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Theoretical study of the II-VI solar cells semiconductor material arrangements effect using the one-dimensional Schrodinger equation

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Abstract: Solar cells are electronic devices that function to convert light energy from sun into electrical energy. Solar cells can work well if the materials used are also right so they can absorb light energy to the maximum. The solar cell materials used in this study are II-VI semiconductors, there are CdS (P), CdSe (Q), and CdTe (R). The purpose of this study was to find the combination of materials has the largest transmission coefficient which was analyzed using the Schrodinger equation (analytic) and Matlab R2022a (numeric). The greater the transmission coefficient, the greater the light energy absorbed by the solar cells, so that the generated electrical energy is also greater. The materials are arranged into 3 uniform arrangements and 6 combined arrangements with a maximum electron energy of 1 *eV*. The results showed that the largest transmission coefficient in the CdS array was 0.9925 at 1.0000 *eV*, the largest transmission coefficient in the CdSe array was 1.0000 at 0.8140 *eV*, and the largest transmission coefficient in the CdTe array was 1.0000 at 0.7330 *eV*. Meanwhile, in the combined arrangement, the biggest transmission value is 0.9823 at 0.9570 *eV* in the QPR and RPQ arrangements.

Keyword: Solar cells, Semiconductor, Transmission coefficient, Schrodinger equation.

1. Introduction

Nanomaterials are an object of study that has a major influence on material devices, which makes researchers try to develop nanomaterials into appropriate technologies. Quantum Dots (QDs), which are also known as nanocrystals, are semiconductor nanostructures that limit the movement of electrons in three spatial directions to a small area such as dots (Suarso, 2013). The manufacture of QDs is divided into 2, self-ensemble QDs and colloidal QDs. In short, colloidal QDs are superior to self-ensemble QDs. The manufacture of colloidal QDs uses a chemical process with easier and cheaper materials and equipment (Kagan et al., 2016). Types of QDs that can be made by this process include semiconductors II-VI, III-V, and IV-VI, examples are CdSe, CdTe, PbS, InP with diameters that can be obtained between 2 to 5 *nm* (smaller than self-ensemble QDs) (Liu et al., 2016; McHugh et al., 2018). In addition, colloidal QDs promising to optoelectronic properties, such as size or shape or composition-dependent absorption edges, high absorption coefficients, large intrinsic dipole moments and high photoluminescence quantum yield (Selopal et al., 2020).

QDs can be applied to semiconductor-based optical devices such as LEDs, laser diodes, and solar cells. The utilization of solar cells in the current era is getting bigger so that the composition of QDs materials having an important things to effectiveness of solar cells (Arquer et al., 2021). Therefore, the material used in this study is a material that has great potential in the utilization of solar cells, there are semiconductor materials from groups II-VI, especially from colloidal QDs, such as CdS, CdSe, and CdTe. CdS has a 2.45 *eV* band gap, has a 0.583 *nm* barrier width, and is often used as a coating in solar cells because of its superior optoelectronic properties (Rahman et al., 2020; Shaikh et al., 2021; Iqbal et al., 2019; Sharma et al., 2021). CdSe has a 1.73 *eV* band gap, has a 0.605 *nm* barrier width, and is often used for solar cells, detector of gamma ray, photo detection and optoelectronics (Rani et al, 2015; Mazing et al., 2015). Meanwhile, CdTe has a 1.44 *eV* wide band gap (Abbaspour et al., 2022; Devendra et al., 2021; Alshahrani et al., 2021), has a 0.648 *nm* barrier width (Kapadnis et al., 2020), and is often used in the manufacture of solar cells (Samoilenko et al., 2020).

QDs have properties like ordinary semiconductors and have properties that resemble those of an atom, such as breakthrough effects, density of states, and energy levels (Alawiyah et al., 2022). The tunneling effect itself occurs when particles try to break through a barrier that has a higher energy than the particle's energy (Lombu et al., 2013; Prastowo et al., 2018; Supriadi et al., 2020). In quantum mechanics, particles with energy E have the opportunity to break through the barrier V which has a greater value (Nasiroh et al., 2020; Ong, 2022). The value of this probability usually called the transmission coefficient, which in this study can be analyzed using the Schrodinger equation that can be used easily to determine the transmission coefficient present in a potential barrier (Huda et al., 2018; Supriadi et al., 2017). Basically the Schrodinger equation compares the normalization constant of the incident wave function and the wave formed after breaking through a potential barrier (Agustin et al., 2019; Abdy et al., 2021).

Research by (Prastowo et al., 2019) shows that the value of the transmission coefficient on graphene material that was searched for using the step or three-barrier matrix propagation method already exists. In addition, research on three barriers using GaN, SiC, and GaAs materials that produced the biggest transmission coefficient of 0.8947 at 0.9000 *eV* energy also used the same principle, but did not have a varied arrangement (Supriadi et al., 2019). Other research which is the main reference for this research is research conducted by (Supriadi et al., 2021) and research by (Supriadi et al., 2023) regarding the transmission in a combination of three semiconductor materials. The two studies both analyzed the transmission coefficient of III-V semiconductor materials and used three materials, however there were significant differences seen in the methods used and the composition of the semiconductor materials analyzed. (Supriadi et al., 2021) uses the matrix propagation method to obtain transmission coefficient values and there is a uniform arrangement and combination of materials used. Meanwhile, research (Supriadi et al., 2023) used the manual Schrodinger equation to obtain the transmission coefficient

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value and the composition of the materials used was only a combination arrangement. If it is concluded from these two studies, the transmission coefficient in the combination arrangement has the same value or is paired with the opposite arrangement so that out there are 3 pairs of the same values of 6 combination arrangements.

This research is intended to combine these two studies, by using the Schrodinger equation to analyze the transmission coefficient values of three barriers in a uniform arrangement and a combination arrangement. The II-VI semiconductor materials are arranged to a triple potential barrier and will be analyzed to get the biggest transmission coefficient value so that it can be used to determine the best arrangement to use in solar cells. Apart from that, this research also has novelty or innovation, there is studying materials that can be applied to solar cells theoretically so that this research can be used as a reference or consideration for a solar cell company in making solar cells that can store and transmit electrons well using a composition of materials which has been carefully analyzed in this study.

2. Method

Researchers collect various literature to conduct research in the form of books and journals on a national and international scale as well as articles from the internet that are relevant to the research topic. At this stage the researcher develops a theory from research that has been done before. Previous research which is conducted by (Supriadi et al., 2023) has analyzed the transmission coefficient using the assumption that the material through which electrons pass is in the form of a spatial structure so that it is assumed to have an x-axis and a y-axis. However, in its application, the research in (Supriadi et al., 2023) only illustrates that electrons only pass through the x axis, so that the resulting picture and equations can be simplified by assuming $y = 0$. Materials that electrons pass through will be depicted as flat shapes with electrons only passing through the x-axis to make analysis easier, as in the following image.

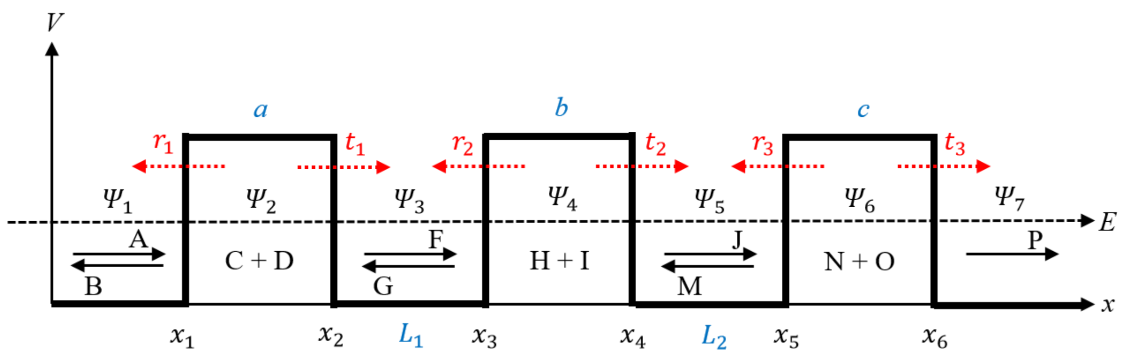

Figure 1. Model of triple potential barrier

In this figure, Ψ is the Schrodinger equation in each region. The symbols A, B, C, D, F, G, H, I, J, M, N, O, and P describe pairs of electron directions assuming that the symbol with the arrow pointing to the right represents that the electron is transmitted and the symbol with the arrow pointing to the the left indicates that the electron will be reflected. The symbols a, b, and c are the barrier width of each material, which are CdS, CdSe, and

CdTe, respectively. Meanwhile, the symbols L_1 and L_2 are the width of the gap between the barrier before and after it.

2.1. Transmission Coefficient Equation for Triple Barriers

From the picture above, the next step is to carry out analytical calculations using the Schrodinger wave function, so that regions 1 to 7 have solutions

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \tag{1}$$

$$\psi_2 = Ce^{k_2x} + De^{-k_2x} \tag{2}$$

$$\psi_3 = Fe^{ik_3x} + Ge^{-ik_3x} \tag{3}$$

$$\psi_4 = He^{k_4x} + Ie^{-k_4x} \tag{4}$$

$$\psi_5 = Je^{ik_5x} + Me^{-ik_5x} \tag{5}$$

$$\psi_6 = Ne^{k_6x} + Oe^{-k_6x} \tag{6}$$

$$\psi_7 = Pe^{ik_7x} \tag{7}$$

with

$$k_1 = k_3 = k_5 = k_7 = \frac{\sqrt{2mE}}{\hbar} \tag{8}$$

$$k_2 = k_4 = k_6 = \frac{\sqrt{2m(V-E)}}{\hbar} \tag{9}$$

The k_2, k_4, and k_2 values will be the same if the material used is the same because the value of V is the potential energy possessed by the material. However, if the materials used are different, then the values of k_2, k_4, and k_6 are different. Another equation needed to analyze the transmission coefficient of triple potential barrier are

$$t_1 = \frac{4ik_1k_2e^{-ik_1a}}{(k_2+ik_1)(ik_1+k_2)e^{-k_2a} + (k_2-ik_1)(ik_1-k_2)e^{k_2a}} \tag{10}$$

$$t_2 = \frac{4ik_1k_4e^{-ik_1b}}{(k_4+ik_1)(ik_1+k_4)e^{-k_4b} + (k_4-ik_1)(ik_1-k_4)e^{k_4b}} \tag{11}$$

$$t_3 = \frac{4ik_1k_6e^{-ik_1c}}{(k_6+ik_1)(ik_1+k_6)e^{-k_6c} + (k_6-ik_1)(ik_1-k_6)e^{k_6c}} \tag{12}$$

$$r_1 = \frac{(k_2+ik_1)(ik_1-k_2)e^{-k_2a} + (k_2-ik_1)(ik_1+k_2)e^{k_2a}}{(k_2+ik_1)(ik_1+k_2)e^{-k_2a} + (k_2-ik_1)(ik_1-k_2)e^{k_2a}} \tag{13}$$

$$r_2 = \frac{(k_4+ik_1)(ik_1-k_4)e^{-k_4b} + (k_4-ik_1)(ik_1+k_4)e^{k_4b}}{(k_4+ik_1)(ik_1+k_4)e^{-k_4b} + (k_4-ik_1)(ik_1-k_4)e^{k_4b}} \tag{14}$$

$$r_3 = \frac{(k_6+ik_1)(ik_1-k_6)e^{-k_6c} + (k_6-ik_1)(ik_1+k_6)e^{k_6c}}{(k_6+ik_1)(ik_1+k_6)e^{-k_6c} + (k_6-ik_1)(ik_1-k_6)e^{k_6c}} \tag{15}$$

$$p = \frac{(k_4+ik_1)(ik_1+k_4)e^{k_4b} + (k_4-ik_1)(ik_1-k_4)e^{-k_4b}}{4ik_1k_4e^{-ik_1b}} \tag{16}$$

From the above equation, the transmission coefficient on the triple barrier can be obtained as follows.

$$T_3 = \left| \frac{t_1 t_2 t_3}{\left(1 - r_2 r_3 e^{2ik_1 L_2}\right) - \left(r_2 + r_3 t_2 e^{2ik_1 L_2} p\right) e^{2ik_1 L_1} r_1} \right|^2 \tag{17}$$

2.2. Arrangements

After knowing the equation to find the transmission of triple potential barrier, we must determine the arrangement of the barrier to be analyzed in this study, which is as follows.

Table 1. Arrangement of barriers

Uniform Arrangements		
PPP	QQQ	RRR
Combination Arrangement		
PQR	QPR	RPQ
PRQ	QRP	RQP

Where P is CdS (Cadmium Sulfide) material, Q is CdSe (Cadmium Selenide) material, and R is CdTe (Cadmium Telluride) material.

2.3. Matlab R2022a Flowchart

In this study there is a numerical analysis carried out using Matlab R2022a. The transmission coefficient equation that has been obtained will be entered into the Matlab R2022a programming language which has the result in the form of a graph of the transmission coefficient to energy as validation. The steps for validating are in the following flowchart.

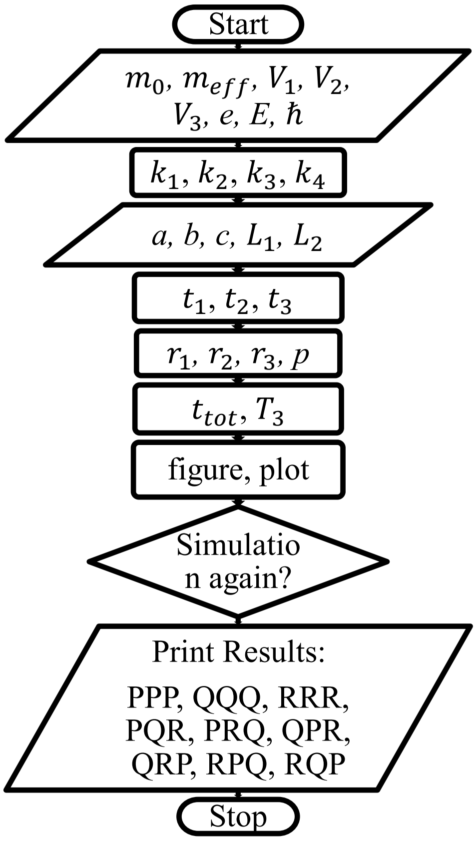

Figure 2. Flowchart Matlab R2022a for transmission coefficient at triple potential barrier

3. Result and Discussion

Based on theoretical research that has been carried out, the following transmission coefficient values are obtained for uniform and combination arrangements, and there is also a relationship between the results that have been obtained and the use of solar cells.

3.1. Transmission Coefficient in Uniform Arrangements

The uniform arrangement in this study are PPP, QQQ, and RRR. The transmission coefficient values of each arrangement are written in the following table.

Table 2. Transmission coefficient in uniform arrangements

Electron Energy *(eV)*	**PPP**	**QQQ**	**RRR**
0.0000	0.0000	0.0000	0.0000
0.2500	0.0003	0.0018	0.0035
0.5000	0.0027	0.0294	0.0791
0.7330	0.0321	0.6503	**1.0000**
0.7500	0.0397	0.7680	0.9876
0.8140	0.0939	**1.0000**	0.8493
1.0000	**0.9925**	0.6720	0.6910

Based on the transmission coefficient table above (**Table 2**), the graph of each arrangement can be described as follows.

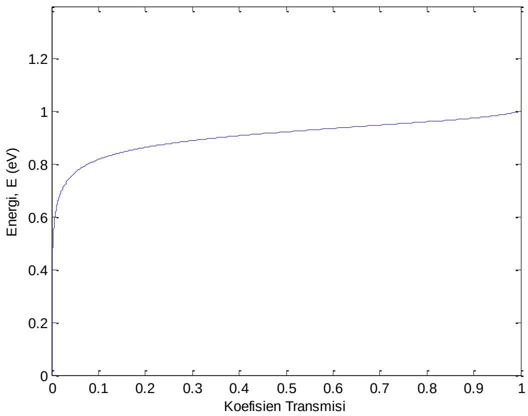

Figure 3. PPP arrangement

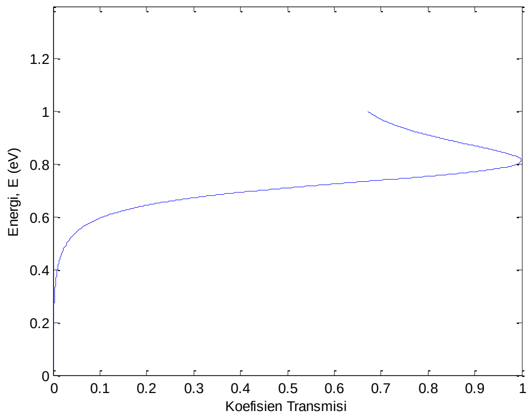

Figure 4. QQQ arrangement

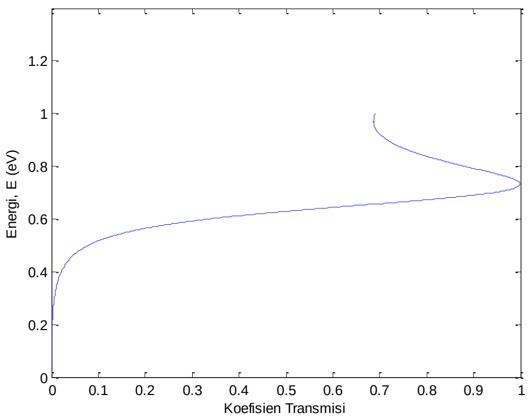

Figure 5. RRR arrangement

It can be seen that the PPP uniform arrangement has the largest transmission value of 0.9925 at 1.0000 eV energy. whereas in the uniform arrangement QQQ and RRR have a transmission value of 1.0000 at energies of 0.8140 eV and 0.7330 eV. In the PPP arrangement, it is difficult for the transmission coefficient to reach its maximum value even though the energy of the particles (electrons) is already at 1.0000 eV. However, in the QQQ and RRR configurations, the transmission coefficient reaches a maximum lift of 1.0000 or maximum when the energy of the particles (electrons) is <1.0000 eV. This is because the QQQ and RRR arrangements have relatively low band gap of 1.73 eV and 1.44 eV compared to the PPP arrangement which has a band gap of 2.45 eV so that the particle energy is more easily transmitted and produces the maximum transmission coefficient value even though the particle energy is not maximum (1.0000 eV).

3.2. Transmission Coefficient in Combination Arrangements

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The combination arrangement in this study are PQR, PRQ, QPR, QRP, RPQ, and RQP. The transmission coefficient of each arrangement are written in the following table.

Table 3. Transmission Coefficient in Combination Arrangement

Electron Energy *(eV)*	**PQR**	**PRQ**	**QPR**	**QRP**	**RPQ**	**RQP**
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.2500	0.0012	0.0012	0.0012	0.0012	0.0012	0.0012
0.5000	0.0183	0.0206	0.0146	0.0206	0.0146	0.0183
0.7500	0.5221	0.7872	0.2545	0.7872	0.2545	0.5221
0.7830	0.6994	**0.8851**	0.3738	**0.8851**	0.3738	0.6994
0.8280	**0.7975**	0.4551	0.9816	0.4551	0.9816	**0.7975**
0.9570	0.5729	0.4474	**0.9823**	0.4474	**0.9823**	0.5729
1.0000	0.5286	0.4160	0.9615	0.4160	0.9615	0.5286

Based on **Table 3**, the graph of each arrangement can be described as follows.

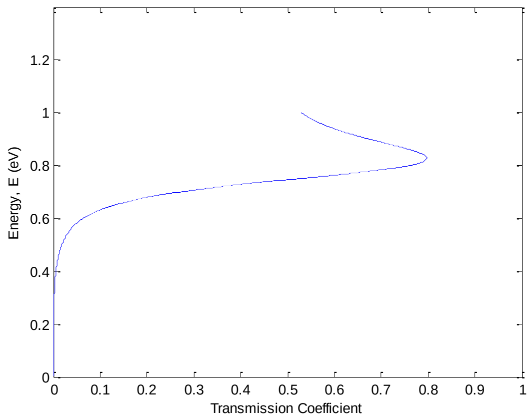

Figure 6. PQR arrangement

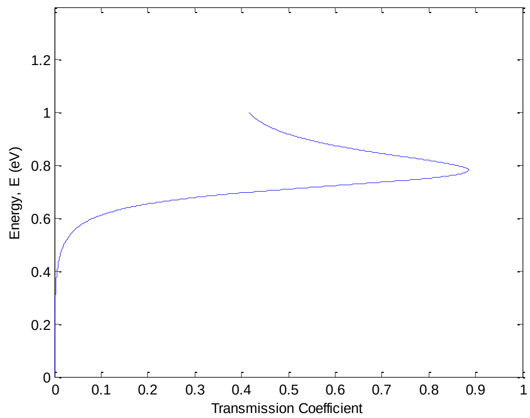

Figure 7. PRQ arrangement

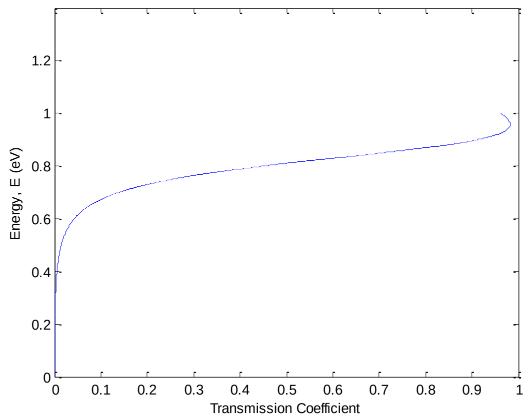

Figure 8. QPR arrangement

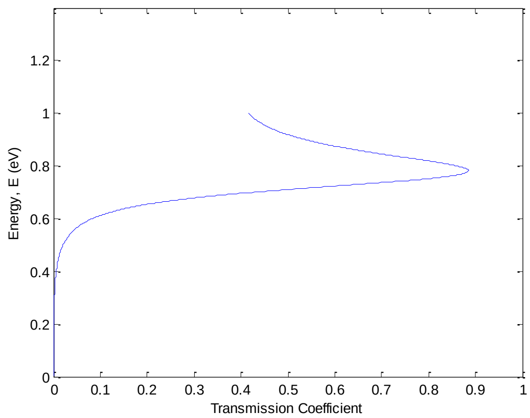

Figure 9. QRP arrangement

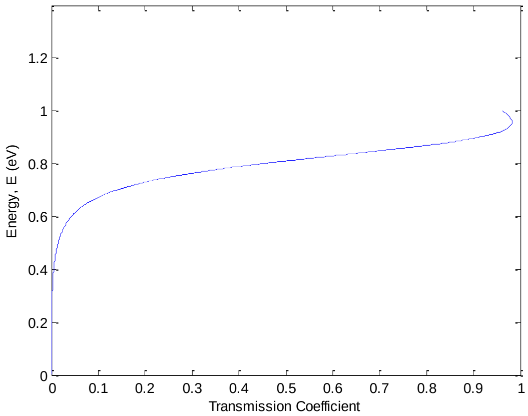

Figure 10. RPQ arrangement

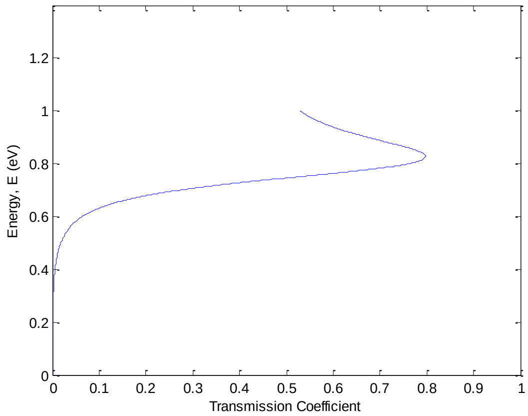

Figure 11. RQP arrangement

It should also be noted that in the combination arrangement, there are two arrangements that opposite which have the same transmission value. These results are the same as the results obtained in previous research with different materials that conducted by (Supriadi et al., 2023) so that there are three values from six combination arrangements. The PQR and RQP arrangements which have a transmission value of 0.7975 at 0.8280 eV energy. The PRQ and QRP arrangement has a transmission value of 0.8851 at 0.7830 eV energy. The QPR and RPQ arrangement has a transmission value of 0.9823 at 0.9570 eV energy. These results illustrate that whatever type of semiconductor material is used, if arranged in opposite directions it will produce the same transmission coefficient value.

3.3. Relationship Between Research Results and Solar Cells

The transmission coefficient that has been obtained from each of these arrangements can facilitate the preparation of materials for solar cells. The greater and faster the transmission coefficient reaches its maximum value, the better the composition of the material for use as a solar cell because it will be easier for the electrons to be stored and channeled into the electric current. The composition of QQQ and RRR has good potential to be used as a solar cell material because basically Q (CdSe) and R (CdTe) materials are materials commonly used for making solar cells, but there has been no research that compiles these materials into threefold as in this study.

In short, a solar cell consists of several parts, there are back contact, absorber, buffer layer, front contact, and substrate (Romeo & Artegiani, 2021). Especially for buffer layers and absorbers, the best materials to use are materials derived from III-V or II-VI alloy semiconductors (Bosio et al., 2020). This part can be described as follows.

Figure 12. Standard structure of solar cells

In several studies, CdS is often used as a buffer layer or as an n-type semiconductor, while CdSe and CdTe are more often used as combined materials in the absorber or as p-type semiconductor materials (Baines et al., 2018). This research further strengthens the reason why CdSe and CdTe are more often used as absorbers than CdS, because of their good properties for storing and transmitting electrons.

As a preliminary illustration for this research, if in previous research there were only two materials used for the buffer layer and absorber or a combination for the absorber, CdS with CdTe (Kapadnis et al., 2020; Devendra et al., 2021 a; 2021b; Romeo & Artegiani, 2021). Then this research will focus more on combining the three materials (CdS, CdSe, CdTe) which are jointly used for the absorber in either a uniform or combined arrangement taking into account the largest transmission value that can be achieved in each arrangement as determined in **Table 1**. When CdSe and CdTe are each arranged into a triple barrier, they have equally large values. However, when CdS stands alone, even though it has been arranged into a triple barrier, it is not able to achieve the greatest transmission compared to the two previous materials.

When CdS, CdSe, and CdTe are jointly arranged into a triple barrier, the highest transmission values are obtained in the QPR and RPQ arrangements, where the real arrangements are CdSe-CdS-CdTe and CdTe-CdS-CdSe. It appears that this arrangement specifically places CdS between CdSe and CdTe so that the transmission value can be maximized. Theoretically, CdS has the largest band gap, so it will be more difficult for electrons to be transmitted and stored in the solar cell when CdS is placed on the outside. However, when CdSe or CdTe is the outermost part, the arrangement will more easily transmit and retain electrons in the solar cell before they are finally transmitted again for household and industrial needs.

Even though in theory the results of this research are in accordance with the literature, the band gap and barrier width values used are a range of values from several previous studies, which have a difference of approximately 0.01 eV. However, in general, CdS with a higher band gap value will certainly be the main difficulty when placed at the beginning of the arrangement because it will be difficult for electrons to reach the maximum value when transmitted. The results of this research certainly still require follow-up with direct experiments so that we can find out how big the relative error of this calculation is.

4. Conclusion

Based on the research and results that have been obtained, it can be concluded that semiconductor materials arranged in opposite directions will produce the same transmission coefficient value. The QQQ (CdSe) and RRR (CdTe) arrangements have relatively low potential energy compared to the PPP (CdS) arrangement so that the particle energy is more easily transmitted and produces the maximum transmission coefficient value even though the particle energy is not yet maximum. The QQQ and RRR arrangements have great potential to be realized in the manufacture of combined solar cells as in this study. The three materials in this research have great potential to be used as absorbers for solar cells which are arranged to form a triple barrier so that more electrons are transmitted and can be stored by the solar cell.

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