vec{G})$ are the form factors and $S(\vec{G})$ is the structure factor,

$$S(\vec{G}) = \frac{1}{N_a} \sum_{i=1}^{N_a} e^{i\vec{G} \cdot \vec{r}_i}. \quad (3)$$

Once the form factors are decided, we solve (1). We can assume that the wave functions $\psi_{\vec{k}}(\vec{r})$ can be expanded in plane waves, with no loss of generality and solve the secular equation, which is the Schrödinger equation (1) in the reciprocal space [Che96] [AM76],

$$\det |H(\vec{k}, \vec{G} - \vec{G}') - E(\vec{k})I| = 0, \quad (4)$$

where

$$H(\vec{k}, \vec{G} - \vec{G}') = \frac{1}{2}(\vec{k} - \vec{G})^2 \delta_{\vec{G}, \vec{G}'} + V(\vec{G} - \vec{G}') S(\vec{G} - \vec{G}'). \quad (5)$$

For tetrahedral semiconductors, the pseudopotential can generally be taken as spherically symmetric. In the Chelikowsky-Cohen pseudopotential [Che96], for diamond or zinc-blende semiconductors, generally only three form factors are enough to determine the pseudopotential, those for $G^2 = 3\left(\frac{2\pi}{a}\right)^2, 8\left(\frac{2\pi}{a}\right)^2, 11\left(\frac{2\pi}{a}\right)^2$. These three values are fitted to optical transition energies and the whole band structure follows from them. The method is the following:

1. Estimate initial $V(|\vec{G}|)$
2. Solve secular equation
3. Calculate band structure and optical properties
4. Compare with experiment
5. If it agrees with experiment stop. If not change $V(|\vec{G}|)$ and start from 2.

The difference between this work and that previous one is, since we are going to describe superlattices, we need to fit the whole curve of the potential, because in a superlattice the \vec{G} vectors may not be constant. As a consequence we have many values of $|\vec{G}|$ for which we require $V(|\vec{G}|)$. Like in the work of reference [WZ95], we will be adjusting an empirical expression to experimental results, but the number of parameters used will be much less and each one will have a physical meaning.

2.3. Non-local and Spin-Orbit Pseudopotentials

If we take into account the spin-orbit effects, we can obtain pseudo-wave-functions $R_{\ell j}^{\text{PP}}(r)$, with energies $\varepsilon_{\ell j}$ and normalization $\int_0^\infty r^2 |R_{\ell j}^{\text{PP}}(r)|^2 dr = 1$ that are constructed from the respective all-electron wave-functions [TM91]. From the inversion of the radial Schrödinger equation we obtain the correspondent ionic pseudopotentials $V_{\ell j}^{\text{PP}}(r)$. The index j takes the values $\ell \pm \frac{1}{2}$, except for $\ell = 0$, where the only allowed value is $j = \frac{1}{2}$. It is in this distinct pseudopotentials for $j = \ell - \frac{1}{2}$ and $j = \ell + \frac{1}{2}$ that the effect of the spin-orbit is included in the calculations, as the major spin-orbit effect is in the core region, since the dominant contribution comes from the motion of electrons in the Coulomb potential in the innermost region of the atomic cores. To restrict the non-local part of the pseudopotential to the core region we define a local potential $V^L(r)$ that is arbitrary in the core region, and is identical to the pseudopotentials $V_{\ell j}^{\text{PP}}(r)$ outside the core region ($V^L = V_{\ell j}^{\text{PP}}$ for $r > r_c$). We define the non local pseudopotential as

$$\Delta V_{\ell j}^{\text{NL}}(\vec{r}) = V_{\ell j}^{\text{PP}}(\vec{r}) - V^L(\vec{r}). \quad (6)$$

The non-local part of the pseudopotential for $\ell > \ell_{\max}$ can be neglected as long as the local part and ℓ_{\max} reasonably chosen.

It is convenient also to separate the pure spin-orbit part from the average non-local pseudopotential, because the spin-orbit can often be treated as a small perturbation, which is often not the case of the non-local component. We therefore define for $\ell > 0$ the degeneracy weighted average

$$\Delta V_{\ell}^{\text{NL}}(\vec{r}) = \frac{\ell}{2\ell+1} \Delta V_{\ell\ell-\frac{1}{2}}^{\text{NL}}(\vec{r}) + \frac{\ell+1}{2\ell+1} \Delta V_{\ell\ell+\frac{1}{2}}^{\text{NL}}(\vec{r}), \quad (7)$$

and the spin-orbit part

$$\Delta V_{\ell j}^{\text{SO}}(\vec{r}) = \Delta V_{\ell j}^{\text{NL}}(\vec{r}) - \Delta V_{\ell}^{\text{NL}}(\vec{r}). \quad (8)$$

In its semi-local form the action of the pseudopotential operator on a spinor is, in a compact notation

$$V^{\text{PP}} = V^L + \sum_{\ell} \sum_m |\ell m\rangle V_{\ell}^{\text{NL}} \langle \ell m| + \sum_{\ell} \sum_j \sum_{m_j} |\ell j m_j\rangle V_{\ell j}^{\text{SO}} \langle \ell j m_j|, \quad (9)$$

where $|\ell m\rangle$ and $|\ell j m_j\rangle$ are angular momentum states, the first with just orbital components the second with the composition of the orbital and spin angular momenta. Semi-local means that it is non-local in the angular but not radial coordinates.

From the computational point of view, the semi-local form of the pseudopotential is less efficient than the full non local form. The procedure of Kleinman and Bylander allows the construction of a fully non-local potential [TM91, TH01, KB82],

$$V_{KB} = \sum_{\ell, m} \frac{|\Delta V_{\ell}^{\text{NL}} \Phi_{\ell, m}^{\text{PP}}\rangle \langle \Phi_{\ell, m}^{\text{PP}} \Delta V_{\ell}^{\text{NL}}|}{\langle \Phi_{\ell, m}^{\text{PP}} | \Delta V_{\ell}^{\text{NL}} | \Phi_{\ell, m}^{\text{PP}} \rangle}, \quad (10)$$

where $\Phi_{\ell, j, m_j}^{\text{PP}}(r, \theta, \phi) = R_{\ell j}^{\text{PP}}(r) Y_{\ell m}(r, \theta, \phi)$.

In the absence of spin terms, we first define a function, referred to as “projector” in the literature. In the EPM, for the non-local part of the potential, we use

$$a_{\ell m}(r, \theta, \phi) = f_{\ell}(r) Y_{\ell m}(\theta, \phi), \quad (11)$$

and

$$V^{\text{KB}} = \sum_{\ell=0}^{\ell_{\max}} \sum_{m=-\ell}^{\ell} |a_{\ell m}\rangle \text{sgn}(b_{\ell}) \langle a_{\ell m}|, \quad (12)$$

where $\text{sgn}(b_{\ell})$ determines if the potential is attractive or repulsive. Considering spin-orbit effects we have for the case $m_j = \pm(\ell + \frac{1}{2})$

$$\begin{aligned} a_{\ell \ell + \frac{1}{2} \ell + \frac{1}{2}}(r, \theta, \phi) &= f_{\ell, \ell + \frac{1}{2}}(r) \begin{pmatrix} Y_{\ell \ell}(\theta, \phi) \\ 0 \end{pmatrix} \\ a_{\ell \ell + \frac{1}{2} - (\ell + \frac{1}{2})}(r, \theta, \phi) &= f_{\ell, \ell + \frac{1}{2}}(r) \begin{pmatrix} 0 \\ Y_{\ell - \ell}(\theta, \phi) \end{pmatrix}, \end{aligned}$$

and for the other case

$$\begin{aligned} a_{\ell \ell + \frac{1}{2} m_j}(r, \theta, \phi) &= f_{\ell, \ell + \frac{1}{2}}(r) \begin{pmatrix} \sqrt{\frac{2\ell+1+2m_j}{4\ell+2}} Y_{\ell m_j - \frac{1}{2}}(\theta, \phi) \\ \sqrt{\frac{2\ell+1-2m_j}{4\ell+2}} Y_{\ell m_j + \frac{1}{2}}(\theta, \phi) \end{pmatrix} \\ a_{\ell \ell - \frac{1}{2} m_j}(r, \theta, \phi) &= f_{\ell, \ell - \frac{1}{2}}(r) \begin{pmatrix} \sqrt{\frac{2\ell+1-2m_j}{4\ell+2}} Y_{\ell m_j - \frac{1}{2}}(\theta, \phi) \\ \sqrt{\frac{2\ell+1+2m_j}{4\ell+2}} Y_{\ell m_j + \frac{1}{2}}(\theta, \phi) \end{pmatrix}, \end{aligned} \quad (13)$$

for which the pseudopotential is calculated,

$$V^{\text{KB}} = \sum_{\ell=0}^{\ell_{\max}} \sum_{j=|l-\frac{1}{2}|}^{l+\frac{1}{2}} \sum_{m_j=-j}^j |a_{\ell m}| \text{sgn}(b_{\ell}) \langle a_{\ell m} \rangle, \quad (14)$$

and $f_l(r)$ and $f_{\ell j}(r)$ are empirical functions.

3. Implementation

3.1. Local pseudopotential

The solid has the diamond crystal structure. The whole crystal has the size $N_1 \vec{a}_1 \times N_2 \vec{a}_2 \times N_3 \vec{a}_3$, where \vec{a}_i are the primitive lattice vectors. To solve the secular equation (4) we use a plane wave basis

$$\langle \vec{r} | \vec{k}, \vec{G} \rangle = \frac{1}{\sqrt{V_{\text{crystal}}}} e^{i(\vec{k} + \vec{G}) \cdot \vec{r}} \quad (15)$$

in which $\vec{k} = \frac{i_1}{N_1} \vec{b}_1 + \frac{i_2}{N_2} \vec{b}_2 + \frac{i_3}{N_3} \vec{b}_3$ with $i_j = 0, \dots, N_j - 1$ and $\vec{G} = I_1 \vec{b}_1 + I_2 \vec{b}_2 + I_3 \vec{b}_3$ is a reciprocal lattice vector to calculate the matrix elements of the kinetic energy operator and \vec{b}_i are the primitive lattice vectors for a fcc lattice. This basis functions are orthogonal among them. The kinetic energy operator will be a diagonal matrix

$$-\frac{1}{2} \nabla^2 \langle \vec{k}, \vec{G} \rangle = \frac{1}{2} |\vec{k} + \vec{G}|^2 \langle \vec{k}, \vec{G} \rangle \quad (16)$$

We start by choosing a simple analytical form for the unscreened local pseudopotential,

$$V_{\text{local}}(r) = -\frac{4}{r} \text{erf}\left(\frac{r}{R_a}\right) + \frac{16\pi}{q_z^2} (\sqrt{\pi} R_a)^{-3} e^{-\frac{r^2}{R_a^2}}. \quad (17)$$

The $-\frac{4}{r}$ (Figure 1, blue line) is the Coulomb potential of the nucleus plus the core electrons for the group IV atoms. The $\text{erf}\left(\frac{r}{R_a}\right)$ (Figure 1, yellow line) term, when it multiplies the Coulomb term, smooths the potential in the origin, so it doesn't diverge as $r \rightarrow 0$ (Figure 1, green line) and $\text{erf}\left(\frac{r}{R_a}\right) \rightarrow 1$ for $r \gg R_a$. We add variational freedom by adding a gaussian function (Figure 1, red line). The strange prefactor will be explained later. The result is the purple line of Figure 1.

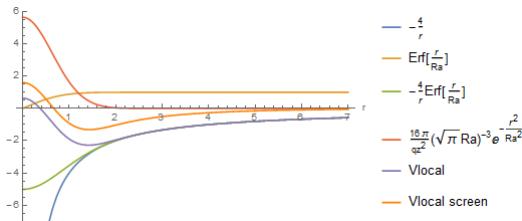


Figure 1: The graphic shows the functions that compose the local pseudopotential and the pseudopotential itself, unscreened and screened

Performing a Fourier transform of this function we get with the local pseudopotential in the reciprocal space,

$$\begin{aligned} V_{\text{local}}(k) &= \int_0^{2\pi} \int_0^\pi \int_0^{+\infty} V_{\text{local}}(k) j_0(kr) r^2 \sin(\theta) dr d\theta d\phi = \\ &= 4\pi \int_0^{+\infty} V_{\text{local}}(k) j_0(kr) r^2 dr = \\ &= 16\pi \left(\frac{1}{q_z^2} - \frac{1}{k^2} \right) e^{-\frac{k^2 R_a^2}{4}}. \end{aligned} \quad (18)$$

We see now that the parameter q_z is when we have $V_{\text{local}}(q_z) = 0$. To obtain the screened pseudopotential we use a very simple Thomas-Fermi screening [Kit76]

$$\epsilon(k) = 1 - \frac{\rho_{\text{ind}}(k)}{\rho(k)} = 1 + \frac{k_{TF}^2}{k^2} \quad \text{with} \quad k_{TF}^2 = \frac{3}{2} n_0 \frac{e^2}{\varepsilon_F \epsilon_0}, \quad (19)$$

obtaining,

$$V_{\text{local,screen}}(k) = \frac{V_{\text{local}}(k)}{\epsilon(k)} = 16\pi \left(\frac{k^2}{q_z^2} - 1 \right) \frac{e^{-\frac{k^2 R_a^2}{4}}}{k^2 + k_{TF}^2}. \quad (20)$$

R_a , q_z and k_{TF} are the parameters to be adjusted to experiment.

3.2. Non local pseudopotential

In expression (11), for the function $f_{\ell}(r)$, consistent with the local form of the pseudopotential and satisfying the desired conditions, we choose again a Gaussian,

$$f_{\ell}(r) = B_{\ell} r^{\ell} e^{-\frac{r^2}{R_b^2}}, \quad (21)$$

where B_{ℓ} and R_b are constants to be adjusted. The reason for including the term r^{ℓ} comes from when $r \rightarrow 0$, $R_{\ell}(r) \rightarrow r^{\ell}$ (eq. (10)). This expression has an analytical Fourier transform,

$$\begin{aligned} F_{\ell}(k) &= \int_0^{+\infty} r^2 j_{\ell}(kr) B_{\ell} r^{\ell} e^{-\frac{r^2}{R_b^2}} dr \\ &= R_b^{\ell} B_{\ell} \frac{\sqrt{\pi} R_b^3}{4} \left(\frac{R_b r}{2} \right)^{\ell} e^{-\frac{R_b^2 k^2}{4}}, \end{aligned} \quad (22)$$

We are going to search for the parameters R_a , q_z and k_{TF} to the local potential from equation (17) and for the parameters R_b and B_{ℓ} to the non-local potential from equation (21). We are going to start for scratch, which means we are lost in a 5-dimensional space of 5 parameters to adjust, without knowing where to start with. So in the beginning, we are going to be based in the LDA pseudopotentials generated with the program from reference [SF] and fit the functions to the pseudopotentials to obtain the first parameters we will work with. We only will use $\ell_{\max} = 0$, so we will use only $Y_{00} = \frac{1}{\sqrt{2\pi}}$ in equation (11) and the projector a_{00} is

$$a_{00}(r) = \frac{1}{\sqrt{2\pi}} B_0 e^{-\frac{r^2}{R_b^2}}, \quad (23)$$

and its 3D Fourier transform

$$A_{00}(k) = \frac{1}{4} B_0 e^{-\frac{1}{4} k^2 R_b^2} \sqrt{\pi} R_b^3. \quad (24)$$

3.3. Spin-Orbit contribution

For the function $f_{\ell j}$ in equation 13 we choose again a gaussian,

$$f_{\ell j} = C_{\ell j} r^{\ell} e^{-\frac{r^2}{R_c^2}}. \quad (25)$$

If the degeneracy averaged perturbation is zero, we have

$$C_{\ell \ell + \frac{1}{2}} = \sqrt{\frac{\ell}{\ell + 1}} C_{\ell \ell - \frac{1}{2}}, \quad (26)$$

and

$$\text{sgn}(b_{\ell\ell+\frac{1}{2}}) = -\text{sgn}(b_{\ell\ell-\frac{1}{2}}) = -1, \quad (27)$$

and we use $\ell_{max} = 2$ because with spin orbit we describe also the contribution of the core electrons, which in Germanium also take part the d ($\ell = 2$) orbitals.

3.4. Density of states

To calculate the density of states and the optical properties it requires the calculation of the eigenvalues and vectors on a cubic grid. First we calculate the density of states,

$$D(E) = \lim_{\sigma \rightarrow 0} \lim_{N_1, N_2, N_3 \rightarrow \infty} \frac{1}{N_1 N_2 N_3} \sum_n \sum_{i_1} \sum_{i_2} \sum_{i_3} G_\sigma(E - E_n(\vec{k}_{i_1, i_2, i_3})), \quad (28)$$

where

$$G_\sigma(E) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{1}{2}(\frac{E}{\sigma})^2}. \quad (29)$$

The joint density of states is also calculated

$$J(E) = \lim_{\sigma \rightarrow 0} \lim_{N_1, N_2, N_3 \rightarrow \infty} \frac{1}{N_1 N_2 N_3} \sum_v^4 \sum_c \sum_{i_1} \sum_{i_2} \sum_{i_3} G_\sigma[E - (E_c(\vec{k}_{i_1, i_2, i_3}) - E_v(\vec{k}_{i_1, i_2, i_3}))], \quad (30)$$

where the indices v and c are correspondent to the valence and conduction bands, respectively.

3.5. Optical properties

We calculate the imaginary part $\epsilon_2(\omega)$ of the dielectric function using [Yu,96]

$$\epsilon_2(\omega) = \left(\frac{2\pi e}{m\omega} \right)^2 \sum_{\vec{k}} |P_{cv}|^2 \delta(E_c(\vec{k}) - E_v(\vec{k}) - \hbar\omega), \quad (31)$$

and the real part $\epsilon_1(\omega)$ from the Kramers-Kroning relation[Lan80]

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{+\infty} \frac{\xi \epsilon_2(\xi)}{\xi^2 - \omega^2} d\xi. \quad (32)$$

4. Results

The search for the pseudopotentials that will describe the elements Si, Ge and C in bulk will be proceeded as follows: We will first fit our theoretical model, the parameterized functions of equations (20) and (24) for the local and non-local pseudopotentials, respectively to an *ab initio* LDA pseudopotential, generated with [SF]. After this fitting, the pseudopotential will be further adjusted to the experimental band structure. Afterwards, the optical properties of each of this elements will be calculated.

4.1. Silicon

For Silicon we use a local and non local pseudopotential with $\ell_{max} = 0$. We start the search by fitting the parameterized functions of equations (20) and (24) to the LDA pseudopotentials of Silicon. After this fit, for both potentials, we find the parameters on Table 1.

R_a	q_z	k_{TF}	R_b	B_0
0.93	2.17	0.54	0.85	10.2

Table 1: The obtained parameters for Silicon after adjusting to the LDA pseudopotentials

After we adjust the results to the experience. The experimental of the band structure are shown in Figure 2 a).

After the process of fitting to experience, the final parameters are on Table 2.

R_a	q_z	k_{TF}	R_b	B_0
0.972	2.17	0.62	1.06	6.1

Table 2: The final parameters for the pseudopotential of Silicon where obtained after adjusting to the experiment

With this parameters we calculate the band-structure (Figure 2 b), the transitions represented on Figure 2 b) (Table 7), the density of states (Figure 3 a)), the joint density of states, b), the dielectric function, c), which we compare to the experiment d)e), and the reflectance, f), that we compare to the experiment as well g).

4.2. Carbon

The same thing was done for the pseudopotentials of Carbon. The results are on Tables, 3 and 4.

R_a	q_z	k_{TF}	R_b	B_0
0.19	5.69	0.70	0.54	46.5

Table 3: The obtained parameters for Carbon after adjusting to the LDA pseudopotentials

R_a	q_z	k_{TF}	R_b	B_0
0.21	5.73	0.70	0.555	47.04

Table 4: The final parameters for the pseudopotential of Carbon where obtained after adjusting to the experiment

The band structure and the optical properties were calculated and are represented on Figures 2 d) and 4, and Table 8.

4.3. Germanium

With Germanium we used not only the local and the non local part of the pseudopotential but also the spin orbit contribution, since it is an heavier element. We used $\ell_{max} = 0$ for the non-local part and $\ell_{max} = 2$ for the spin-orbit. To search for the local and the non-local pseudopotentials we did as previously for Silicon and Carbon. The results are on Table 5.

R_a	q_z	k_{TF}	R_b	B_0
0.94	1.83	0.52	0.71	10.5

Table 5: The obtained parameters for Germanium, used to be adjusted to the experimental values on Figure 2 e)

After we introduce the spin-orbit splitting. We set $R_c = R_b$ and adjust $C_{\ell j}$ in a way that the splitting of the most energetic valence bands is $T_0 = 0.296$. This value is $C_{\ell j} = 0.279$ for all ℓ and j . The parameters used to draw the band structure (Figure 2 f)), calculate the energy transitions indicated on Figure 2 c) (Table 9) and calculate the optical properties of Germanium (Figure 5) are on Table 6

R_a	q_z	k_{TF}	R_b	B_{00}	R_c	$C_{\ell j}$
0.94	1.83	0.52	0.74	12.0	0.71	0.279

Table 6: The final parameters for the pseudopotential of Germanium where obtained after adjusting to the experiment

5. Conclusions

In this research project we obtained a description of bulk Silicon, Carbon and Germanium, group IV elements, using the Empirical Pseudopotential Method. We obtained a successful description for Silicon, since the band structure was pretty well adjusted, and we did that by using parameters in a pseudopotential model that have physical meaning. The reflectance and the imaginary part of the dielectric function could be better, but the calculation of this properties allowed us to diagnose a problem with the band structure that was drawn. As a future work, the pseudopotential should also be adjusted to the experimental reflectance data. For Germanium, the results are similar to Silicon. The band structure and the density of states was pretty well adjusted to the experimental values, but in the future we should also try to adjust to the optical properties such as reflectance, to obtain better results. To Carbon (Diamond), we obtained the least successful description, since it was very difficult to adjust the band structure with just a small number of parameters. This element requires some extra work and, in the future the research could go into finding a pseudopotential model with more parameters to describe it.

All the tools where developed to continue this research and improve each of the descriptions. As a next step we can introduce the pseudopotentials in a FORTRAN program and increase the number of points in the cubic grid, to obtain better results. After having the best description possible of each of the elements, as a future research the pseudopotentials will be used to be introduced in a supercell composed with these elements. This was already tested for a Si₂₉C supercell, a supercell of Si with a C impurity. Figure 6 shows the calculated unfolded band structure for that system.

With an improvement of the fit to the optical properties, these EPM could be used to search for the material with the best optoelectronic properties that is compatible with Si technology.

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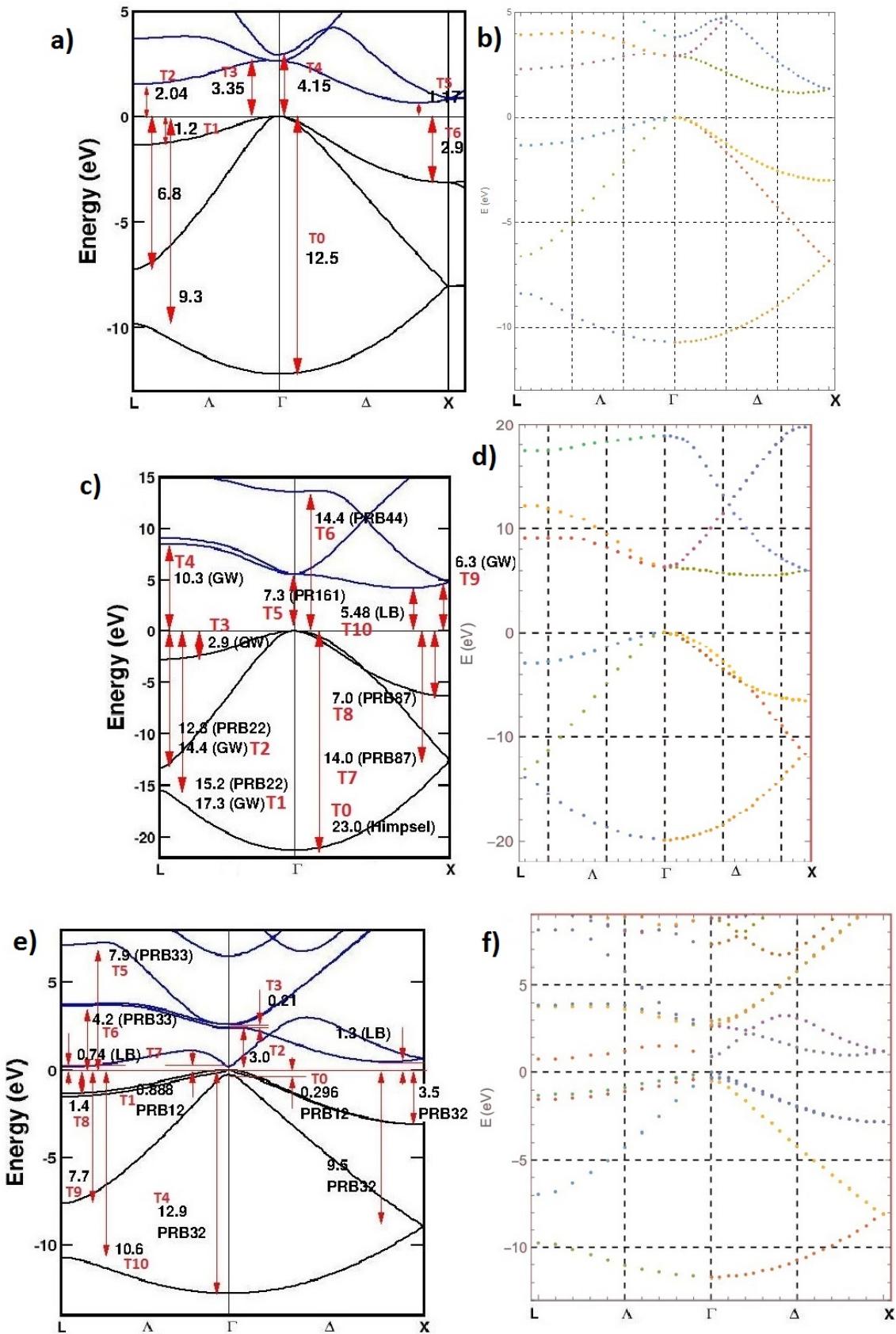


Figure 2: The figure shows the band structure of Silicon a) calculated using LDA with the values of some important transitions in eV, from [ea] and b) calculated using the parameters on Table 2, the band structure of Carbon c) form reference [ea] with the values of some important transitions in eV and d) calculated with the parameters in Table 4 and the band structure of Germanium d) using reference [ea] and with the values of some important transitions in eV, e) with the program, using the parameters of Table 6

	T_0	T_1	T_2	T_3	T_4	T_5	T_6
Experience	12.5	1.2	2.04	3.35	4.15	1.17	2.9
Calculated	10.7	1.3	2.29	3.91	3.83	1.17	3.0

Table 7: Experimental and calculated in the current work transitions of Silicon in eV are calculated with the parameters on Table 2

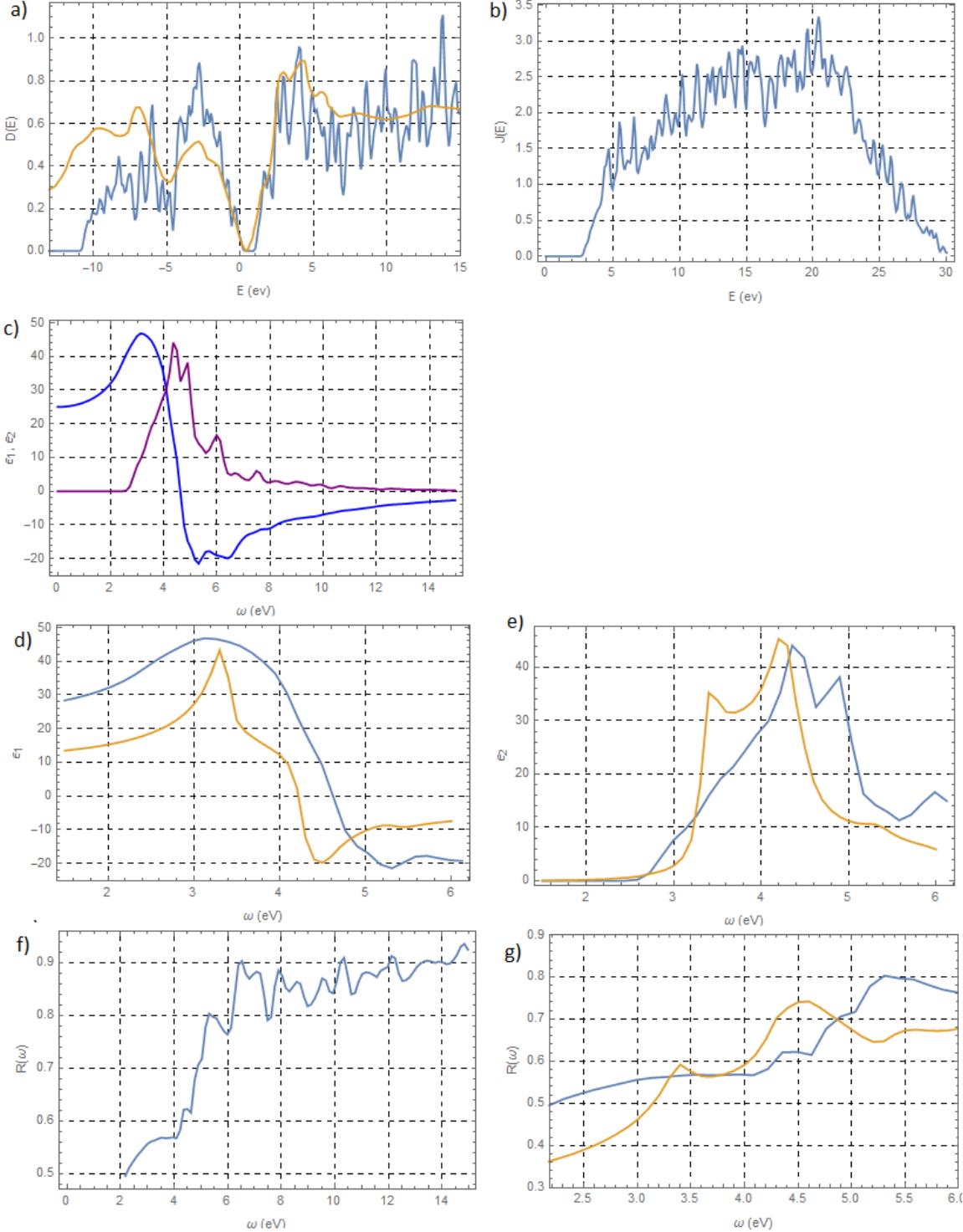


Figure 3: It is represented a) the calculated density if states (blue line),the photo emission spectroscopy and inverse photo emission data obtained from reference [Che89] (yellow line), b) the calculated joint density of states, c) calculated dielectric function, d) calculated (blue line) and experimental (yellow line, [AS83]) ϵ_1 , e) calculated (blue line) and experimental (yellow line, [AS83]) ϵ_2 f),g) calculated (blue line) and experimental (yellow line, [AS83]) reflectance for Silicon with the local pseudopotential of equation (17) and non-local projector for the pseudopotential of equation (23) with the parameters written in Table 2

	T_0	T_1	T_2	T_3	T_4	T_5	T_6	T_7	T_8	T_9	T_{10}
Experience	23.0	17.3	14.4	2.9	10.3	7.3	14.4	14.0	7.0	6.3	5.48
Calculated	19.8	13.9	13.1	2.9	9.1	6.3	18.8	11.6	6.5	6.1	5.48

Table 8: Experimental and calculated in the current work transitions of Diamond in eV , calculated with the parameters on Table 4

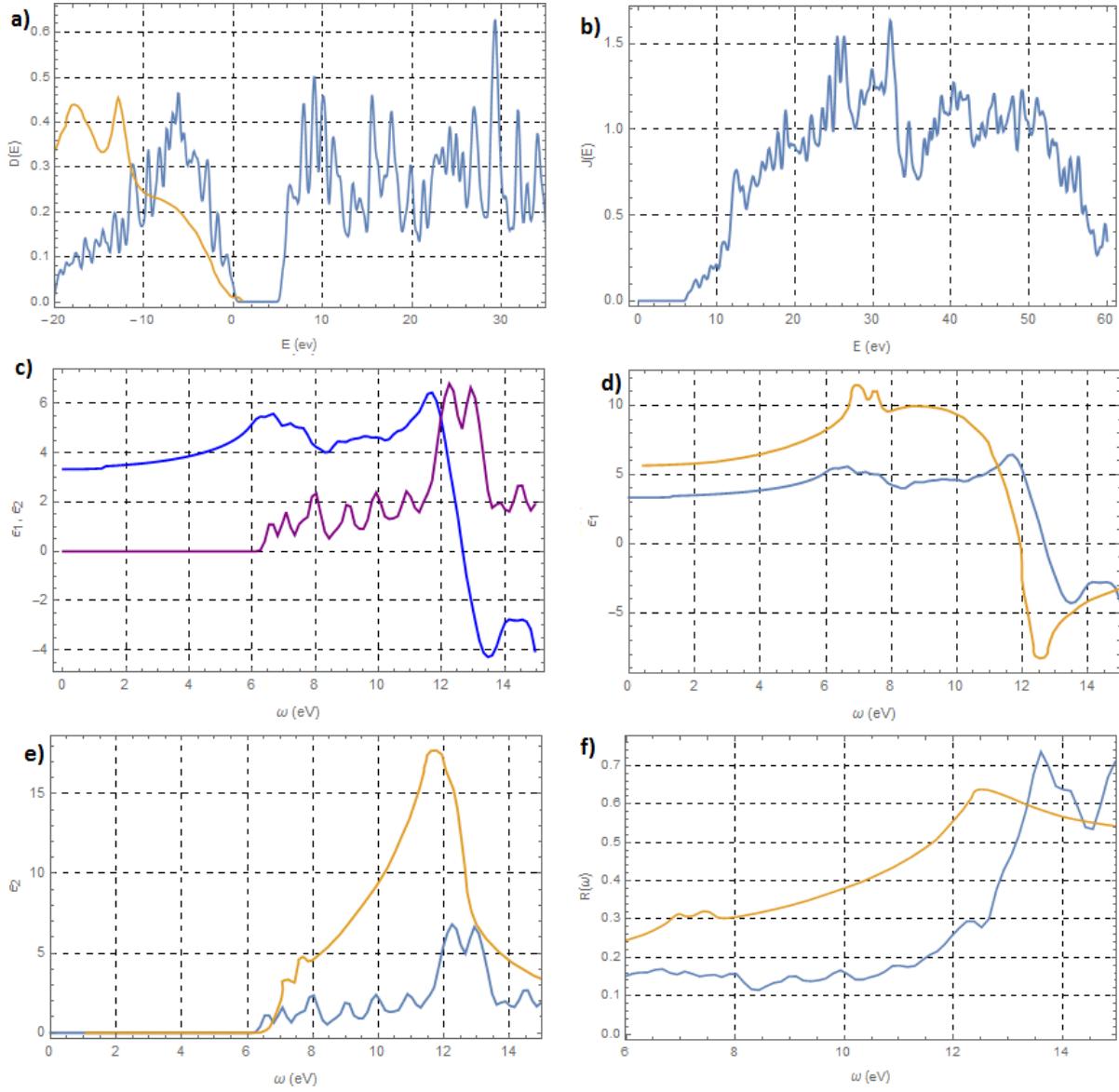


Figure 4: It is represented the a) DOS of Carbon, calculated here (blue line), the photo emission spectroscopy data from reference [ea74] (yellow line) divided by a factor of 20, b) the calculated joint density of states, the c) real part (blue line) and imaginary part (purple line) of the dielectric function, d) the comparison between the calculated (blue) and experimentally obtained (yellow, [RW67]) ϵ_1 , e) comparison between the calculated (blue) and experimental (yellow, [RW67]) ϵ_2 and f) the calculated (blue) and experimentally obtained (yellow, [RW67]), divided by a factor of 100, reflectance. The parameters on Table 4 were used in the calculations

	T_0	T_1	T_2	T_3	T_4	T_5	T_6	T_7	T_8	T_9	T_{10}	LB	PRB32	PRB32
Experience	0.296	0.888	3.0	0.21	12.9	7.9	4.2	0.74	1.4	7.7	10.6	1.3	3.5	9.5
Calculated	0.296	0.882	2.6	0.23	11.7	8.1	3.8	0.76	1.3	6.9	9.8	1.0	2.9	8.1

Table 9: Important optical transitions of Germanium where calculated in eV using the parameters of Table 6

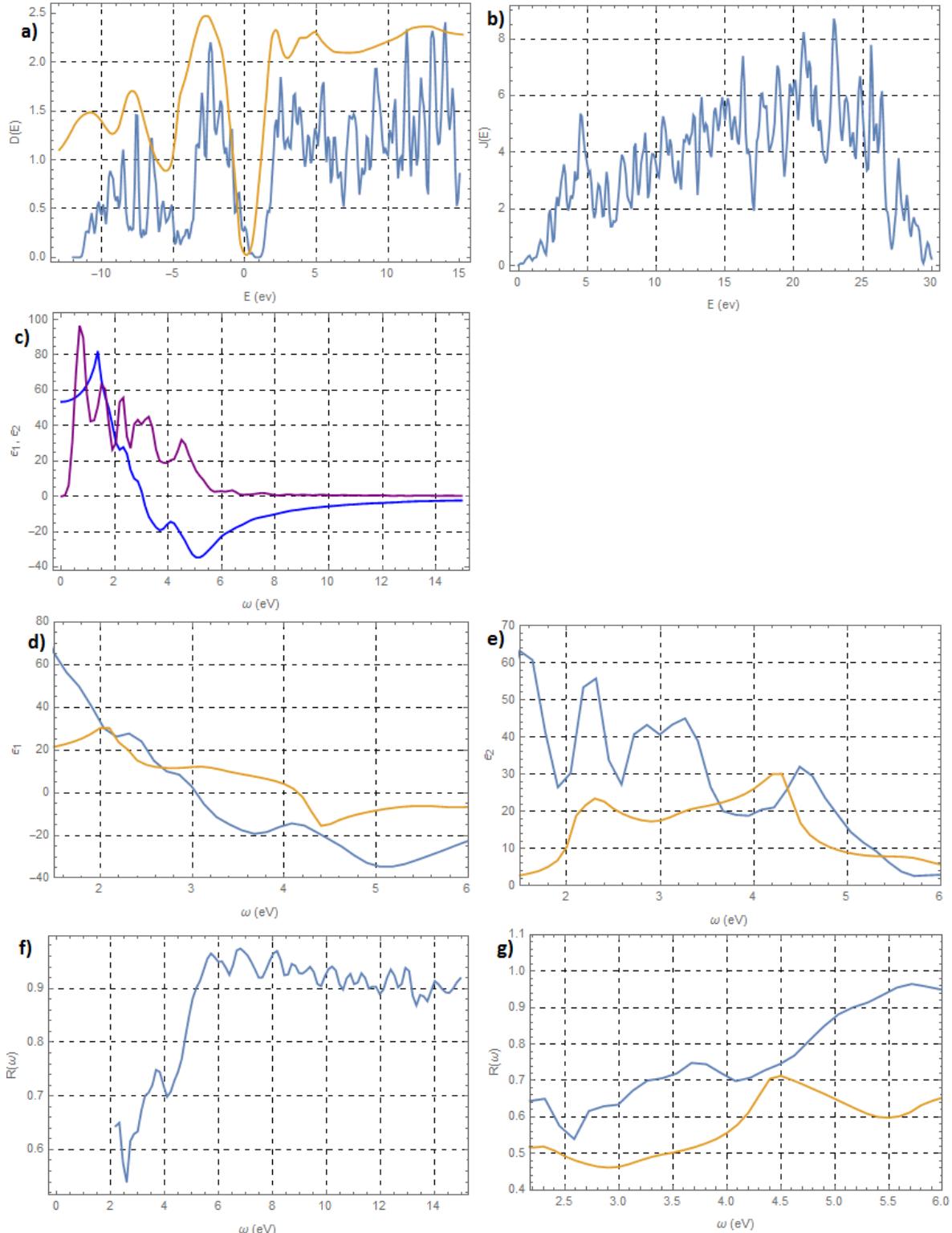


Figure 5: It is represented a) the calculated density if states (blue line),the photo emission spectroscopy and inverse photo emission data obtained from reference [Che89] (yellow line) divided by a factor of 3, b) the calculated joint density of states, c) calculated dielectric function, real part (blue) and imaginary (purple), d) calculated (blue line) and experimental (yellow line, [AS83]) ϵ_1 , e) calculated (blue line) and experimental (yellow line, [AS83]) ϵ_2 , f,g) calculated (blue line) and experimental (yellow line, [AS83]) reflectance for Germanium with the local pseudopotential of equation (17), the non-local projector for the pseudopotential of equation (23) with the parameters written in Table 6 and the spin-orbit projectors using equations (13) and (25-27) with $l_{max} = 2$

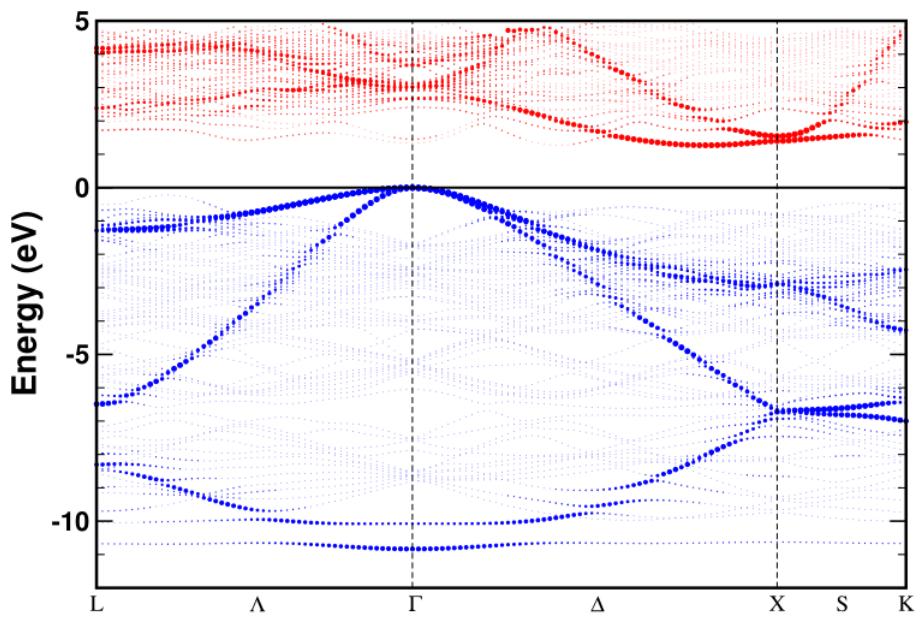


Figure 6: The figure shows the unfolded band structure of $Si_{29}C$