Study on the Property of Electron-Transport Layer in the Doped Formamidinium Lead Iodide Perovskite Based on DFT

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ABSTRACT: The electron-transport layer in planar perovskite solar cells plays an important role in improving photoelectric conversion efficiency. At present, the main electronic transmission materials in perovskite solar cells include TiO₂, ZnO, WO₃, ZrO₂, SnO₂, ZnO₂, etc. This work mainly studies the electron-transport characteristics of six different electron-transport layers in perovskite solar cells. Based on the density functional theory, the electron-transport model of a solar cell doped with formamidinium iodide lead compound perovskite under six different electron-transport materials was constructed, and their effective electron mass and the mobility of carriers were obtained by optimizing the structure and theoretical calculations. The results show that the mobility of electrons in TiO₂ crystal is slightly higher than that of FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ carriers. Because of their high matching degree, it can be reasonably explained that titanium dioxide has been widely used in perovskite solar cells and achieved higher photoelectric conversion efficiency. In addition, the mobility of carriers in WO₃ and SnO₂ crystals is also high, so they also have great advantages in carrier transport. Due to its abundant, nontoxic, and low-pollution content, TiO₂ has become the most widely used electronic transmission layer material for solar cells. Furthermore, we have explored eight new semiconductor materials that have not yet been used in perovskite solar cells as the electron-transport layer. The calculation results show that Ta₂O₅ and Bi₂O₃ are promising materials for the electron-transport layer. This study provides a theoretical basis for seeking better electronic transmission materials for solar cells in the future.

1. INTRODUCTION

In the past 10 years, sensitized solar cells that use perovskite doped with formamidinium iodide lead as an optical absorption layer have become a hot spot in the field of solar cells due to their low cost and high conversion efficiency.¹⁻⁶ Lately, Newport has been authorized by the National Renewable Energy Laboratory of the United States to update the certification of perovskite solar cells with a maximum efficiency of 23.7%.⁷ The mechanism of electron–hole pairs excitation after absorbing photons in perovskite solar cells has been reported in many references.⁸⁻¹⁰ Theoretically, the main ways to improve the efficiency of dye-sensitized solar cells are as follows: (1) increase the absorption of light by sensitizer, (2) improve the transport efficiency of electron and hole, and (3) reduce the recombination of charge. One of them is to improve the electron-transfer efficiency of electronic transmission materials and the electron-transport layer plays an important role in n–i–p perovskite solar cells. However, different electronic transmission materials have different transmission efficiencies. Jun Hong Noh and colleagues reported that perovskite solar cells using TiO₂ thin film mesoporous structure as the electron-transport material can achieve an efficiency of 12.3% under standard solar light.¹¹ Kim and his co-workers reported the photovoltaic characteristics of perovskite solar cells with nanostructure ZrO₂ as the electron-transport material.¹² A method of gradually injecting electrons into ZnO via exciplex intermediates at the surface was reported in ref 13. So far, the main materials used for electronic transmission are TiO₂, ZnO, WO₃, ZrO₂, SnO₂, ZnO₂, and so on. Among these electron-transport layer materials, TiO₂ is one of the ideal materials in the structure of perovskite solar cells. Waleed Abu Laban et al. analyzed the CH₃NH₃PbI₃/TiO₂–layered polaronic hybrid perovskite solar cells using the Mott–Schottky method and expounded the operation mechanism of CH₃NH₃PbI₃/TiO₂ in a solar cell.¹⁴

To find a kind of electron-transfer material that matches the carrier rate of the photosensitive absorber for improving the photoelectric conversion efficiency (PCE), many researchers have focused on the properties of nanoporous TiO₂ films immersed in electrolytes¹⁵⁻²⁵ due to their unique role in dye-sensitized solar cells (DSSCs). Others have tried to use different electron-transport materials to match the band structure of the doped organic–inorganic perovskite materials (CH₃NH₃PbI₃) and (NH₄CH₃—NH₃PbI₃) to increase the carrier transport rate.²⁶⁻³⁵ Giles E. Eperon et al. obtained 20.3% efficiency of
reaching the back electrode, and then mass and carrier transfer electronic theory (DFT) used to analyze the effective electron transport materials in the future. hole pairs are produced. The free electrons diffuse to the perovskite absorption layer and are injected into the conduction band of TiO₂ propagating in the TiO₂ layer and reaching the back electrode, and then flowing through the external circuit to the metal electrode. When free electrons are excited into the perovskite conduction band, holes are generated in the perovskite valence band and diffused into the perovskite/hole-transport layer interface and then injected into the HTM valence band. Holes travel in the hole-transport layer and reach the metal.

Figure 2 shows the bonding and charge distribution of FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ and TiO₂. The gray and blue portions of the figure are the probability distributions of electrons on both sides of the equilibrium position. According to quantum mechanics theory, the position of electrons is random and therefore cannot accurately describe the position of electrons. Therefore, statistical methods can only be used to predict the probability of occurrence at a certain location, so the gray and blue portions represent the probability. Different colors represent different orbits, and the same color represents the same orbit, which can also be said to be the probability of electrons appearing. Gray/blue indicates how much the two orbits overlap, showing different colors to distinguish, and the density of the electron cloud. Gray and blue are the probabilities of the emergence of electronic clouds, many of which are electronic clouds that are generally considered to be more active. According to Figure 2a, the electron density around FA and Cs is relatively small, and the charge density is quite different from that of adjacent atoms. The electron density distributions of lead ions and iodide ions are not much different, and the bonding types between atoms are mainly covalent bonds or metal bonds. It can be seen that the distribution of electronic states is related to the atomic gap and structure from the structure of TiO₂ shown in Figure 2b. The unbound part is the boundary with a lower electron density. The difference of electron density between oxygen and titanium bond regions is large, and the bonding type is ionic bond.

The lattice matching parameters in Figure 3 of the two crystal interfaces are as follows: FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ TiO₂ (a × 7; b × 7; c × 1); FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ ZnO (a × 5; b × 5; c × 1); FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ WO₃ (a × 5; b × 5; c × 1); FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ ZrO₂ (a × 5; b × 5; c × 1); FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ SnO₂ (a × 5; b × 3; c × 1); FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ SnO₂ (a × 5; b × 3; c × 1); FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃ (a × 2; b × 2; c × 1) @ ZnO (a × 5; b × 5; c × 1). All the mismatch ratio of lattices interface are less than 4%, except that of FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃@ZnO, which is about 8%.

3. COMPUTATIONAL METHODS

The structure of the doped formamidinium lead iodide perovskite oxide (FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃) and TiO₂ was constructed by Material Studio software. The electron density of states, energy band structure, and optical properties are calculated by Dmol³ package. Also, the details of the calculations were as follows: the exchange-correlation effects were treated by Generalized Gradient Approximation (GGA) version of Perdew-Wang-1991 (PW91), and the basis set was 4.4 double Numerical plus d-functions basis (DND), the qualities were selected as “fine”, SCF tolerance is at 10⁻⁴ eV/atom, the other sets were the default.

All planar heterostructures of FA₀.₇₅Cs₀.₂₅Sn₀.₅Pb₀.₅I₃/(TiO₂, ZnO, WO₃, ZrO₂, SnO₂, ZnO₂) and eight new semiconductor crystals were constructed by Visualizer module in Material Studio software, as shown in Figure 3. The band gaps of TiO₂/ZnO/WO₃/ZrO₂/SnO₂/ZnO₂ and eight new semiconductor crystals were calculated using CASTEP module. The exchange-correlation effects were still treated by the Perdew–Burke–Ernzerhof function in the generalized gradient approximation (GGA). The cutoff energy of plane wave basis set is 340 eV, and the parameters of convergence tolerance are as follows: energy 10⁻⁵ eV/atom and maximum force 0.01 eV/Å. The calculation and optimization structure in this paper are based on the principle of lowest energy. Also, the quantum effects are taken into account in both CASTEP and Dmol³ computational modules. Moreover, the Generalized Gradient Approximation (GGA) is an empirical describing function, which attributes the electron–electron interaction to exchange-correlation energy (EXC). The main parameters calculated in
this paper are band gaps and elastic modulus, which do not involve additional magnetic field.

4. RESULTS AND DISCUSSION

4.1. Calculation Results of Six Crystals. The effective mass of electrons directly affects the efficiency of electron transport in the electron-transport layer, which, in turn, affects the conversion efficiency of perovskite solar cells. The effective mass of electrons depends on the K state and band structure of electrons. According to the theory of solid physics, if the band width is wider, the effective mass is smaller. The band gaps of the above six crystal structures were calculated by first principles and is shown in Figure 4.

According to the theory of solid-state physics. The holes appear at the top of the valence band. The electrons appear at the bottom of the conduction band. The effective masses of electrons and holes can be determined from the curvature of the dispersion curve at the extreme value. Since the effective mass is inversely proportional to the second derivative of energy, the smaller the extreme value of the curve, the heavier the electron or hole. The effective mass of carriers indicates the mobility of carriers under the action of external electric fields. If the effective mass is light, it shows that the carrier mobility is very high, and the corresponding material conductivity will be large. The effective mass of electrons is relative to the mass of free electrons. It contains the physical effects of all interactions between electrons and the surrounding environment. The electron (or hole) of crystal can be considered as a particle (as quantum wave packet) with momentum \( P = \hbar k \) (\( k \) is the quasi-momentum of crystal electrons or holes) and energy \( E = \frac{p^2}{2m^*} \). That is, the electrons or holes in crystals are free particles with effective masses, and their effective masses are, respectively, \( m_e^* \) and \( m_h^* \).

According to the solid physics, we can estimate the effective mass \( m^* \) of carriers near the bottom of the conductive band or the top of the valence band by fitting the dispersion relation.\(^{37}\)

\[
m^* = \hbar^2 \left[ \frac{\partial^2 \varepsilon(k)}{\partial k^2} \right]^{-1}
\]

Here \( \varepsilon(k) \) is the band edge eigenvalue and \( k \) is the wave-vector. The unit of \( \frac{\partial^2 \varepsilon(k)}{\partial k^2} \) is \( \frac{\text{eV}}{\pi a^2} \). The value of effective mass depends on the second derivative near the bottom of the conduction band and the top of the valence band from formula 2. Therefore, the function \( \varepsilon(k) = A + Bk + CK^2 \) was fitted using the parameters near the bottom of the conduction band and the top of the valence band.\(^{39}\) Because of \( \frac{\partial^2 \varepsilon(k)}{\partial k^2} = 2C \), the effective mass can be obtained through below formula

\[
m^* = \frac{\hbar^2}{2C \times (1.6 \times 10^{-19}) \times 9.1 \times 10^{-31}} = \frac{3.01 \times 10^2}{2a^2C}
\]

The effective mass electrons and holes can be calculated by adding the corresponding parameters, as shown in Tables 1 and 2.

If the effective mass is very small, the carrier mobility is very high and the corresponding material conductance is relatively large. The effective mass of electrons depends on the band structure and the electrons in the K states. From Tables 1–3, it can be seen that the transmission efficiency of most crystals along the z-axis is higher than that along the x-axis and y-axis except for ZnO and ZrO with a large electronic effective mass. Therefore, we have constructed the plane heterojunction structure of perovskite FA\(_{0.75}\)Cs\(_{0.25}\)Sn\(_{0.5}\)Pb\(_{0.5}\)I\(_3\) and electron-
transport layer (TiO$_2$, ZnO, WO$_3$, ZrO$_2$, SnO$_2$, and ZnO$_2$) according to the lattice parameters shown in Figure 3.

In semiconductor materials, the coherent wavelength of thermally activated electrons or holes is much longer than the lattice constant at room temperature and is close to that of phonon. The electron–phonon coupling can lead to scattering in the low-energy region, which can be optimized by the deformation potential (DP) theory proposed by Bardeen and Shockley. Through the effective mass approximation, the DP theory has been widely used to study the carrier mobility in two-dimensional materials.

$$\mu = \frac{e\hbar C_{2D}}{k_BTm^*_0(E_f)^2}$$

where $m^*_0$ is the effective mass along the transmission direction, $m_\alpha$ is the average effective electron mass along the other two directions perpendicular to the transmission direction $m_\alpha = \sqrt{m_x^*m_y^*}$ (where $\alpha, \beta$ are $x$, $y$, or $z$) and $T$ is the

Figure 3. Planar heterostructures of FA$_{0.75}$Cs$_{0.25}$Sn$_{0.5}$Pb$_{0.5}$I$_3$/[(TiO$_2$, ZnO, WO$_3$, ZrO$_2$, SnO$_2$, ZnO$_2$)].
$E_i = \Delta E_g / (\Delta l / l)$ is the deformation potential constant and $\Delta E_g$ is the displacement of the band edges (the bottom of the electron conduction band and the top of the hole valence band) caused by strain. The elastic modulus along the $z$-axis and the uniform deformation along the $y$-axis are calculated to simulate the lattice distortion induced by strain activation. For the 2D model, the in-plane stiffness can determined as $C_{2D} = [\partial^2 \omega / \partial \delta^2] / S_0$, here $\omega$ is the total energy of the supercell, $\delta$ is the applied uniaxial strain, and $S_0$ is the area of the equilibrium supercell. The elastic modulus follows the $z$-axis of the Forcite Code. In the $y$-$z$ plane, the lattice constants of the crystals FA$_{0.75}$Cs$_{0.25}$Sn$_{0.5}$Pb$_{0.5}$I$_3$, TiO$_2$, ZnO, WO$_3$, ZrO$_2$, SnO$_2$, and ZnO$_2$ along the transmission direction, i.e., $z$-axis, are 12.8, 3.77, \[\ldots\]
4.63, 5.42, 5.29, 4.73, and 4.96 Å, respectively. Using formula 3, we obtain the carrier mobility of the above crystals, as shown in Tables 4 and 5.

The carrier mobility can be estimated by means of another way according to the refs 46, 47, which reads

\[
\mu = \frac{e\hbar \rho S^2}{k_B T m_e m_d (E_i^*)^2}
\]  

(4)

where \( \rho \) is the mass density and \( S \) is the sound velocity. The other parameters in eq 4 are same as those in formula 3. Using formula 4, we have calculated the carrier mobility such as in Tables 6 and 7.

Using formulas 3 and 4, we have calculated the mobility of carriers and obtained the carrier mobility of the seven crystals along the \( x \)-axis and \( z \)-axis, respectively, as shown in Tables 3–6. The results obtained by the two methods are basically consistent. The calculated results of ZnO carrier mobility are in good agreement with refs 48, 49. It was also reported that the mobility of mesoporous TiO\(_2\) structure was 10\(^{-5}\) cm\(^2\)/(V s) in the above references. It is well-known that the mobility of carriers is an important characteristic parameter of semiconductor materials. Theoretically, the carrier mobility of inorganic semiconductors is 10\(^2\)–10\(^6\) cm\(^2\)/(V s). Because the carrier mobility of titanium dioxide in a two-dimensional space is
much higher than that of the mesoporous structure, the above calculation results are relatively reliable (Figure 5).

![Effective mass of electrons of six kinds of crystals](image)

**Figure 5. Effective mass of electrons of six kinds of crystals.**

### 4.2. Exploration of New Transport Materials

There are many other new semiconductor materials, such as Ta₂O₅, Bi₂O₅, Nb₂O₅, Pr₂O₃, Sb₂O₃, V₂O₅, In₂S₃, ZnS₂, and so on, which have not yet been used in perovskite solar cells as the electron-transport layer. They have attracted much attention because of their good physical or chemical properties. Ta₂O₅ has a strong corrosion resistance and ductility, Bi₂O₅, Nb₂O₅, and V₂O₅ have better heat resistance, and In₂S₃ is a new type of two-dimensional material with wide spectral response and photoelectric detection performance. Most of these materials have good stability and are widely used in electronic devices or high-temperature superconducting materials. There are a lot of literatures exploring their relevant characteristics. In this section, we explore the band gap structure, optical absorption properties, and electron mobility along the x-axis and y-axis of eight crystals. The crystal structure is shown in Figure 6.

The band gaps of the above eight crystals were calculated by first principles and are shown in Figure 7. The carrier mobility can be estimated according to the band gap structure. If the curve at the top of the valence band (VB) is relatively flat, it indicates that the effective mass of electrons is relatively large, and vice versa from the top-of-the-price curve in Figure 7. The curves of V₂O₅ and In₂S₃ at the top of the valence band (VB) is relatively flat, but the curves of Ta₂O₅ and Bi₂O₃ fluctuate considerably. Furthermore, we calculate the band gap by considering the quantum effect and spin–orbit coupling (SOC) by the CASTEP package of Material Studio 2017. The precision parameter settings remain unchanged with the Dmol³, and the results are shown in Tables 3 and 8. Comparing the results of the two methods with those of the refs 40–44 and 56–63, we find that the band width will change to narrower. However, it cannot calculate the other properties of crystal when considering SOC. Comparing the results of the above references, we find that the results obtained by DMOL³ package are reliable; in this part, we use the results of the DFT energy gap to study the electron-transport characteristics of the electron-transport layers in perovskite solar cells.

### 5. CONCLUSIONS

The speed of carrier transmission in the electron-transport layer plays an important role in improving the power conversion efficiency of solar cells. It is well-known that the dye molecule absorbs the incident light, and the ground-state electron changes to the excited state when the solar light is irradiated to the organic–inorganic lead iodide perovskite. The unstable excited dye molecules rapidly inject electrons into the TiO₂ conduction band. The free electrons propagate in the electron-transport layer and reach the back electrode and then flow through the external circuit to the metal electrode. The high mobility of electrons in the transport layer can realize charge separation and reduce the charge recombination as soon as possible, which is helpful to improve the photoelectric conversion efficiency of solar cells. At present, the commonly used electronic transmission materials are TiO₂, ZnO, WO₃, SnO₂, ZrO₂, and SnO₂, and so on. Based on the structure of the electron-transport layer of perovskite solar cells, the electron-transport characteristics of six different materials have been studied in this paper. First, the crystal structures of perovskite and titanium dioxides were constructed by Studio software, and the distribution of electronic states in the crystal was investigated by first principle. Then, the energy band structures of six kinds of crystals are calculated, and according to the distribution of the energy-level curves at the top of the valence band and the bottom of the conduction band, the effective mass of the six kinds of holes and electrons are obtained. It is found that the effective mass of the electrons along the y-axis and x-axis is similar. In most of the above crystals, the transmission speed of electrons along the z-axis is slightly higher than that along the x-direction. On this basis, FA₀.₇₅Cs₀.₂₅Pb₀.₇₅I₃/(TiO₂, ZnO, WO₃, SnO₂, SnO₂, ZnO₂) plane heterostructures along the z-axis are constructed and their electron mobility along the z-axis and x-axis are calculated. The mobility of the carriers along the z-axis and the x-axis of the six electron-transport materials are shown in Tables 4–7. Respectively. From the above parameters, we found that the mobility of electrons in TiO₂ is slightly higher than the carrier mobility of FA₀.₇₅Cs₀.₂₅Pb₀.₇₅I₃. This can reasonably explain the reason why TiO₂ is widely used in perovskite solar cells and which can perovskite solar cells to achieve the high power conversion efficiency. In addition, from the data in Tables 4–7, the mobility of carriers in WO₃ and SnO₂ crystals are also high. Therefore, they also have advantages in carrier transport. Due to its abundance, nontoxicity, and low pollution content, TiO₂ has become the most widely used electronic transmission layer material for solar cells (Figure 8).

Furthermore, we have explored eight new semiconductor materials that have not yet been used in perovskite solar cells as the electron-transport layer. Using the above method of calculating the carrier mobility, the data in Table 8 are substituted into formula 4. We can calculate the carrier mobility of these eight crystals, which is show in Table 7. The order of the electron mobility along the x-direction from large to small is Ta₂O₅ > Nb₂O₅ > Bi₂O₅ > Sb₂O₃ > Nb₂O₅ > In₂S₃ > ZnS₂ > ZnO₂, and that along y is Ta₂O₅ > Bi₂O₅ > Sb₂O₃ > Nb₂O₅ > Pr₂O₃ > In₂S₃ > ZnS₂ > V₂O₅, which can be shown as Figure 9. Ta₂O₅ and Bi₂O₅ have good heat resistance and a relatively good electron-transfer rate. They are mostly used in electronic ceramics, electrolyte materials, photoelectric materials, high-temperature superconducting materials, catalysts, and so on.

Comparing the calculation results in Tables 3 and 8, it is found that the band gaps of ZnO, WO₃, SnO₂, ZnS₂, and ZnO₂ change obviously when considering the spin and orbit coupling (SOC). We further analyze the energy band structure in Figure 8. When considering the spin and orbit coupling, the band gap moves to the other energy value or the band width changes. The band gap
Figure 6. Planar heterostructures of FA$_{0.75}$Cs$_{0.25}$Sn$_{0.5}$Pb$_{0.5}$I$_3$/(Ta$_2$O$_5$, Bi$_2$O$_3$, Nb$_2$O$_5$, Pr$_2$O$_3$, Sb$_2$O$_3$, V$_2$O$_5$, In$_2$S$_3$, and ZnS$_2$). The lattice matching parameters in (A) of the two crystal interfaces are abbreviated as: 1 × 2 × 3 / 2 × 5 × 3, Triclinic_Ta$_2$O$_5$ (110). 1 × 2 × 3 / 2 × 2 × 3, Triclinic_Bi$_2$O$_3$ (110). 1 × 2 × 3 / 1 × 7 × 5, Triclinic_Nb$_2$O$_5$ (110). 1 × 2 × 3 / 3 × 7 × 3, Triclinic_Pr$_2$O$_3$ (110). 1 × 2 × 4 / 2 × 2 × 2, Triclinic_Sb$_2$O$_3$ (110). 4 × 3 × 2 / 5 × 2 × 2, Triclinic_V$_2$O$_5$ (110). 1 × 2 × 3 / 2 × 2 × 3, Triclinic_In$_2$S$_3$ (110). 1 × 2 × 3 / 2 × 4 × 3, Triclinic_ZnS$_2$ (110).

The lattice matching parameters in (A) of the two crystal interfaces are abbreviated as: 1 × 2 × 3 / 2 × 5 × 3, which means: FA$_{0.75}$Cs$_{0.25}$Sn$_{0.5}$Pb$_{0.5}$I$_3$ (a × 1; b × 2; c × 3) @ Ta$_2$O$_5$ (a × 2; b × 5; c × 3), the following three items are the crystal type, crystal name, and crystal face information in turn. Also, those of other subparts are the same as those for (A). The heterojunction we constructed the layer-structure as a crystal and kept constant volume with the vacuum as 0.
of the ZnO, ZnS becomes three band gaps. Also, the band structure of WO₃ moves to the energy value from −7.44 and −20.23 eV and the SnO₂ moves between −8.93 and −17.94 eV. The band gaps are 12.78 and 8.99 eV, respectively. The band gap of ZnO₂ is similar to the band gap structure of ZnO and ZnS. It can be shown that the main contribution to the band gap

**Figure 7.** Band structures of eight crystals.

**Table 8. Carrier Mobility along x-Axis and y-Axis of Eight Crystals**

| Crystal | a (Å)  | b (Å)  | c (Å)  | DFT energy gap (eV) | band gap (eV) in references | SOC energy gap (eV) | S/0 (x) (eV) | S/0 (y) (eV) | ρ (10^4 kg/m^3) | S/0 (x) (km/s) | S/0 (y) (km/s) | μx (10⁴ cm²/(V s)) | μy (10⁴ cm²/(V s)) |
|---------|--------|--------|--------|---------------------|-----------------------------|----------------------|-------------|-------------|----------------|----------------|----------------|------------------|------------------|
| Ta₂O₅   | 5.74   | 5.25   | 13.09  | 2.243 eV            | 2.243 eV                    | 1.83                 | 1.88        | 8.98        | 8.98          | 2.43           | 1.59           | 2.59              | 0.942            |
| Bi₂O₃   | 5.74   | 12.81  | 3.87   | 2.244 eV            | 2.244 eV                    | 1.54                 | 3.94        | 8.03        | 8.03          | 2.43           | 2.50           | 0.487              | 0.08             |
| Nb₂O₅   | 6.09   | 5.72   | 4.06   | 2.292 eV            | 0.934 eV                    | 1.852                | 1.14        | 4.29        | 4.29          | 2.32           | 1.98           | 0.45               | 0.048            |
| Pr₂O₃   | 8.13   | 10.31  | 6.97   | 2.597 eV            | 1.184 eV                    | 2.73                 | 4.06        | 6.78        | 6.78          | 2.22           | 1.81           | 0.621              | 0.557            |
| Sb₂O₃   | 8.13   | 5.70   | 12.17  | 1.184 eV            | 1.777 eV                    | 3.9                 | 1.04        | 3.89        | 3.89          | 2.17           | 1.18           | 0.18               | 0.506            |
| V₂O₅    | 8.13   | 11.04  | 6.91   | 1.777 eV            | 6.00 eV                     | 3.2                 | 1.04        | 2.97        | 2.97          | 2.22           | 1.81           | 0.45               | 0.249            |
| In₂S₃   | 10.31  | 5.70   | 12.17  | 6.00 eV             | 6.00 eV                     | 3.3                 | 1.04        | 2.97        | 2.97          | 2.22           | 1.81           | 0.45               | 0.249            |
| ZnS₂    | 6.97   | 6.97   | 6.00   | 6.00 eV             | 6.00 eV                     | 3.3                 | 1.04        | 2.97        | 2.97          | 2.22           | 1.81           | 0.45               | 0.249            |
structure when considering the SOC is a heavy element. Then, we calculate the optical absorption properties of these crystals. The absorption spectra are shown in Figure 10. The absorption of light is mostly concentrated in the range of 100–500 nm. The absorption spectra range of Nb₂O₅ and V₂O₅ is distributed in 300–800 nm. However, carrier mobility of V₂O₅ is relatively low. Although the electron-transport materials are not the main optical absorption layer, it still contributes to the photoelectric conversion efficiency. Considering the factors of electron-transmission characteristics and spectral absorption, Ta₂O₅ and Bi₂O₃ are promising materials for the electron-transport layer. This study provides a theoretical basis for finding better electronic transmission materials for solar cells in the future.

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Notes
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