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ORIGINAL RESEARCH ARTICLE

Synthesis of hybrid semiconductors based on modified polyethylene and $SrTiO_3$ with improved electronic and optical properties

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ABSTRACT

The fabrication of hybrid semiconducting materials comprising polymers and ceramics is a novel approach that has gained significant traction for designing multifunctional materials with improved electronic and optical properties. In this research, the design of a heterojunction hybrid material comprising polyethylene (PE) and Strontium Titanate ($SrTiO_3$) was explored through extensive simulations using Materials Studio. $SrTiO_3$ nanoparticles were dispersed in the polyethylene matrix at specific filler loadings to analyze the structural compatibility and charge-transfer phenomenon between the two constituents. The structural analysis showed increased structural compatibility and stability in the hybrid system, with improved molecular packing and reduced free volume at the interface. Electronic properties analysis revealed a heterojunction formed by the interaction between PE and $SrTiO_3$, which altered the band structure, reduced the energy gap, and improved charge-carrier mobility compared to pristine polyethylene.

Keywords: $SrTiO_3$; polyethylene; hybrid semiconductors; structural properties; electronic properties; optical properties

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1. Introduction

With the rapid development of semiconductor technologies, the quest for innovative hybrid materials that offer flexibility, cost-effectiveness, and enhanced functional performance is gaining momentum. In this regard, polymeric-inorganic hybrid semiconductor systems are among the most attractive material systems owing to their adjustable properties and complementary benefits arising from the integration of organic and inorganic components[1].

One example of a readily available, highly stable polymer is polyethylene (PE), among many other commonly employed materials such as polystyrene (PS), polyvinyl alcohol (PVA), and polymethyl methacrylate (PMMA). Polyethylene (PE) possesses several advantages, including low dielectric losses, mechanical flexibility, affordable price, and availability in the industry. Besides, PE constitutes a chemically resistant matrix material for incorporating inorganic particles like $SrTiO_3$ into the matrix. However, despite the electrical insulating property of pure PE, the formation of a heterojunction between PE and oxide semiconductors could change its electrical and optical properties. featured by such benefits as mechanical flexibility, workability, and minimal dielectric losses. At the same time, its inherent insulating properties limit its use in electronics and optoelectronics. One efficient way to overcome this challenge is to use oxide semiconductor fillers to enhance the electrical and optical properties of polymers[2-4]. Among many inorganic compounds, strontium titanate ($SrTiO_3$), an oxide semiconductor of the perovskite type, has gained popularity for its distinctive electronic properties, high dielectric constant, and adjustable electronic band structure. Strontium titanate is considered a representative oxide for oxide electronics and has been extensively investigated for photocatalysis, sensing, and optoelectronics. Strontium titanate exhibits exceptional properties, including the ability to form heterostructures with other materials, thereby enabling efficient charge separation and transport. Furthermore, strontium titanate-based heterojunctions exhibit pronounced improvement in photodetection efficiency owing to charge distribution at the interface[5,6].

The phenomenon of heterojunction formation is extremely important for improving the efficiency of semiconductor devices by enabling effective charge-carrier separation and reducing recombination. Through heterojunction formation in p-n or type-II configurations, the creation of an internal electric field allows for directional charge transport. It enhances the electronic and optical behaviour of the materials. Heterojunction research using $SrTiO_3$ has demonstrated that, when combined with appropriate compounds, the efficiency of photocatalysis, photoelectrochemistry, and electrochemistry can be markedly enhanced, owing to improved bandgap alignment, increased active surface area, and enhanced carrier transport properties[7,8].

Recent developments in the use of polymer matrices combined with semiconducting nanostructures have led to innovative strategies for developing flexible, lightweight electronic hybrid materials. In this regard, by combining $SrTiO_3$ nanoparticles with polymer matrices such as polyethylene, we can achieve new hybrid heterojunction structures whose material properties are determined by the interfaces. Some potential advantages of these hybrids may include superior dielectric properties, greater optical absorptivity, and an altered electronic band structure compared to those of isolated materials. It is worth noting that some oxide thin films, in combination with polymers, have been found to exhibit high mechanical flexibility, among other favorable electrical properties[9].

Though considerable advancements have been made in hybrid semiconductor materials, little has been done on the synthesis and characterization of polyethylene-$SrTiO_3$ heterojunction systems. For instance, previous studies have shown that organic-inorganic hybrids exhibit tailorable electrical and optical properties; however, achieving uniform dispersion of ceramic particles within polymer blends and manipulating interfacial phenomena can be difficult[9]. In $SrTiO_3$-containing hybrids, problems such as particle agglomeration, poor interfacial adhesion, and inefficient charge-transport processes may compromise device functionality. Moreover, the construction of efficient heterojunctions with optimized band alignments and charge mobility in polymer hybrids is a relatively new concept [10]. Thus, a comprehensive study of the structure-property relationships of the polyethylene-$SrTiO_3$ hybrid system is crucial to unravel its potential electronic and optoelectronic capabilities[10]. This research concerns the synthesis of polyethylene-based $SrTiO_3$ heterojunction hybrid semiconductors using both theoretical and experimental methods. The objective of the study is to understand the structural arrangement, band alignment, and optical characteristics of the semiconductor alloy. Through the integration of heterojunction technology and the interaction between polymers and inorganic materials, this research sheds light on the potential of flexible hybrid semiconductors and their applications in advanced electronic devices[11,12].

2. Materials and methods

Polyethylene (PE) was selected as the polymer matrix due to its maximum availability, low price, chemical stability, flexibility, and widespread use in electronic insulation systems. The polymer model was constructed using a linear chain of repeating –CH_2– units in an all-trans configuration to represent crystalline polyethylene segments. The inorganic component, strontium titanate ($SrTiO_3$), was modeled in its cubic perovskite phase (space group $Pm\bar{3}m$), which is its most stable structure at room temperature. The initial crystal structure parameters were obtained from standard crystallographic databases and validated against literature values. To construct the hybrid heterojunction, a slab model of $SrTiO_3$ (001) surface was generated with periodic boundary conditions in the x-y plane and a vacuum layer of approximately 15-20 Å along the z-direction to eliminate spurious interactions between periodic images. The polyethylene chain was placed above the $SrTiO_3$ surface and geometrically aligned to form an interface suitable for interaction analysis. The initial interface distance was set to 3-4 Å to allow relaxation during optimization. All structural models were built using the *Materials Studio* software package. The crystal structure of the polyethylene (PE) material, strontium titanate ($SrTiO_3$), and the heterojunction (PE/$SrTiO_3$) were generated and optimized by using the Materials Studio software. The strontium titanate ($SrTiO_3$) crystal structure was generated using the lattice parameters of a = 5.5223 Å, b = 5.5223 Å, and c = 7.8453 Å, while the lattice dimensions used in generating the polyethylene repeating unit (-CH_2-) structure were set at a = 2.44588 Å, b = 4.925811 Å, and c = 7.158763 Å **(Table 1)**. The lattice parameters of the optimized heterojunction (PE/$SrTiO_3$) were observed to be a = 5.224056 Å, b = 4.033444 Å, and c = 36.875659 Å. All lattice structures had lattice angles set at $\alpha = \beta = \gamma = 90°$, implying that orthogonal simulation cells were considered. Geometry optimization of all materials was conducted to ensure that the total energy of the system and other unfavourable atomic interactions were minimized prior to conducting optical property calculations. Periodic boundary conditions were implemented throughout the simulation, and a sufficient interface distance was created.

Table 1. Optimized lattice parameters of $SrTiO_3$- PE heterojunction calculated using GGA–PBE functionals compared with experimental data.

Crystal	A Å	B Å	C Å	α	β	γ
$SrTiO_3$	5.5223	5.5223	7.8453	90	90	90
PE	2.44588	4.925811	7.158763	90	90	90
$SrTiO_3$- PE heterojunction	5.224056	4.033444	36.875659	90	90	90

3. Results and discussion

3.1. Structural Optimization and Interfacial Properties

Figure 1 presents the optimized atomic configurations of the three key components used to construct the hybrid semiconductor system: (a) polyethylene (PE) chain, (b) cubic perovskite $SrTiO_3$ crystal, and (c) the combined PE/$SrTiO_3$ heterojunction. Together, these subfigures illustrate the structural foundation and interfacial interactions that govern the hybrid material's electronic and optical behavior.

In **Figure 1(a)**, the optimized structure of the polyethylene chain is shown within a simulation cell. The polymer backbone consists of repeating –CH_2– units arranged in an all-trans conformation, which represents the energetically favorable configuration for crystalline polyethylene. The hydrogen atoms are symmetrically distributed around the carbon backbone, minimizing steric hindrance and stabilizing the chain through σ-bonding interactions. The large space in the simulation box reflects the low density and insulating nature of polyethylene, which is characterized by a wide band gap and the absence of intrinsic charge carriers. This structural simplicity and chemical stability make PE an ideal matrix for hosting inorganic fillers, although its electronic inactivity necessitates modification for semiconductor applications.

Figure 1(b) depicts the cubic crystal structure of $SrTiO_3$, a well-known perovskite oxide semiconductor. In this structure, titanium (Ti) atoms occupy the middle of oxygen (O) octahedra, forming TiO_6 units, while strontium (Sr) atoms are positioned at the corners of the cubic lattice. The periodic arrangement of these atoms results in a highly symmetric structure (space group $Pm\bar{3}m$), which is responsible for its excellent dielectric and electronic properties. The strong Ti–O bonding interactions and the overlap between the O 2p and Ti 3d orbitals are crucial in determining the electronic band structure of $SrTiO_3$. This configuration enables efficient charge transport and contributes to its semiconducting behavior with a band gap of approximately 3.2 eV. The presence of well-defined atomic coordination and periodicity also makes $SrTiO_3$ highly suitable for forming heterojunction interfaces with other materials.

In **Figure 1(c)**, the combined PE/$SrTiO_3$ heterojunction is illustrated, highlighting the interfacial interaction between the polymer and the inorganic semiconductor. The polyethylene chains are positioned above the $SrTiO_3$ (001) surface, forming a layered hybrid structure. The interface is primarily governed by weak van der Waals forces and electrostatic interactions rather than strong covalent bonding. However, despite the absence of strong chemical bonds, the proximity of the polymer chains to the oxide surface enables interfacial electronic coupling. This interaction can induce charge redistribution at the interface, thereby generating an internal electric field that enhances charge separation. The structural arrangement also suggests that the inorganic $SrTiO_3$ phase serves as the primary pathway for charge transport, while the polymer matrix provides mechanical flexibility and structural support. Such hybrid architectures are known to facilitate heterojunction formation, which is essential for improving optoelectronic performance by reducing recombination and enhancing carrier mobility.

Overall, **Figure 1** demonstrates the successful construction and optimization of a polymer inorganic hybrid system, where the distinct structural characteristics of polyethylene and $SrTiO_3$ are preserved while enabling interfacial interaction. The transition from isolated components (a and b) to the integrated heterojunction (c) provides a clear visualization of how structural design at the atomic level can influence the functional properties of hybrid semiconductors. This structural framework serves as the basis for subsequent analysis of electronic structure, charge-transfer behavior, and optical response in the PE/$SrTiO_3$ system.

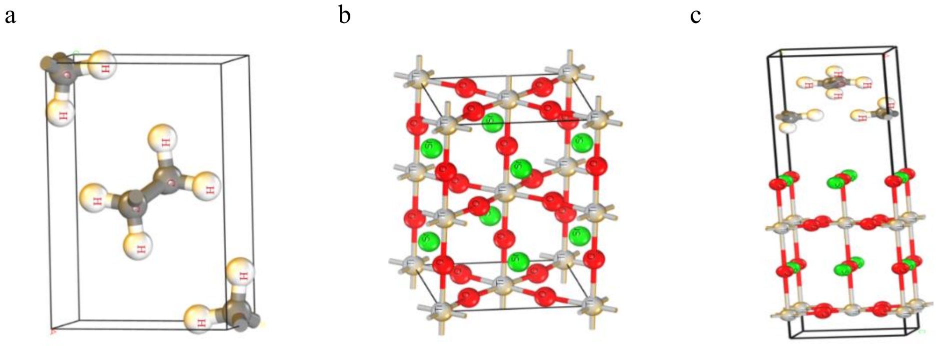

Figure 1. Optimized atomic structures of (a) Poly Ethylene (PE) chain, (b) cubic perovskite $SrTiO_3$, and (c) PE/$SrTiO_3$ hetero junction. The composite structure illustrates the interfacial interaction between the polymer matrix and the inorganic $SrTiO_3$ phase.

3.2. Band Structure Analysis

The band structure refers to the graphic illustration of the permissible energy levels of the electron in the material based on its momentum. This graph provides information about the movement of the electrons from the valence band (VB) to the conduction band (CB). Through band structure, it is possible to find out the physical characteristics of the material, such as whether the material can act as an insulator, conductor, or semiconductor. **Figure 2** illustrates the electronic band structure of the PE/$SrTiO_3$ heterojunction, showing the energy distribution of electrons along the high-symmetry points (G–F–Q–Z–G) in the Brillouin zone. The figure indicates that the heterojunction exhibits a narrow band gap of approximately 0.151 eV, as marked between the conduction band (CB) and valence band (VB) near the Fermi level (EF). The significant reduction in band gap after heterojunction formation suggests enhanced electronic interaction between PE and $SrTiO_3$, which can improve charge carrier mobility and facilitate electron excitation under low-energy photon absorption. This behavior makes the PE/$SrTiO_3$ heterojunction promising for optoelectronic and photocatalytic applications due to its improved electronic conductivity and charge transfer characteristics.

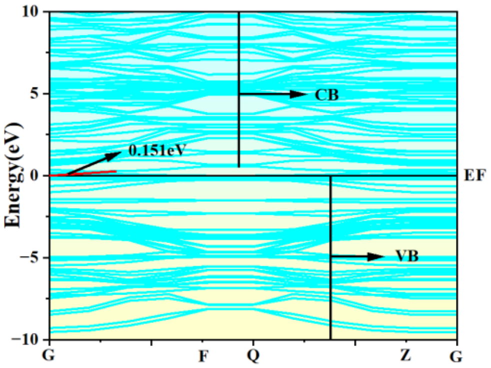

Figure 2. Electronic band structure and band alignment of the PE/$SrTiO_3$ heterojunction. The plot illustrates the distribution of energy states, highlighting the conduction band (CB) and valence band (VB) positions of both PE and $SrTiO_3$. The band gap is observed from the separation between the VB and CB regions, indicating the heterojunction's potential for efficient charge separation and photocatalytic activity.

3.3. The Total Density of States (DOS)

The density of states (DOS) is a fundamental concept in solid-state physics that describes the number of available electronic states at each energy level that electrons can occupy. It helps determine how electrons are distributed in a material and directly influences its electrical, optical, and thermal properties. In DOS plots, the energy is typically shown along the horizontal axis, while the vertical axis represents the number of states. Regions with zero DOS indicate energy gaps (band gaps), while peaks correspond to high availability of electronic states.

The PE/$SrTiO_3$ heterojunction density of states (DOS) has been presented in **Figure 3** below. It shows the electronic state distribution of various energy levels in CH_2 and $SrTiO_3$. The Fermi level is at 0 eV. There are many electronic states that occur near the Fermi level. This shows that there is a good interaction of electrons of PE and $SrTiO_3$ after the formation of heterojunctions. This will provide good electron flow in PE and $SrTiO_3$ because of low band gap values.

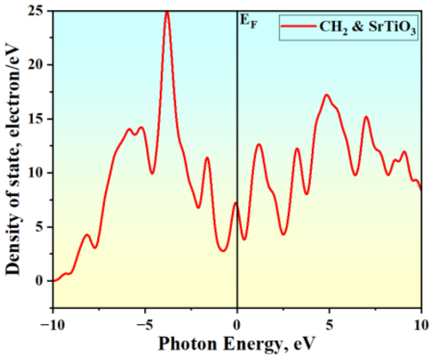

Figure 3. Density of states (DOS) of the PE/$SrTiO_3$ heterojunction showing the contribution of each component near the valence and conduction bands, indicating effective electronic interaction and charge transfer across the interface.

3.4. Projected Density of State (PDOS)

The projected density of states (PDOS) is an extension of the total DOS that decomposes the contribution of specific atoms or orbitals (e.g., s, p, d) to the overall electronic structure. It provides more detailed insight into which elements and orbitals dominate at different energy levels, helping to understand bonding, charge distribution, and the origin of a material's electronic properties.

Figure 4 gives the partial density of states (PDOS) of the PE/$SrTiO_3$ heterojunction, where the influence of each atomic orbital (s, p, d, and f orbitals) on the electronic structures of the material has been illustrated.

The Fermi level (EF) is present at 0 eV. It was seen that the p orbital plays a major role in the valence band area, whereas the d orbital plays the most prominent role in the conduction band area. The overlapping behavior of orbital influences in the vicinity of the Fermi level indicates the existence of high orbital mixing and electronic interactions between PE and $SrTiO_3$, which enhance charge transfers and decrease the bandgap.

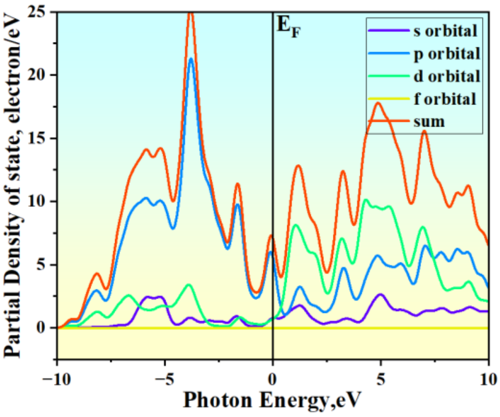

Figure 4. Projected density of states (PDOS) of the $PE/SrTiO_3$ heterojunction, showing orbital contributions from constituent atoms. The valence band is mainly dominated by O 2p and C 2p states, while the conduction band is largely contributed to by Ti 3d states, indicating interfacial electronic interaction and modified charge distribution in the hybrid system.

3.5. Optical Properties

The optical response of the $SrTiO_3$-PE heterojunction was investigated through the frequency-dependent complex dielectric function:

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

Where ε_1 (ω) represents the real part (dispersion) and ε_2 (ω) denotes the imaginary part (absorption). All optical constants, including absorption coefficient, refractive index, reflectivity, optical conductivity, and energy loss function, were derived from ε(ω).

The dielectric properties of $PE/SrTiO_3$ heterojunction show a clear improvement over pure polyethylene due to interfacial polarization and the high dielectric constant of $SrTiO_3$. Polyethylene is a low-k insulating polymer, while $SrTiO_3$ is a high-k dielectric material. When combined, the heterojunction enhances overall polarization under an applied field, increasing the dielectric constant and improving energy storage capability.

Dielectric function shows interaction of the $PE/SrTiO_3$ heterojunctions under illumination and consists of two types: the real part (ε_1) and the imaginary part (ε_2). The real dielectric function (blue graph) shows polarization ability of materials, whereas the imaginary dielectric function (red graph) describes optical absorbance and energy dissipation. According to **Figure 5**, the peaks of ε_1 and ε_2 at low photon energies (0–1 eV) show significant electronic polarization and interband electronic transitions taking place within this range of photon energy. In addition, the ε_1 part obtains rather high values of dielectric constant, which demonstrates good charge polarization in $CH_2/SrTiO_3$ heterojunctions. After the first peak of the dielectric constant, both functions begin their rapid decrease and make a couple of other oscillations from 2 to 8 eV. This process demonstrates interband transitions between valence and conduction bands, but after certain energies, the graphs become flat, which means small photon interactions. Taking into account the significant dielectric response and high absorption ability of the heterojunction at low energies, we can state that it is optically active and has good charge-carrying capacity.

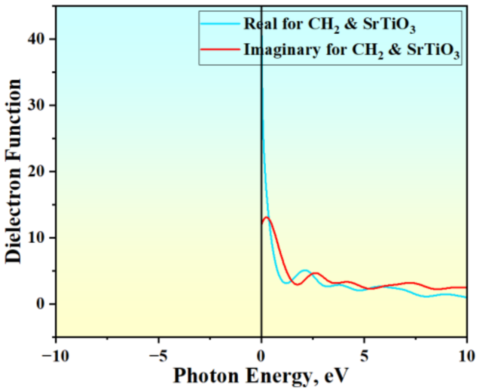

Figure 5. Real (ε_1) and imaginary (ε_2) dielectric functions of the PE/$SrTiO_3$ heterojunction as a function of photon energy, illustrating its polarization behavior and optical absorption characteristics.

The absorption coefficient (α) measures how effectively a material absorbs incident electromagnetic radiation and is directly linked to the imaginary part of the dielectric function, reflecting electronic transitions from the valence to the conduction band. In the CH_2/$SrTiO_3$ heterojunction, absorption is strongly influenced by interfacial charge transfer and band alignment, thereby enhancing light-harvesting efficiency and broadening the optical response.

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c}\left[\sqrt{\varepsilon_1^2 + \varepsilon_2^2} - \varepsilon_1\right]^{1/2}$$

As shown in **Figure 6**, the absorption coefficient of the PE/$SrTiO_3$ heterojunction varies significantly with respect to the photon energy. The absorption coefficient starts increasing from zero til reaching 10 eV and shows a steady increase over an extensive range of energy levels, implying better photon absorption within these energy levels. This can be attributed to the fact that low-energy photons cause weak absorption because there is limited electronic transition due to the lower energy level. However, as the photon energy increases, some peaks and fluctuation regions appear in the plot, which represent the transitions of electrons from the valence band to the conduction band. In the high-energy region, the absorption coefficient exceeds 1×10^5 cm^{-1}, reflecting the efficiency of the heterojunction in harvesting energy from light. This implies that there is strong absorption of photons in the heterojunction system and hence the efficient utilization of ultraviolet and visible light energy. These photons will help generate electron-hole pairs that are needed for catalytic processes.

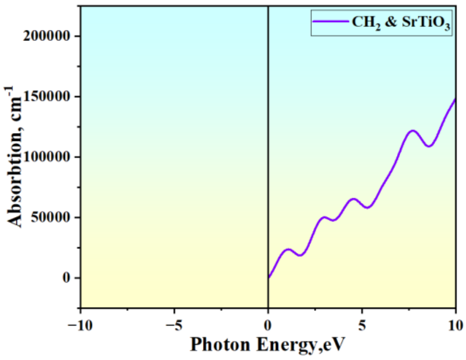

Figure 6. Absorption coefficient (α) of the PE/$SrTiO_3$heterojunction as a function of photon energy, showing strong optical absorption and enhanced light-harvesting capability across a wide energy range.

The electrical conductivity of PE/$SrTiO_3$ heterojunction is significantly improved compared to pure polyethylene due to the formation of an interface that facilitates charge transport. Polyethylene is an insulating polymer with very low conductivity, whereas $SrTiO_3$ is a semiconductor that can support charge carriers under excitation. When combined, the heterojunction creates pathways for electron movement and reduces charge recombination, leading to enhanced conductivity.

As seen from **Figure 7**, the optical conductivity of the PE/$SrTiO_3$ heterojunction is described as a dependence on the photon energy. The real part of the optical conductivity rises with an increase in the energy of the photons used and is positive at all the considered ranges of the photon energy. Some peaks and oscillations recorded for the real conductivity are caused by the interband electronic transitions. As for the imaginary part, it demonstrates the oscillating character of change and takes predominantly negative values. It is concluded that the PE/$SrTiO_3$ hetero structure has good photon-induced properties that can be useful for optoelectronic devices.

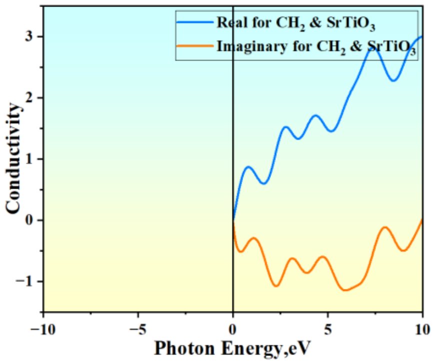

Figure 7. Real and imaginary optical conductivity spectra of the PE/$SrTiO_3$ heterojunction as a function of photon energy, illustrating enhanced photon-induced charge transport and interfacial optical response.

In **Figure 8**, the refractive index spectrum of the PE/$SrTiO_3$ heterojunction has been plotted against photon energy. The real refractive index has a high value in the lower range of photon energies and then rapidly drops until it becomes stable with increasing energy. This signifies a high level of light interaction in the lower range of photon energies. On the other hand, the imaginary refractive index has oscillating values over all ranges of energy, which means that there are fluctuations in the absorption of light by the material, as well as the dissipation of energy.

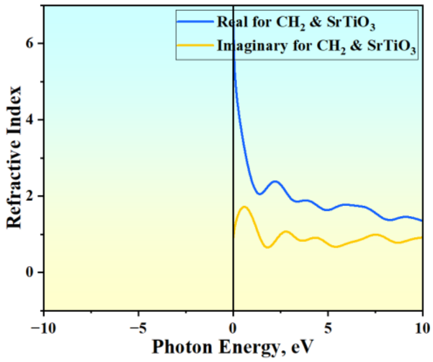

Figure 8. Real and imaginary refractive index spectra of the PE/$SrTiO_3$ heterojunction as a function of photon energy, illustrating dispersion behavior and optical interaction across the interface.

The reflectivity spectrum of the PE/$SrTiO_3$ heterojunction in relation to the photon energy is depicted in **Figure 9**. As shown in the figure, the reflectivity increases at low photon energies, up to a maximum value of about 0.5 at 0 eV, after which it decreases steeply with increasing photon energies. There are various minor peaks and oscillations that occur as photon energies increase, indicating interband electronic transitions and changes in optical properties within the heterojunction. It is evident from the results above that the reflectivity of the material is relatively low at high photon energies, meaning the material can absorb light effectively.

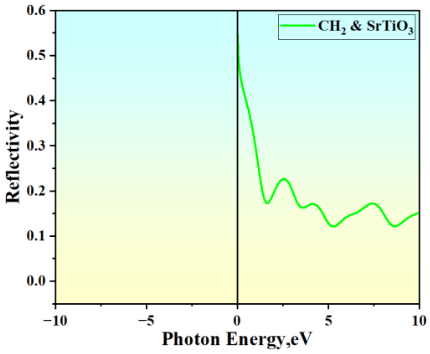

Figure 9. Reflectivity spectrum of the PE/SrTiO$_3$ heterojunction showing variation of reflectivity (Y) as a function of photon energy (X), highlighting reduced reflection and enhanced absorption at higher energies.

The energy loss function (ELF), expressed as In [-1/ε(ω)], describes the rate of electron energy loss and is closely associated with plasmon excitations and interband transitions. For the PE/SrTiO$_3$ heterojunction, the ELF reflects the combined dielectric response of both components and their interface. **Figure 10** displays the energy loss function of the PE/SrTiO$_3$ heterojunction as a function of photon energy. The energy loss function is very close to zero in the negative energy region, but increases gradually when the photon energy enters the positive region. There are small oscillations in the graph, which imply differences in the photon-electron interactions of the heterojunction. This implies that there is a high loss of energy when the photon energy increases. It might be due to the formation of plasmon or other collective electronic excitation modes. Thus, the PE/SrTiO$_3$ heterojunction has relatively low energy loss in the negative photon energy region and increases gradually with an increase in photon energy.

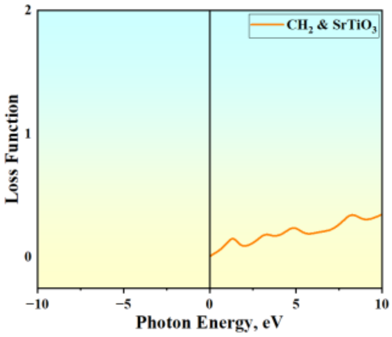

Figure 10. Energy loss function spectrum of the PE/SrTiO$_3$ heterojunction as a function of photon energy, showing plasmonic excitations and interband electronic transitions.

4. Conclusion

In this study, a PE/SrTiO$_3$ hetero-semiconductor was designed and investigated using Materials Studio simulations and electronic structure analysis. The incorporation of SrTiO$_3$ into the polyethylene matrix produced significant changes in the structural, electronic, and optical properties of the composite. Structural analysis confirmed a stable interface heterojunction in which PE molecules interact effectively with the SrTiO$_3$ surface, preserving polymer flexibility while introducing semiconducting characteristics. Electronic structure calculations demonstrated a reduced band gap in the PE/SrTiO$_3$ composite relative to pure polyethylene, indicating enhanced electrical conductivity and charge transfer capability. Band structure and DOS/PDOS analysis revealed that the valence bands are predominantly composed of O-2p and C-2p orbitals, while the conduction bands are dominated by Ti-3d orbitals, confirming substantial interfacial orbital interactions. Optical analysis further showed marked improvements in dielectric performance, absorptivity, refractive index, conductivity, reflectivity, and energy loss characteristics. The composite exhibited strong light-matter interaction, high polarization efficiency, and notable optical absorption at low-to-medium energy ranges, making it particularly suitable for optoelectronic and photocatalytic applications. The observed dielectric stability and conductivity enhancements also indicate potential utility in flexible electronics and energy conversion technologies. The electronic and optical properties of PE/$SrTiO_3$ heterojunction achieved in this research correlate well with those reported in previous investigations dealing with other hybrid polymer/oxide semiconductor materials. Previous investigations of polyethylene-based nanocomposites and $SrTiO_3$ heterostructures have shown that the addition of oxide semiconductors improves dielectric response, charge transport efficiency, and band structure. These results are consistent with prior studies on hybrid polymer/oxide semiconductor systems, wherein oxide semiconductor incorporation has been shown to improve dielectric response, charge transport efficiency, and band structure modification. The present findings, reduced bandgap, increased dielectric polarization, and enhanced optical absorbance are attributed to the coupling effect at the PE/$SrTiO_3$ interface, reinforcing the viability of combining insulating polymers with perovskite oxide semiconductors to engineer advanced hybrid materials with tunable properties. Future work should prioritize experimental synthesis and characterization of the PE/$SrTiO_3$ heterostructure to validate the simulation-derived results. Recommended techniques include XRD, FTIR, SEM, TEM, UV-Visible spectroscopy, impedance spectroscopy, and electrical conductivity measurements. Optimization of $SrTiO_3$ nanoparticle loading, size distribution, and dispersion homogeneity within the polyethylene matrix is essential for maximizing interface quality and charge transport. Surface modification strategies and coupling agents should be explored to enhance compatibility and long-term stability. Computational investigations should be extended to defect engineering, elemental doping, and surface functionalization of $SrTiO_3$ for precise band structure control. The effects of temperature, pressure, and external electric fields on heterojunction behavior warrant further examination. Finally, the hybridization methodology applied here may be extended to other polymer–perovskite and polymer–oxide systems, potentially yielding a broader class of flexible, multifunctional semiconductor materials applicable to photovoltaics, photodetection, solar energy conversion, and wearable electronic devices.

Author contributions

Ismat Jahan Jony: Conceptualization, methodology, investigation, writing- original draft; Bakhodir Abdullayev: Visualization, project administration, writing-reviewing and editing; Murodjon Samadiy: Supervision, visualization, project administration, writing-reviewing and editing, reformatting, grammar editing; Umida Shabarova; Anora Jumayeva; Aziz Salimov; Eldor Togayev; Gulkhayo Umidjonova; Umida Abdurakhmatova; Akbar Abdiev; Madina Murodillayeva; Sirojiddin Kengboev; Erkin Yakubov; Barat Abdurahmanov; Axmad Nurmuxamedov: Investigation and resource. All authors have read and agreed to the published version of the manuscript.

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Conflict of interest

The authors declare no conflict of interest.

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