IOSR Journal Of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 16, Issue 1 Ser. I (Jan. – Feb. 2024), PP 48-54
www.Iosrjournals.Org

Transmission And Reflection Of Two Dimensional Arrangements Of Four-Barrier Semiconductor Materials (Pbse, Znte, Pbte, Zns) Using The Schrodinger Equation

Tamara Pingki[1], Bambang Supriadi[1], Muhammad Syafa Tirtana Sanjaya[2]
[1](Department Of Physics Education, Faculty Of Teacher Training And Education, University Of Jember, Indonesia)
[2](Department Of Business Statistic, Faculty Of Vocational, Institute Of Technology Sepuluh Nopember, Indonesia)

Abstract:
This research is based on previous research which has never used semiconductor materials from two different groups, only analyzing the effect of arrangement on transmission values without reflection values, the method used is very mathematical so it eliminates the physical meaning of electrons. So this research aims to find the transmission and reflection values in alloy semiconductor materials from groups IV-VI and II-VI using the Schrodinger equation. The materials that have been selected are arranged according to their partners to avoid band gap spikes so that the final arrangement used is PbSe – ZnTe – PbTe – ZnS. This research was carried out using an analytical method, calculating the final equation to find the transmission and reflection values manually. Next, numerical calculations were carried out using Matlab 2022b. From the result, it was obtained that the largest transmission value occurred at 0.5280 eV, it is 0.6171, while the lowest reflection value was 0.3829 at the same energy. In general, the results of the research are in accordance with theory and the transmission value is greater than the reflection value so that this material composition can be tested concretely for electronic devices.

Key Word*: Transmission; Reflection; Four Barrier, Semiconductor; Schrodinger*.

Date of Submission: 07-01-2024 Date of Acceptance: 17-01-2024

I. Introduction

The study of quantum mechanics continues to develop over time. This study begins with the postulate of wave-particle duality, which states that a particle (electron) can act as a particle itself or as a wave[1,2]. One of the characteristics of a quantum wave is that it can be reflected or reflected and transmitted or forwarded through a boundary or medium[3]. This study is the background to the creation of new technology that is increasingly sophisticated and modern, one of which is the creation of semiconductor materials which play an important role in various electronic devices and systems such as transistors, diodes and integrated circuits (IC) which can be found in LEDs, cellphones, laptops, computers, television, and many more[4,5,6,7]. Of course, not all semiconductor materials from various periodic elements can be used in making electronic devices, the choice of material depends on the size of the band gap and the lattice constant of each material[8,9]. It is not uncommon for certain electronic devices to utilize alloy semiconductors, by combining two or even more semiconductor materials from the same or different groups so as to obtain adequate band gaps and electronic factors.

Previous research[10] which is the main basis for this research was carried out on four alloy semiconductor materials from the same group, there are AlAs (A), GaAs (B), GaSb (C), and InP (D) which come from groups III-V. This research analyzed the effect of changing the composition of materials on the transmission value and it was found that in the opposite arrangement there were the same values, the highest transmission was 0.8078 in the ADCB and BCDA arrangements, while the lowest transmission was 0.4267 in the BCAD and DACB[10] arrangements. However, so far there has been no research that analyzes the reflection and transmission values by combining four materials from two different groups. This research will combine semiconductors from groups IV-VI, there are PbSe and PbTe with groups II-VI, there are ZnTe and ZnS.

A good material or arrangement to be used as a semiconductor electronic device is a material that produces a transmission value that is greater than the reflection value. A large transmission value indicates that electrons can be transmitted to the material or structure well enough so that the large number of electrons can be used optimally in electronic devices. So the aim of this research is to find out at what energy the transmission value of the material arrangement determined above is greater than the reflection value using a certain method.

If previous research[10] used the matrix propagation method to analyze the transmission that occurs in the composition of materials, this research uses a method that is considered manual, this is using the Schrodinger equation during data analysis. The matrix propagation method only focuses on simple mathematical forms so as to obtain more concise equations but ignores the physical meaning of moving electron waves[11]. In contrast to the matrix propagation method, the use of the Schrodinger equation in this research is quite long but does not eliminate the physical elements of the wave. The form of the wave equation that will be analyzed is still original so you can see how electrons travel in this equation. In general, this research continues previous research[12] which analyzed transmission in three semiconductor materials II-VI, whereas in this research four materials were used so that more barriers were formed and the equations used were also different.

II. Material and Methods

The materials used in this research are PbSe, ZnTe, PbTe, and ZnS which have band gaps, lattice constants, and certain electronic uses as semiconductor materials. PbSe (Lead Selenide) is a semiconductor with a narrow band gap of around 0.27 eV[13,14] and a lattice constant of around 0.615 nm[15], making it suitable for infrared (IR) applications[16]. ZnTe (Zinc Telluride) is a II-VI semiconductor with a medium band gap of around 2.23 eV[17,18] and a lattice constant of around 0.609 nm[19]. ZnTe is used in optoelectronic devices such as light-emitting diodes (LEDs) and detectors[20,21]. PbTe (Lead Telluride) is a narrow band gap semiconductor of approximately 0.32 eV for a cubic crystal structure[22,23] and a lattice constant of approximately 0.6379 nm[24]. PbTe is widely used in thermoelectric generator devices and cooling devices[25]. ZnS (Zinc Sulfide) is a wide band gap semiconductor of approximately 3.68 eV for a cubic crystal structure[26,27] and a lattice constant of approximately 0.5409 or 0.541 nm[28]. ZnS is used as a phosphor in cathode-ray tubes (CRTs), optoelectronics, catalysts and other display technologies to emit light when excited by electrons[29,30].

This research will not analyze the effect of the arrangement on the reflection and transmission values, so there is only one arrangement because the material chosen has a crucial problem if the arrangement is varied because the band gap of each material has quite a large difference. The PbSe material with a small band gap (0.27 eV) will be doped with ZnTe which has a large enough band gap (2.23 eV) so that they complement each other, dampen each other, so that large band gap spikes do not occur. Meanwhile, the PbTe material with a small band gap (0.32 eV) will also be doped with ZnS which has a quite large band gap (3.68 eV). The two pairs of doped materials arranged in the order PbSe – ZnTe – PbTe – ZnS will be analyzed for their reflection and transmission values to see how good and efficient these materials and arrangements are when used as building materials for LEDs and thermoelectric devices. So if the arrangement is depicted in graphical form according to the band gap of each material, it will look like the image below.

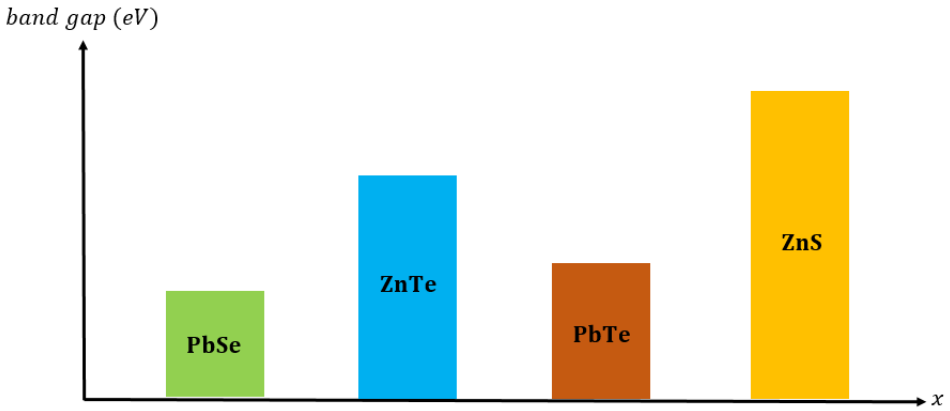

Figure 1. Arrangement of materials based on band gap

The materials in this research will be analyzed in two dimensions so that the illustration of electrons ways in the four materials above in accordance with their sequence forms parallel barriers as follows.

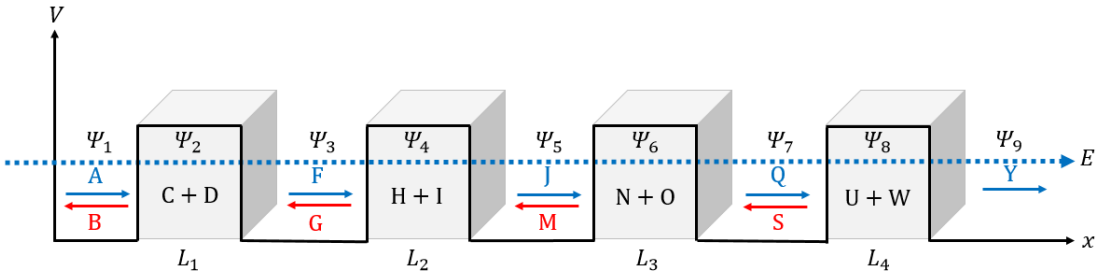

Figure 2. Model of four-barrier materials in two dimensions

To find the transmission and reflection values on the barrier or on the four materials, it is necessary to analyze the equations that will be used. Before that, it is necessary to limit this research so that the resulting equation has a clear physical meaning and the values obtained do not deviate from what was planned. The following are several limitations and conditions in this research.

1. The Schrodinger equation used is the Schrodinger equation which does not depend on time.
2. The wave function meets the requirements by behaving well and meeting the normalization requirements.
3. The wave function used is the free electron wave function.
4. The height and width of the barrier in Matlab analysis are accordance for PbSe, ZnTe, PbTe, and ZnS materials.
5. The distance between each material is fixed, it is 1 nm.
6. The electron energy used is in the range 0 to 1 eV.

Based on the limitations and conditions above, the first step that needs to be taken is to find the final equation to find the transmission and reflection values. But before that, it is necessary to first know the wave function that acts on the material and the composition of these four materials, there are

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \quad (1)$$

$$\psi_2 = Ce^{k_2x} + De^{-k_2x} \quad (2)$$

$$\psi_3 = Fe^{ik_3x} + Ge^{-ik_3x} \quad (3)$$

$$\psi_4 = He^{k_4x} + Ie^{-k_4x} \quad (4)$$

$$\psi_5 = Je^{ik_5x} + Me^{-ik_5x} \quad (5)$$

$$\psi_6 = Ne^{k_6x} + Oe^{-k_6x} \quad (6)$$

$$\psi_7 = Qe^{ik_7x} + Se^{-ik_7x} \quad (7)$$

$$\psi_8 = Ue^{k_8x} + We^{-k_8x} \quad (8)$$

$$\psi_9 = Ye^{ik_9x} \quad (9)$$

Equations (1) to (9) above are analyzed according to the barrier boundary conditions, which total 8 boundaries and then produce the main equation as follows.

$$\frac{Y}{Q} = t_4 \quad (10)$$

$$\frac{Q}{J} = \frac{t_3}{\left(1 - r_3 r_4 e^{2ik_1 L_3}\right)} \quad (11)$$

$$\frac{J}{F} = \frac{t_2\left(1 - r_3 r_4 e^{2ik_1 L_3}\right)}{\left(1 - r_3 r_4 e^{2ik_1 L_3}\right) - \left(r_3 + r_4 t_3 e^{2ik_1 L_3} p\right) e^{2ik_1 L_2} r_2} \quad (12)$$

$$\frac{F}{A} = \frac{t_1\left(\left(1 - r_3 r_4 e^{2ik_1 L_3}\right) - \left(r_3 + r_4 t_3 e^{2ik_1 L_3} p\right) e^{2ik_1 L_2} r\right)}{\left(1 - r_3 r_4 e^{2ik_1 L_3}\right) - \left(r_3 + r_4 t_3 e^{2ik_1 L_3} p\right) e^{2ik_1 L_2} r_2 - \left(\left(1 - r_3 r_4 e^{2ik_1 L_3}\right) r_2 + \left(r_3 + r_4 t_3 e^{2ik_1 L_3} p\right) e^{2ik_1 L_2} p t_2\right) e^{2ik_1 L_1} r_1} \quad (13)$$

The T or transmission value can be found by substituting equation (10) to equation (13) into the following equation.

$$T = \left|\frac{F}{A} \times \frac{J}{F} \times \frac{Q}{J} \times \frac{Y}{Q}\right|^2 = \left|\frac{Y}{A}\right|^2$$

The above equation can be simplified to

$$T = \left|\frac{Y}{A}\right|^2$$

So the final equation for T is

$$T = \left| \frac{t_1 t_2 t_3 t_4}{\left(1 - r_3 r_4 e^{2ik_1 L_3}\right) - \left(r_3 + r_4 t_3 e^{2ik_1 L_3} p\right) e^{2ik_1 L_2} r_2 - \left(\left(1 - r_3 r_4 e^{2ik_1 L_3}\right) r_2 + \left(r_3 + r_4 t_3 e^{2ik_1 L_3} p\right) e^{2ik_1 L_2} p t_2\right) e^{2ik_1 L_1} r_1} \right|^2 \quad (14)$$

In general, adding the transmission value to the reflection value will produce a value of 1[31] so that the mathematical form can be written as follows.

$$T + R = 1 \quad (15)$$

If the transmission value has been obtained from equation (14), then the reflection value can be found using the following equation.

$$R = 1 - T \quad (16)$$

After obtaining all the equations from manual analysis, the next step is to analyze the transmission values using Matlab 2022b with the following flowchart.

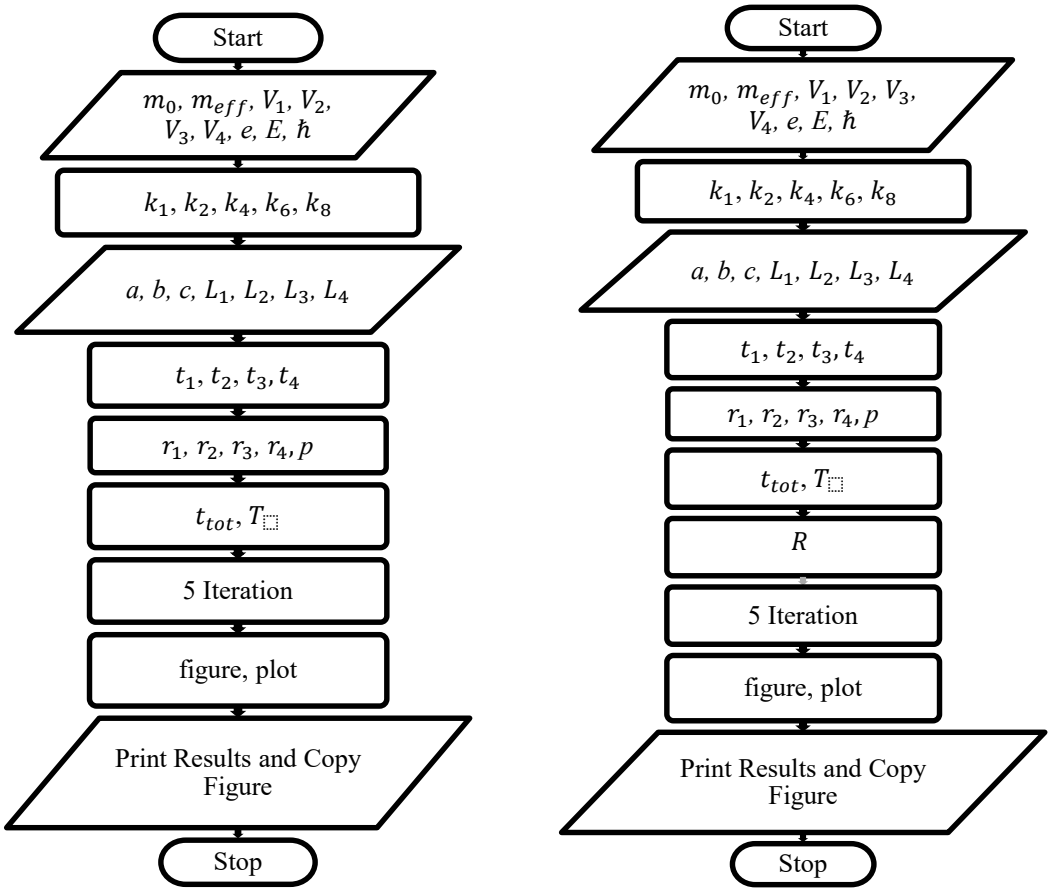

Figure 3. Flowchart Matlab 2022b for transmission (a) and reflection (b)

III. Result and Discussion

In **Figure 2**, it has been completely illustrated what the wave components are that pass through each material or two-dimensional barrier with electrons only given to the x-axis. Odd wave functions, such as Ψ_1, Ψ_3, Ψ_5, and Ψ_7 have electrons that are successfully transmitted and those that are reflected. Electrons that are successfully transmitted are written in blue and arrows to the right, there are A, F, J, and Q. Meanwhile electrons that are reflected are written in red and arrows to the left, there are B, G, M, S. Meanwhile in Ψ_9 there are only one characteristic of electrons, that there is transmitted from the previous barrier without being reflected, this is Y because there is no barrier to the right which could be the reason for the electron reflection to occur. Meanwhile, even wave functions such as Ψ_2, Ψ_4, Ψ_6, dan Ψ_8 are in a barrier or material so they have the

sum of the transmitted and reflected wave properties because electrons are trapped in them, there are C + D, H + I, N + O, and U + W.

Based on the results of numerical calculations using Matlab 2022b and iterated 5 times so that the results were more valid, the results were obtained in the form of a transmission graph below.

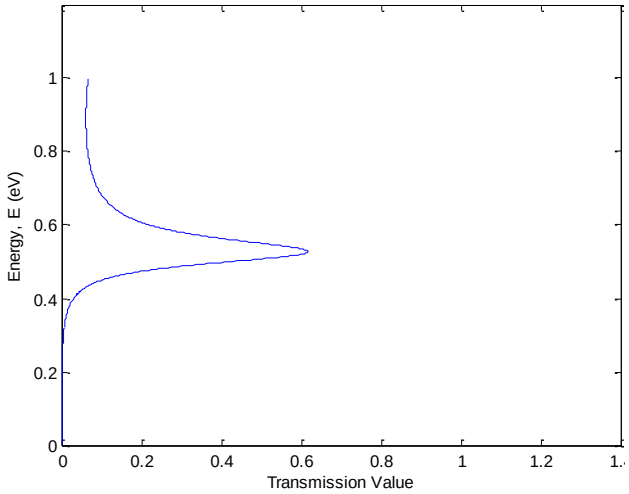

Figure 5. Graph of the transmission value of the PbSe – ZnTe – PbTe – ZnS array

Meanwhile, the graph for reflection is as follows.

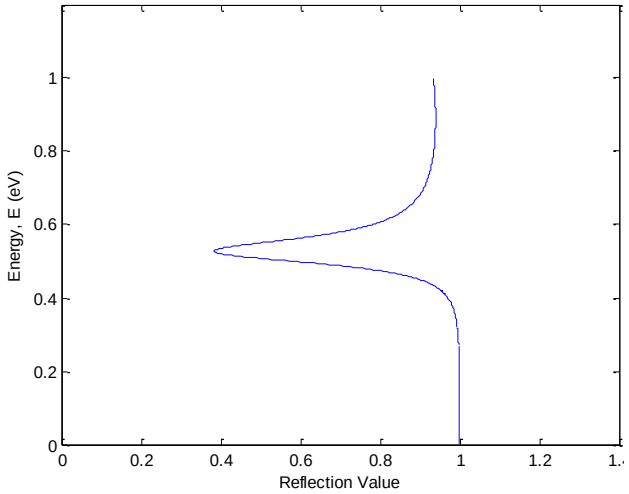

Figure 6. Graph of the reflection value of the PbSe – ZnTe – PbTe – ZnS array

The graph obtained shows that the transmission and reflection values of the PbSe – ZnTe – PbTe – ZnS material composition are very different. The transmission graph in **Figure 5** shows that the transmission value rises slowly along with the increase in energy and then reaches its maximum value and falls again slowly and will rise again. This is because there is an exponential function in equation (14) which is input into the system so that a very visible up and down graph occurs. If continued until the energy is above 1 eV, it is likely that more than one up and down graph will be visible. The time used for transmission is 0.015423 seconds and for reflection is 0.012063 seconds.

This is different from the reflection graph in **Figure 6** which shows a decrease at the beginning and then a gradual increase over a certain energy range and then if it continues again, there will be a decrease. It can also be seen directly that the energy range of 0 to 0.4 eV and the energy range above 0.6 eV the reflection value is in the range of 1 or maximum, which means that in this energy range it is not recommended for use in making electronic devices because it is almost all electrons are reflected and almost nothing can break through the material or barrier that has been arranged. If this material arrangement is applied concretely, it would be better to use a safe energy range, where the reflection graph shows the smallest value and the transmission graph shows the largest value. Based on theory and equations (15) (16), it is very common for this to happen, when

transmission increases in a certain energy range, reflection decreases. It is theoretical to show that the equations obtained in the method produce appropriate graphs of the results.

Based on **Figure 1**, it can be seen that PbSe will be side by side or will be doped with ZnTe so that the band gap resulting from the combination of the two is smaller compared to the subsequent doping of the material, namely PbTe with ZnS. This makes it easier for electrons to penetrate the barrier, provided that the energy used must not be too small or too large because the electrons must penetrate two pairs of barriers resulting from doping which has a band gap value that gets bigger to the right or as it progresses the band gap also gets bigger. In **Figure 2** and also in accordance with the research limitations, the width of the barrier used is the same, L_1, L_2, L_3, and L_4 The value is 1 nm and this does not have much impact on equation (14) on the various materials that are passed through. Basically, transmission and reflection are absolute opposites, so that when transmission reaches the largest value, this is 0.6171 at an energy of 0.5280 eV, whereas at this energy the reflection produced is only 0.3829. If added together, transmission and reflection will get the result is 1, in accordance with the theory commonly used in waves. It can be seen that the transmission value is greater than the reflection value, so it can be said that the composition of the materials analyzed in this study is good enough to be used as the main constituent of electronic devices such as LEDs, photodetectors, thermoelectric generators, etc., adjusted to the needs and external support materials.

IV. Conclusion

Based on the results of this research, the highest transmission value of the PbSe – ZnTe – PbTe – ZnS material arrangement is at an energy of 0.5280 eV, this is 0.6171, while the lowest reflection value of 0.3829 also occurs at the same energy. This research has several limitations and conditions that apply so that the results obtained are straight to the point. Iteration was also carried out in this study with the time used being 0.015423 seconds for transmission and 0.012063 seconds for reflection. In general, the results obtained are in accordance with theory because at the same energy, the transmission value is greater than reflection, so these results can be followed up concretely so that they can be used as an alternative material for making increasingly sophisticated and modern electronic devices.

References

[1]. Orefice A, Giovanelli R, Ditto D. The Dynamics Of Wave-Particle Duality. Journal Of Applied Mathematics And Physics. 2018;6(9): 1840-1859.

[2]. Chang Dc. Review On The Physical Basis Of Wave–Particle Duality: Conceptual Connection Between Quantum Mechanics And The Maxwell Theory. Modern Physics Letters B. 2021;35(13): 1-34.

[3]. Zhang L., Wu Ry, Bai Gd, Wu Ht, Ma Q, Chen Xq, Cui Tj. Transmission-Reflection-Integrated Multifunctional Coding Metasurface For Full-Space Controls Of Electromagnetic Waves. Advanced Functional Materials. 2018;28(33): 1802205.

[4]. Perez G, Maréchal A, Chicot G, Lefranc P, Jeannin Po, Eon D, Rouger N. Diamond Semiconductor Performances In Power Electronics Applications. Diamond And Related Materials. 2020;110: 1-43.

[5]. Park Jh, Kim Dy, Schubert Ef, Cho J, Kim Jk. Fundamental Limitations Of Wide-Bandgap Semiconductors For Light-Emitting Diodes. Acs Energy Letters. 2018;3(3): 655-662.

[6]. García De Arquer Fp, Talapin Dv, Klimov Vi, Arakawa Y, Bayer M, Sargent Eh. Semiconductor Quantum Dots: Technological Progress And Future Challenges. Science. 2021;373(6555): 1-16.

[7]. Haneef Hf, Zeidell Am, Jurchescu Od. Charge Carrier Traps In Organic Semiconductors: A Review On The Underlying Physics And Impact On Electronic Devices. Journal Of Materials Chemistry C. 2020;8(3): 759-787.

[8]. Chaves A, Azadani Jg, Alsalman H, Da Costa Dr, Frisenda R, Chaves Aj, Song Sh, Kim Yd, He D, Zhou K, Castellanos-Gomez A, Peeters Fm, Liu Z, Hinkle Cl, Oh Sh, Ye Pd, Koester Sj, Lee Yh, Avouris Ph, Wang X, Low T. Bandgap Engineering Of Two-Dimensional Semiconductor Materials. Npj 2d Materials And Applications. 2020;4(1): 1-29.

[9]. Woods-Robinson R, Han Y, Zhang H, Ablekim T, Khan I, Persson Ka, Zakutayev A. Wide Band Gap Chalcogenide Semiconductors. Chemical Reviews. 2020;120(9): 4007-4055.

[10]. Chilwatun N, Supriadi B, Handayani Rd. Tunnelling Effect For Quadruples Potential Using Matrix Propagation Method. Indonesian Review Of Physics. 2020;3(2): 66-73.

[11]. Agustin Nc, Nugroho Ciw, Pratama Ma. Koefisien Transmisi Inn (Indium Nitrit) Penghalang Tunggal Hingga Penghalang Tiga Dengan Metode Schrodinger. Seminar Nasional Pendidikan Fisika 2019. 2019;4(1): 102– 106.

[12]. Supriadi B, Pingki T, Mardhiana H, Faridah N, Istighfarini Et, Subiki. Transmission Coefficient Of Triple Potential Barrier Combination Structure Using Two-Dimensional Schrodinger Equation. Series Title: Advances In Physics Research. 2023;6: 146-155.

[13]. Zhang X, Shen Jx, Van De Walle Cg. Anomalous Auger Recombination In Pbse. Physical Review Letters. 2020; 125(3): 1-5.

[14]. Haq Bu, Alfaify S, Ahmed R, Laref A, Mahmood Q, Algrafy E. Optoelectronic Properties Of Pbse Monolayers From First-Principles. Applied Surface Science. 2020; 525: 1-7.

[15]. Liu X, Wang J, Riney L, Bac Sk, Smith Dj, Mccartney Mr, Khan I, Hoffman Aj, Dobrowolska M, Furdyna Jk, Assaf Ba. Unraveling The Structural And Electronic Properties Of Strained Pbse On Gaas. Journal Of Crystal Growth. 2021; 570: 1-7.

[16]. Maskaeva Ln, Yurk Vm, Markov Vf, Kuznetsov Mv, Voronin Vi, Muhamediarov Rd, Zyrianov Gv. Composition, Structure And Functional Properties Of Nanostructured Pbse Films Deposited Using Different Antioxidants. Materials Science In Semiconductor Processing. 2020; 108: 104867.

[17]. Hossain Mi, Siddiquee Kamh, Islam O, Gafur Ma, Qadir Mr, Ahmed Na. Characterization Of Electrodeposited Znte Thin Films. Journal Of Optics. 2019; 48: 295-301.

[18]. Shobana M, Meher Sr. Experimental And Ab-Initio Study Of The Structural, Electronic And Vibrational Properties Of Znte. Journal Of Alloys And Compounds. 2018; 762: 260-271.

[19]. Shobana M, Meher Sr. Experimental And Ab-Initio Study Of The Structural, Electronic And Vibrational Properties Of Znte. Journal Of Alloys And Compounds. 2018; 762: 260-271.
[20]. Panaitescu Am, Antohe Va. Study Of Optical And Electrical Properties Of Rf-Sputtered Znse/Znte Heterojunctions For Sensing Applications. Coatings. 2023; 13(1): 208.
[21]. You D, Xu C, Zhang W, Zhao J, Qin F, Shi Z. Photovoltaic-Pyroelectric Effect Coupled Broadband Photodetector In Self-Powered Zno/Znte Core/Shell Nanorod Arrays. Nano Energy. 2019; 62: 310-318.
[22]. Cao J, Querales-Flores Jd, Fahy S, Savić I. Thermally Induced Band Gap Increase And High Thermoelectric Figure Of Merit Of N-Type Pbte. Materials Today Physics. 2020; 12: 1-12.
[23]. Akinlami Jo, Omeike Mo, Akindiilete Ja, Abdulfatai Lo. Electronic Properties And The Phonon Band Structure Of Pbte. Computational Condensed Matter. 2018; 15: 90-94.
[24]. Yu Y, Kong Xg, Shen Yh, Yin Gq. First-Principles Calculations Of The Dynamical And Thermodynamic Properties Of Lead Chalcogenides Pbx (X= S, Se, Te). Chalcogenide Letters. 2022; 19(11): 1-11.
[25]. Guo D, Li C, Li K, Shao B, Chen D, Ma Y, Sun J, Cao X, Zeng W, Yang R. The Strain-Induced Excellent Thermoelectric Performance Of Pbte. Physica E: Low-Dimensional Systems And Nanostructures. 2021; 130: 114685.
[26]. Alwany Ab, Youssef Gm, Samir Om, Algradee Ma, Yahya Naa, Swillam Ma, Humaidi S, Abd-Shukor R. Annealing Temperature Effects On The Size And Band Gap Of Zns Quantum Dots Fabricated By Co-Precipitation Technique Without Capping Agent. Scientific Reports. 2023; 13(1): 10314.
[27]. Bhushan M, Jha R, Bhardwaj R. Reduced Band Gap And Diffusion Controlled Spherical N-Type Zns Nanoparticles For Absorption Of Uv-Vis Region Of Solar Spectrum. Journal Of Physics And Chemistry Of Solids. 2019; 135: 109021.
[28]. Heiba Zk, Albassam Aa, Mohamed Mb. Effect Of Zn/S Non-Stoichiometric Ratio On The Structural, Optical And Electronic Properties Of Nano-Zns. Applied Physics A. 2020; 126: 1-13.
[29]. Alvarado-Hernández L, Lapidus Gt, González F. Recovery Of Rare Earths From Waste Cathode Ray Tube (Crt) Phosphor Powder With Organic And Inorganic Ligands. Waste Management. 2019; 95: 53-58.
[30]. Xu X, Li S, Chen J, Cai S, Long Z, Fang X. Design Principles And Material Engineering Of Zns For Optoelectronic Devices And Catalysis. Advanced Functional Materials. 2018; 28(36): 1-24.