



Research Article

Ab-initio Study of the Optoelectronic Properties of a Semiconductor Under the Influence of an External Electric Field: The Case of Silicon (Si)

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Abstract

DFT calculations are performed on the structural, electronic, and optical properties of fcc silicon (Si). The plane wave (PW) method using Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) exchange correlation potentials is applied to solve the Kohn-Sham equations. Energy convergence was examined to study ground-state properties. Band structure and total density of states (TDOS) diagrams are plotted from the calculated equilibrium lattice parameters. An electric field on the order of $E=0$ V/Å and $E=1$ V/Å is applied to the silicon surface. Band structure and energy density of Si at electric field $E=0$ V/Å and $E=1$ V/Å is studied in this paper. We also studied variation of the Fermi energy of Si as a function of the applied electric field. On simulate real part of the dielectric function $\epsilon_1(\omega)$ and Imaginary part of the dielectric function $\epsilon_2(\omega)$ as a function of the photon energy for Si with electric field $E=0$ V/Å and $E=1$ V/Å (10 GV/m). General profiles of the optical spectra under ambient conditions with and without an electric field are calculated. This study shows that applying an electric field normal to the surface of silicon modifies its electronic and optical properties. The band gap of silicon contracts, with the appearance of band degeneracy. The peak amplitude of its absorption coefficient, the dielectric function and the refractive index decrease in the ultraviolet range and increase in the visible range.

Keywords

Silicium, Ab-initio, DFT Calculations, TDOS

1. Introduction

Optical properties play a crucial role in understanding the nature of materials and inform their use in optoelectronic devices. Applying a strong external electric field to the surface of a semiconductor is expected to induce significant changes in band structures and, consequently, in the material's optical properties [1].

Applying an intense electrostatic field to silicon can induce

a modification of its band structure, a phenomenon often linked to the Stark effect or structural polarization in nanoscale devices (such as nanowires or ultrathin films) [2, 3].

The resulting reduction in the band gap width offers several strategic advantages for electronic and optoelectronic components [4-6].

In this work, we consider the case of silicon subjected to

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fields of $E=0$ V/Å and $E=1$ V/Å. The objective is to study the electronic and optical properties and the energy modification of states at the silicon surface under these conditions, specifically the optical properties, the band gap, and the total density of states (TDOS), using ab initio calculations with the QANTUM ESPRESSO software. Fundamental principles calculations are used to study the influence of applying an electric field on the electronic structure and optical properties of silicon. In the case of an electric field (E_z) normal to the silicon crystal surface, a perturbation of the electron Hamiltonian by the electrostatic potential is expected. This leads to the modification of the system's Hamiltonian H according to the following equation:

$$H = H_0 + eE_z$$

Where H_0 is the Hamiltonian of the system without an external electric field.

Our article can be summarized as follows: Section 2 presents the details of the calculations and a brief description of the calculation method. Section 3 presents the results of this calculation. Finally, the conclusions are presented in Section 4.

2. Methology

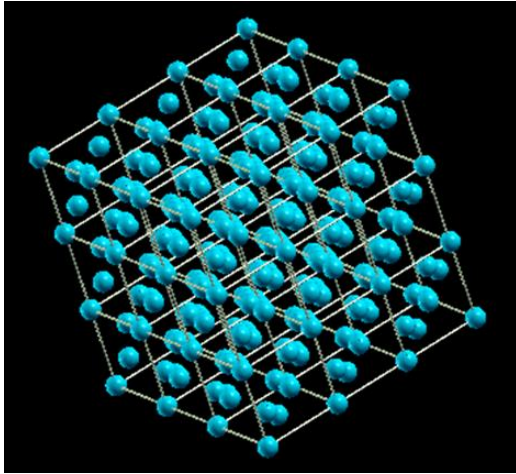


Figure 1. Structure of the silicon crystal lattice for 280 Si atoms.

We performed first-principles calculations based on density functional theory (DFT) to predict the electronic and optical properties of silicon Si. All DFT calculations reported in this manuscript are obtained using the Quantum ESPRESSO suite [7], with plane-wave expansion and norm-preserving relativistic scalar pseudopotentials [8]. The electron exchange and correlation functionals were treated using the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation [9, 10]. The system under study is a fcc cube with periodic boundary

conditions. After a convergence test, a plane-wave basis kinetic energy cutoff of 30 Ry, a $4 \times 4 \times 4$ Monkhorst-Pack k-point uniform mesh [11], and the equilibrium lattice parameter $a = 5.486$ Å are used. We introduce an electric field in the (z) direction normal to the plane of the Si crystal and then discuss how the band structures change under the effect of this external electric field.

It is generally accepted that the interaction of a photon with the electrons of the system can be described by temporal perturbations of the ground electronic states. The transitions between occupied and unoccupied states are caused by the electric field of the photon. The spectra resulting from these excitations can be described as a joint density of states between the valence and conduction bands.

The optical response of a material to the electromagnetic field, at all energy levels, can be described by the complex dielectric function $\varepsilon(\omega)$ as follows:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

Where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real and imaginary parts of the dielectric function. The real part of the dielectric function represents the scattering of incident photons by the material, while the imaginary part of the dielectric function corresponds to the energy absorbed by the material. The calculation of these components of the dielectric function is associated with the energy eigenvalue and the energy wave functions, which are the direct output of the band structure calculation. From knowledge of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, all other optical properties, such as reflectivity $R(\omega)$, refractive index $n(\omega)$, extinction coefficient $\kappa(\omega)$, energy loss function $L(\omega)$, absorption coefficient $\alpha(\omega)$, and optical conductivity $\sigma(\omega)$, can be calculated [12].

$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

Where n and k are respectively the real and imaginary parts of the complex refractive index.

$$n(\omega) = \frac{\sqrt{\left(\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega)\right)}}{\sqrt{2}}$$

$$k(\omega) = \frac{\sqrt{\left(\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right)}}{\sqrt{2}}$$

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)}$$

$$\alpha(\omega) = \omega\sqrt{2} \sqrt{\left(\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right)}$$

$$\Re[\sigma(\omega)] = \frac{\omega}{4\pi} \varepsilon_2(\omega)$$

3. Results and Discussion

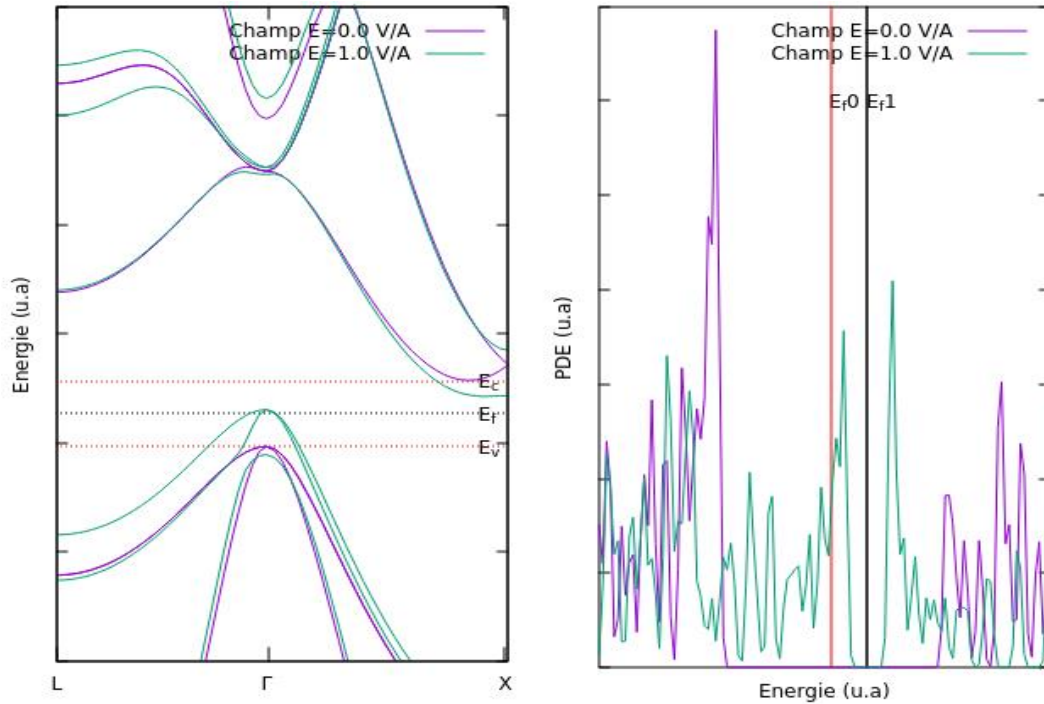


Figure 2. Band structure and energy density of Si at electric field $E=0$ V/Å and $E=1$ V/Å.

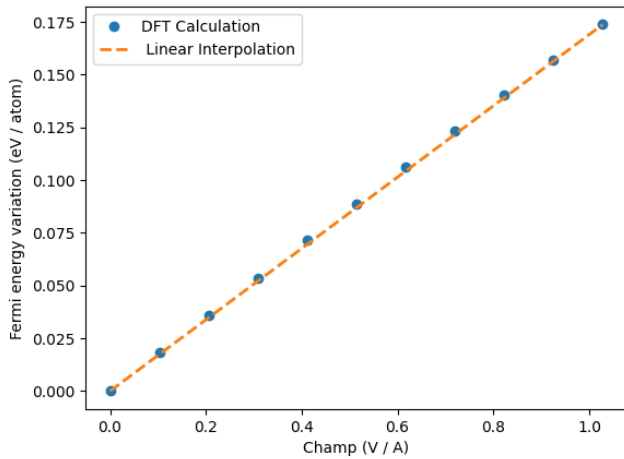


Figure 3. Variation of the Fermi energy of Si as a function of the applied electric field. The Fermi level follows the following relationship: $E_f = E_{f0} + 0.169E_z$, where E_z is the electric field strength and E_{f0} is the Fermi energy with zero electric field.

The electronic properties of Si are studied using the band structure and the total density of states (TDOS) calculated with optimized values [10]. Spin-unpolarized calculations are performed [13]. The calculations are carried out along the L- Γ -X top symmetry points in the Brillouin zone. Our results in Figure 2 show a contraction of the band gap between the valence and

conduction band states, leading to a significant curvature of the band structure at a strong electric field of 1 V/Å. We also observe the emergence of new energy states (degeneracy) and the Fermi level shift under the effect of this applied electric field [14]. Figure 3 shows that this Fermi level shift follows a linear law with the amplitude of the electric field. This is due to the electric polarizability, which is proportional to the E_z field. The maximum of the valence band E_V and the minimum of the conduction band E_C are located at points Γ and X, respectively, resulting in an indirect band gap. $E_V = 5.9638$ and $E_C = 6.5703$ without a field, and $E_V = 6.3025$ and $E_C = 6.4249$ at $E_z = 1$ V/Å. Therefore, the band gap of undoped Si is $E_g = 0.6056$ eV without an electric field. This band gap value, lower than the experimental value of 1.12 eV for pure Si, is expected because the DFT calculation with Quantum Espresso systematically underestimates energy gaps. When the electric field increases from 0 to 1 V/Å, the band gap decreases from 0.6056 eV to 0.1224 eV, a reduction of $x = 79.79\%$. Therefore, the predicted experimental value of the band gap is $1.12(1-x/100)$, or 0.2223 eV under an E_z field of 1 V/Å. The band gap response of silicon under the influence of an electric field modifies the electronic properties of silicon. We observe that the inclusion of E_z changes the energy level of silicon. Consequently, under the effect of E_z on the order of a few tenths of a V/μ, the band gap still indicates the semiconducting properties of silicon. Thus, the band gap can be significantly controlled by the influence of E_z .

Figure 2b illustrates the total density of states of silicon as

a function of E_Z . The description of these states defines the conductive properties of silicon. The state of all atoms in the silicon crystal structure near the Fermi level is primarily derived from the 3pz orbital of silicon 3p. Due to the decrease in

band gap energy, the probability of occupation of electrons near the Fermi level increases.

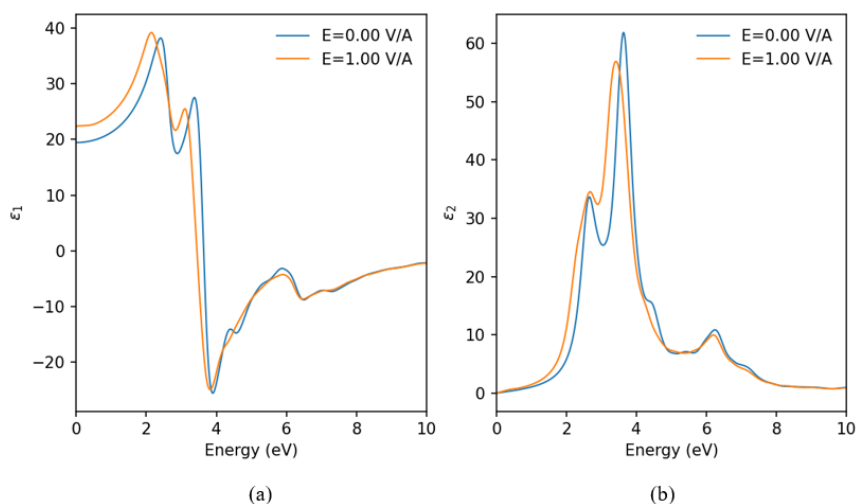


Figure 4. (a) Real part of the dielectric function $\epsilon_1(\omega)$ and (b) Imaginary part of the dielectric function $\epsilon_2(\omega)$ as a function of the photon energy for Si with electric field $E=0$ V/Å and $E=1$ V/Å i.e. 10 GV/m.

Figure 4 shows the complex dielectric function $\epsilon(\omega)$ as a function of frequency in the range of 0 to 10 eV. It describes the optical properties of silicon interacting with light. Its real part, $\epsilon_1(\omega)$, determines the dispersion effects, and its imaginary part, $\epsilon_2(\omega)$, determines the absorption effects.

It can be observed that under the effect of E_Z , the peaks of $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ increase in the visible region while they decrease in the UV region. These results demonstrate the ability of silicon to absorb photons in the visible range when E_Z is applied in the Z direction normal to the crystal surface. The

$\epsilon_2(\omega)$ portion exhibits two prominent peaks in the range of 2 to 10 eV, related to interband transitions. The maximum peak is recorded for an incident photon energy of 3.79 eV, where absorption is maximal. It is important to note that for values of $\epsilon_2(\omega) = 0$, at low energy and towards the end of the UV there is no absorption, because electrons cannot react at E_Z . The value of the static dielectric constant (the value of the dielectric constant at zero energy) $\epsilon_1(0)$ is 19.4475 without an electric field and 22.2660 at $E_Z = 1$ V/Å.

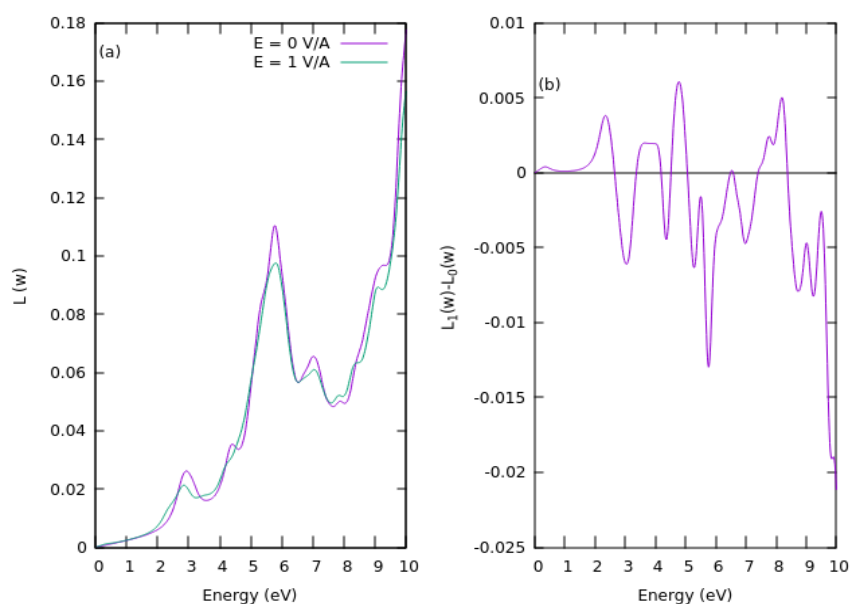


Figure 5. Energy loss function $L(\omega)$ as a function of photon energy for Si with electric field $E=0$ V/Å and $E=1$ V/Å.

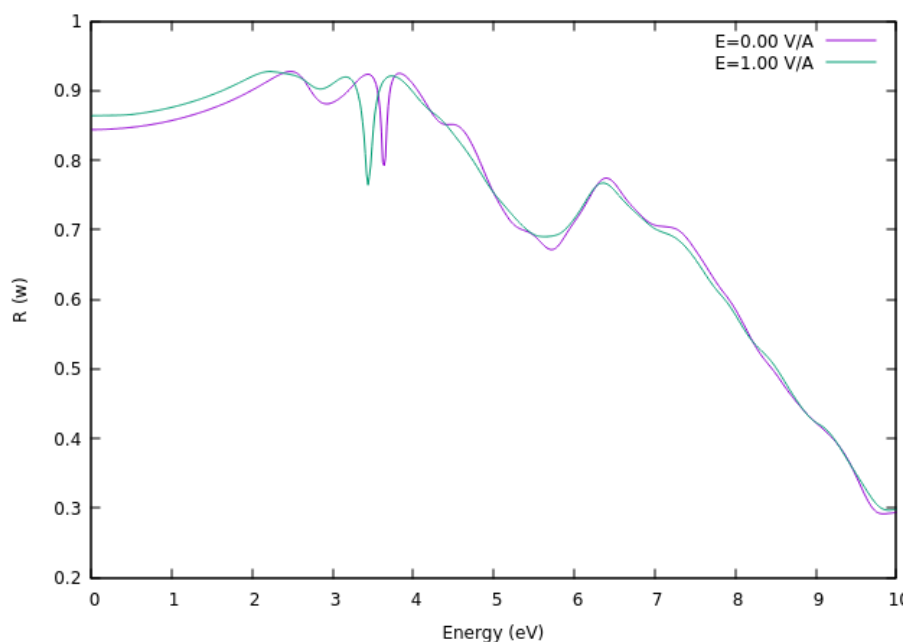


Figure 6. Reflectivity spectra $R(\omega)$ as a function of photon energy for Si at electric field $E=0 \text{ V/\AA}$ and $E=1 \text{ V/\AA}$.

Figures 5 and 6 show the reflectivity and energy loss spectra of silicon. Reflectivity is significant at low photon energies. The reflectivity of pure silicon as a function of the applied electric field is illustrated in Figure 6. It can be seen that the reflectivity is higher at low energies, therefore the transition

probability is lower at low energies. The static refractive index (the refractive index value at zero energy) is 4.40208 without an external electric field, while it is 4.7330 when an electric field is applied, as shown in Figure 7a.

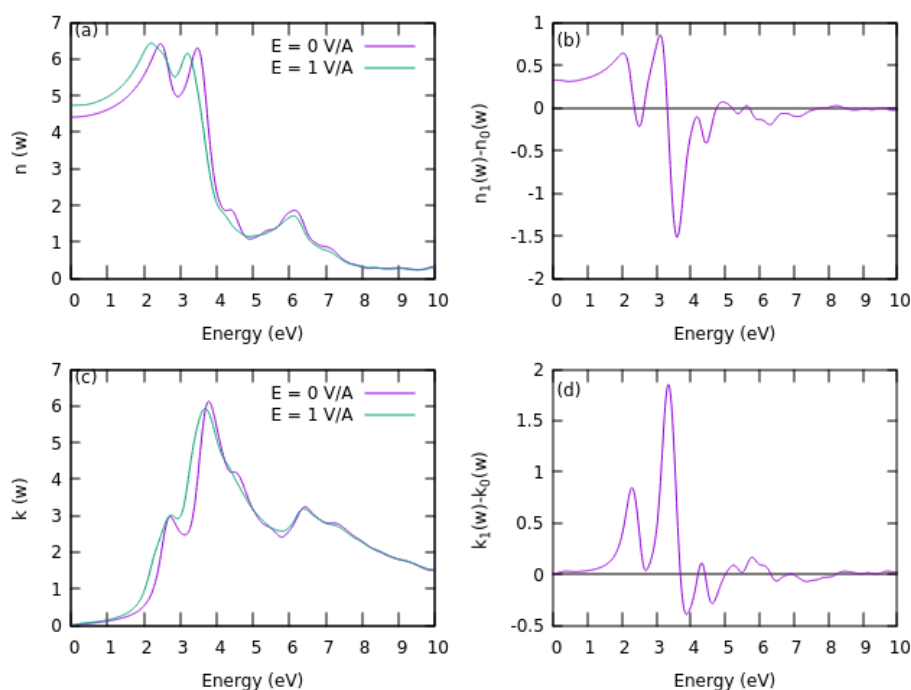


Figure 7. (a), (b) real part of the refractive index and (c), (d) Imaginary part of the refractive index as a function of the photon energy for Si, at electric field $E=0 \text{ V/\AA}$ and $E=1 \text{ V/\AA}$.

Figure 6 illustrates the complex refractive index $n^*(\omega) = n(\omega) + ik(\omega)$ of Si, which describes the propagation of light in

this absorbing material. The imaginary part $k(\omega)$ deals with attenuation, while the real part $n(\omega)$ deals with refraction [15].

The above values of the static dielectric constant $\epsilon_1(0)$ and the static refractive index $n(0)$ satisfy the relation $n = \sqrt{\epsilon_1}$ (Table 1). When E_z is applied to the surface of Si, the part $n(\omega)$ varies with frequency. Therefore, Si is a dispersive material, and its dispersion is affected by E_z . The refractive index increases in the visible and decreases in the ultra violet (UV), because the application of E_z causes collisions and interactions between incident photons and electrons within Si. Furthermore, the component $k(\omega)$ increases in the visible. Analysis of the graphs of $\epsilon_2(\omega)$ and $k(\omega)$ shows similar physical behavior in Figures 5 and 6. These two physical quantities provide information on the absorption of light by the Si crystal structure. Without an external E_z field, the absorption spectrum consists of three peaks of different intensities. The intensity of the first peak is 2.71 eV, that of the second is 3.79 eV, and that of the third is 6.44 eV [16]. The first two peaks originate from two fundamental (interband) transitions between the electronic states of Si. The first peak corresponds to the transition from the occupied to the unoccupied state in the conduction band. The second peak corresponds to the Si-Si transition from the π - π^* state near the Fermi level in the sp^3 hybrid region [17]. The third peak originates from the intraband transition. Based

on these three peaks, the Si crystal exhibits strong light absorption, capable of absorbing in the visible and UV ranges. In the visible range, the intensity of the absorption peak increases when a voltage $E_z = 1 \text{ V/\AA}$ is applied in the z-direction normal to the Si crystal, due to the decrease in the band gap energy. When E_z is applied, it causes a shift of the absorption peak towards the infrared (IR) range, due to the decrease in the band gap energy [16]. This behavior suggests that E_z can be used effectively to tune the absorption of Si. Furthermore, its application to Si increases its light absorption capacity in the visible range. According to our absorption spectrum calculation results, silicon possesses optical properties dependent on the effect of E_z .

Table 1. The static dielectric constant $\epsilon_1(0)$ and the static refractive index $n(0)$ of Si under an external electric field E_z .

$E \text{ (V/\AA)}$	0	1
$n(0)$	4.40208	4.7330
$\epsilon_1(0)$	19.4475	22.2660

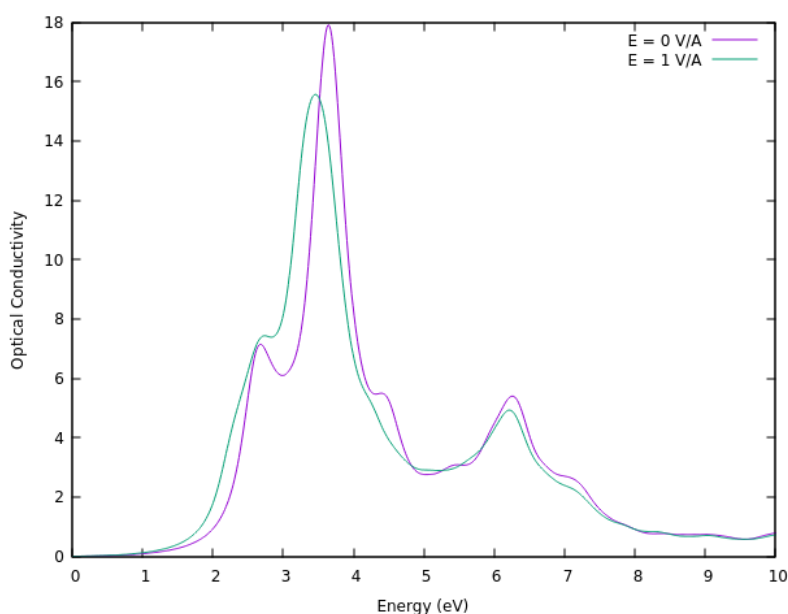


Figure 8. Optical conductivity $\sigma(\omega)$ as a function of photon energy for Si at electric field $E=0 \text{ V/\AA}$ and $E= 1 \text{ V/\AA}$.

4. Conclusion

This ab initio study quantified the impact of an external electric field ($E_z=1 \text{ V/\AA}$) on the properties of silicon.

Applying the field induces a strong perturbation of the Hamiltonian, resulting in an 80% band gap contraction (from 0.61 to 1.12 eV) and the lifting of band degeneracy. The Fermi

level exhibits a linear shift proportional to the field intensity.

The band gap reduction promotes increased absorption in the visible range, while a decrease is observed in the ultraviolet. This intensity shift towards lower energies (redshift) is confirmed by the evolution of the imaginary parts of the dielectric function $\epsilon_2(\omega)$ and the refractive index $k(\omega)$.

By validating the relation $n \approx \sqrt{\epsilon_1}$ under a strong electric field, we demonstrated the consistency of our calculations.

In summary, these results demonstrate that silicon, under the influence of an intense electric field, becomes an optically tunable material. This property paves the way for the design of electro-optical modulators and controlled absorption photovoltaic devices.

Abbreviations

PWX	Plane Wave
PBE	Generalized Gradient Approximation
GGA	Perdew-Burke-Ernzerhof
TDOS	Total Tensity of States
DFT	Density Functional Theory

Conflicts of Interest

The authors declare no conflicts of interest.

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