Volume 2, Issue 11 November 2016 ISSN NO: 2454 - 2326

North Asian International Research Journal Consortium

North Asian International Research Journal

Of

Multidisciplinary

CIF IMPACT FACTOR: 4.465

NAIRJC JOURNAL PUBLICATION

North Asian International Research Journal Consortium

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ISSN NO: 2454 - 2326

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CIF IMPACT FACTOR: 4.465

Theoretical Models used in Calculation of Electronic Polarizability and Refractive Index of Ternary Chalcopyrite Semiconductors: A Comparative Study

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ABSTRACT

In this work, comparative analysis was done; comparing the values of refractive index and values of electronic polarizability calculated from the theoretical models proposed by different researchers with the known values of refractive index and electronic polarizability of ternary chalcopyrite semiconductors. The Statistical Package for Social Science (SPSS) analysis tool and Microsoft excel data analysis tool was used in order to know the model that gave values of refractive index and electronic polarizability that are in perfect agreement with the known values or closest to the known values. From the result of the analysis the best model for calculating refractive index is that of Kumar and Singh ; the best model for calculating electronic polarizability is that of Moss employing the refractive index calculated from his model gave values of electronic polarizability closest to the known values for ternary chalcopyrite semiconductors, both in the range of energy gap 0.26ev≤E_g≥3.50ev; which can be extended to all other semiconductors in the range of energy gap 0.26ev≤E_g≥3.50ev.

Keywords: ***Refractive index ; Energy gap; Electronic polarizability ; SPSS analysis tool; Microsoft excel data analysis tool.***

1.0 INTRODUCTION

Ternary chalcopyrite is a type of semiconductor with the general formula $A^{I}B^{III}C_2^{VI}$ (A=Li, Cu, Na, Ag; B=Al, Ga, ln,; C= S, Se, Te) and $A^{III}B^{IV}C_2^{V}$ (A= Zn, Cd, B=Si, Sn, Ge; C=P_2,As_2). They are of considerable interest because of their potential optoelectronic applications as solar energy converters, nonlinear optical (NLO) devices, light emitting diodes (LED), and detectors. Recently, the (Cu, Ag)GaX_2 alloy system has attracted considerable attention, because this material has direct band gaps between 1.68 and 2.65ev, which is the range desirable for application in solid state lighting and high-efficiency tandem solar cells [1-2].

The refractive index and energy gap of semiconductors represent two fundamental physical aspects that characterize their optical and electronic properties .The applications of semiconductors as electronic, optical and optoelectronic devices are

very much determined by the nature and magnitude of these two elementary properties. These properties also aid in the performance assessment of band gap engineering structures for continuous and optimal absorption of broad band spectral sources. Devices such as photonic crystals, waveguides, solar cells and detectors require a pre-knowledge of refractive index and energy gap [3-4]. The refractive index of a semiconductor typically decreases with increasing energy gap E_g.

Polarizability determines the dynamical response of a bound system to external fields, and provides insight into a molecule's internal structure [5]. Electronic polarizability is the response of electrons to an applied alternating electric field. Electronic polarizbility is usually calculated using the refractive index.

Several researchers have proposed different theoretical models for calculating refractive index of semiconductors; which in turn gives different values of electronic polarizability of semiconductors. But there is a need to know which one of these models that can give values of refractive index and electronic polarizability closest to the known values of refractive index [6] .

In this work, a comparative study of the values of refractive index and electronic polarizability of ternary chalcopyrite semiconductors calculated from the theoretical models of different researchers with the known values of refractive index and electronic polarizability are done. The Statistical Package for Social Science (SPSS) [7] and Microsoft Excel [8] data analysis tool are used. The aim of the analysis is to know which model gives values of refractive index and electronic polarizability closest to the known values of refractive index and electronic polarizability.

2.0 THEORY

They have been various theoretical models relating the refractive index and Energy gap of semiconductors. The first model is of Moss [9] given as:

$$n^4 E_g = 95ev \qquad (1)$$

where n and E_g are refractive index and energy gap respectively. Moss proposed that all energy levels in a solid are scaled down by a factor $1/\varepsilon^2_{opt}$ or $1/n^4$, where n is the refractive index and ε_{opt} is the optical dielectric constant, which is equal to the square root of the refractive index.

The model of Herve and vandemme [10] given as:

$$n^2 = 1 + \left(\frac{A}{E_g + B} \right)^2 \qquad (2)$$

where A is the hydrogen ionization energy equal to 13.6ev and B =3.4ev is a constant to be the difference between UV resonance energy and band gap energy and E_g is energy gap. The relation of

equation (2) was proposed based on the assumption that ultra-violet resonance energy has a constant difference with the energy gap.

The model of Reddy *et al.* [11] given as:

$$n^2 = \left(\frac{12.417}{E_g - 0.365} \right) \qquad (3)$$

Equation (3) is the modified form of the original moss equation with a secondary arbitrary constant (0.365). The refractive index becomes negative when energy gap is less than 0.365ev; that is the disadvantage of equation (3)

The model of Ravindra *et al.* [12] given as:

$$n = 4.084 + \beta E_g \qquad (4)$$

where $\beta = -0.62 ev^{-1}$. The Ravindra *et al*. relation do not hold for high energy gap from the equation (4), n = 0, if E_g = 6.5ev which shows that semiconductors whose energy gap is high; the refractive index cannot be calculated.

The moss formula was modified for solar cells by Ravindra and Srivastava which was used to evaluate the refraction loss in order to improve the conversion efficiency of semiconductors.

The model of Anani *et al.* [13] given as:

$$n^4 = 1 + \frac{A}{E_g^{\,2}} \qquad (5)$$

Where A = 40.8ev

The model of Kumar and Singh [14] given as:

$$n = KE_g^{\,C} \qquad (6)$$

where K = 3.3668 and C = −0.32234 are the constants. They used simulation software and simulated experimental values of energy gap and refractive index and obtained the relation between n and E_g.

The model of Ahmad and Haq [15] given as:

$$n = \left(\frac{44}{E_g} \right)^{1/3} \qquad (7)$$

where n is the refractive index and E_g is the energy gap.

Tripathy [16] fitted an exponential empirical formula to the experimental values of refractive index and energy gap of some elemental and binary semiconductor over a wide range of energy gap ranging from low value of E_g= 0.1ev to a reasonably high value E_g = 8.5ev.

The proposed relationship for those data is:

$$n = n_0 + n_1 e^{(-Eg/\mu)} \qquad (8)$$

The parameters of the above relation for the best fit are found to be n_0 = 1.65752 ± 0.14605, n_1 = 3.78368 ± 0.21302, and μ = 1.85447 ± 0.25777ev. However,

in order to provide the formula to a better shape, equation (8) can be rewritten as:

$$n = n_0[1+\alpha e^{-\beta Eg}] \qquad (9)$$

The new parameters α, β and n_0 appearing in the above equation are adjusted so as to get good agreement with the experimental values of elemental and binary semiconductors over a wide range of energy gap. The parameters of the modified relation are $n_0 = 1.73$, $\alpha = 1.9017$ and $\beta = 0.539(ev)^{-1}$. While modifying the fitted relation in equation (8) the general behaviour of the model was kept intact by retaining the exponential term. Only the first term in equation (8) has been readjusted with certain normalization so as to get a better shape and results.

The Lorentz local field (E_L) can be approximated to the average local field through the dielectric polarization **P** [17] as:

$$\mathbf{F} = <\mathbf{E}_L> + L<\mathbf{P}> \qquad (10)$$

where L is the dimensionless Lorentz factor depending on the structure of the material phase and can be equated to $\frac{4\pi}{3}$. The Lorentz Lorenz formula for refractive index can be expressed as:

$$\left(\frac{n^2-1}{n^2+2}\right) = \frac{4\pi N\alpha}{3} \qquad (11)$$

N is the number of dipoles per unit volume of the material. Since refractive index for semiconductor can be determined from energy gap, its electronic polarizability (in the unit of $Å^3$; $Å = 10^{-8}cm$) can be determined using the Lorentz- Lorenz formula

$$\alpha = 0.3965\left(\frac{n^2-1}{n^2+2}\right)\frac{m}{d} \qquad (12)$$

Where m is the molecular weight and d is the mass density of the material and n is the refractive index.

Ahmad and Haq [15] proposed a model to calculate electronic polarizability expressed in terms of energy gap given as:

$$\alpha = 0.395\left[1-0.242\left(E_g - 0.4\right)^{1/2}\right]\frac{m}{d} \qquad (13)$$

electronic polarizability (in the unit of $Å^3$; $Å = 10^{-8}cm$), Eg is the energy gap, m is the molecular weight and d is the mass density.

Also, Tripathy and Anup [18] proposed a model where the electronic polarizability can be expressed in terms of the energy gap given as:

$$\alpha\left(E_g\right) = \left[\frac{0.3965}{a + bE_g{}^C}\right]\frac{m}{d} \qquad (14)$$

where a = 1.1776, b = $0.137ev^{-1}$, c = 1.0388 and E_g is the energy gap.

3.0 METHOD OF ANALYSIS

The data in table 1 containing the values of the refractive index (n) calculated from the models or relations stated above (equations: 1,2 ,3 ,4 ,5 ,6 ,7 ,9)

were analyzed using the SPSS analysis tool. Before carrying out the statistical analysis; the data were tested for normality or non normality. The reason for this test is to know the right statistical test (parametric or non parametric) to use. So, homogeneity of variance test is used to test for non normality; that is, to see if the variance across the data are homogeneous.

This was carried out in four steps as described below:

i. The ranking of the data was done: That is, the values of refractive index (n) of each models or relations are ranked. ii. The mean values of n of each model was found. iii. The absolute difference was computed; that is, ABS (Rank of values of n of each model – Mean values of n of each model). Iv. The one-way analysis of variance (ANOVA) was done in order to see if there is any difference in the variance or the variance across the values of n of each model is homogeneous. After computing the ANOVA, the significance value(p) for the variance across the data was greater than the significance level(p) or threshold value of 0.05; so, the null hypothesis (The variance across the data is homogeneous) was accepted.

The one-way ANOVA [19] is a statistical test that is carried out on two or more samples or groups to see if there is a difference of variance across those samples or groups. The significance level (α) is a probability, with a value ranging from 0.01 to 1.00 and it is used to evaluate the significance of the sample result. The null hypothesis (H_0) simply sates that there is no difference between the two groups; using this term, one can define the P value to be the probability of observing a difference as large or larger than one observed if the null hypothesis were true. So, before carrying out any statistical test one usually set a threshold α value and traditionally or mostly the α value is set to 0.05. So, if $P \leq \alpha$, the null hypothesis (H_0) is rejected and vice versa.

After confirming that the data are non-normally distributed; the Friedman two way analysis of variance by ranks [20] and Kendall's coefficient of concordance test [21] were used to see if the distribution of values of refractive index (n) across the data were the same. Results are shown in table 2. Also, the Wilcoxon signed rank test [22] was performed to test for the median difference between two related groups. . Results are shown in table 3.

The data in table 4 and table 5 containing the values of the electronic polarizability calculated from the models stated above equation (12) and equations (13 and 14) were analyzed using the SPSS analysis tool. Before carrying out the statistical analysis; the data were tested for normality or non normality. That is, are the data distributed normally or not. The reason for this test is to know the right statistical test (parametric or non parametric) to use. So, using the Shapiro Wilki test [23] to see whether the data are

normally distributed or not. After conducting the test, the P value across the data were greater than the significance level (α) or threshold value of 0.05; so, the null hypothesis (The data are normally distributed) was accepted.

After confirming that the data are normally distributed; Using Microsoft Excel the single factor analysis of variance test (ANOVA: Single factor) was used to compare the means between the values of electronic polarizability employing the refractive index calculated from the models and known values to see if there is any difference in their means. Results are shown in table 6. Before using the t-test, the F-test [24] was used to compare the variance of the known values and each of the models separately in order to know which of the two samples (known values and the calculated values from each of the models) that have equal variances or unequal variances; so that, the right t-independent test will be used because there are of two types; two sample t-test: unequal variances and two sample t-test: equal variances.

The t-independent test two-sample assuming unequal variances [25] was used to compare the means between the known values and each value of electronic polarizability using the refractive index calculated from the models separately to ascertain if there is any difference in their mean. Results are shown in table 7 and again, the t-independent test two-sample assuming unequal variances [25] was used to compare the means between the known values and values of electronic polarizability calculated from the models of Ahmad and Haq, Tripathy and Anup (equations: 13 and 14). Results are shown in table 8.

4.0 RESULT AND DISCUSSION

From table 2 the Friedman two analysis of variance by ranks the distributions of values calculated from the models and known values are not the same, since the P-value is 0.000 which is below the significance level (α) set at 0.05. So, the null hypothesis was rejected indicating that the distributions are not the same. Also, from the Kendall's coefficient test; the distributions of values from the models and known values are not the same since the P-value is below the significance level (α) set at 0.05. So, the null hypothesis was rejected indicating that the distributions are not the same.

From table 3 the related samples Wilcoxon signed rank test shows that the median of differences between values calculated from models of Moss, Herve and Vandemme, Kumar and Singh, Ahmad and Haq, Tripathy, Ravindra *et al*., Reddy *et al*. and known values equals zero since their P-values 0.052, 0.289, 0.762, 0.161, 0.088, 0.466, 0.111 are greater than the significance level (α) set at 0.05; so, the null hypothesis was accepted indicating that the median of differences between known values and values calculated from each of models are equal to zero.

The result of the median of difference between values calculated from model of Anani *et al*. and known values are not equal to zero. Since the P-value is 0.000 which is less than the significance level (α) set at 0.05; so, the null hypothesis was rejected indicating that the median of differences between values calculated from model of Anani *et al*. and known values are not equal to zero.

From table 6 the single factor analysis of variance by ranks the mean of differences between the calculated values of electronic polarizability and known values are not the same, since the P-value is 0.000, which is below the significance level (α) set at 0.05. So, the null hypothesis was rejected indicating that the means are not the same.

From table 7 the t- independent test two-sample assuming unequal variances showed that the mean of differences between values calculated from models of Moss, Herve and Vandemme, Kumar and Singh, Ahmad and Haq, Tripathy, Ravindra *et al.*, Reddy *et al.*, and known values equals zero since their P-values 0.079, 0.48, 0.40, 0.23, 0.23, 0.34, 0.14 are greater than the significance level (α) set at 0.05; so, the null hypothesis was accepted indicating that the mean of differences between known values and values calculated from each of the models are equal to zero. The result of the mean of difference between values calculated from model of Anani *et al.* and known values are not equal to zero. Since the P-value is 0.01, which is less than the significance level (α) set at 0.05; so, the null hypothesis was rejected indicating that the mean of differences between Anani et al. and known values is not equal to zero.

Also, from table 8 the result of the mean of differences between values calculated from model of Ahmad and Haq, model of Tripathy and Anup and known values equals zero. Since their P-values 0.32 and 0.41 are greater than the significance level (α) set at 0.05; so, the null hypothesis was accepted indicating that the mean of differences between known values and values calculated from each of the models equals zero.

From the result it showed that values calculated from the models of Moss, Herve and Vandemme, Kumar and Singh, Ahmad and Haq, Tripathy, Ravindra *et al.*, Reddy *et al.*, are closely related to the known values while values calculated from the model of Anani *et al.*, are not closely related to the known values. The Kumar and Singh model gave the closest values of refractive index to known values of refractive index since its P-value is 0.762 which is the highest from the rest models.

From the result it showed that values of electronic polarizability calculated from the models of Moss, Herve and Vandemme, Kumar and Singh, Ahmad and Haq, Tripathy, Ravindra *et al*., Reddy *et al.*, model of Ahmad and Haq, model of Tripathy and Anup are closely related to the known values while

the values of electronic polarizability calculated from the model of Anani *et al.* are not closely related to the known values. The Moss model gave the closest values of electronic polarizability to the known values of electronic polarizability since its P-value is 0.79 which is the highest from the rest models.

Table 1: Refractive index (n), Energy gap (E_g (ev)) and the known values of (n) of the ternary chalcopyrites

Ternary Chalcopyrites	Moss(n)	Herve&Vand.(n)	Kumar&Singh(n)	Ahmad&Haq (n)
$CUAlS_2$	2.28	2.21	2.25	2.33
$CUAlSe_2$	2.44	2.45	2.45	2.55
$CUAlTe_2$	2.61	2.68	2.67	2.78
$CUGaS_2$	2.50	2.54	2.53	2.63
$CUGaSe_2$	2.74	2.86	2.85	2.97
$CUGaTe_2$	1.06	3.10	3.15	3.30
$CUlnS_2$	2.81	2.93	2.94	3.06
$CUlnSe_2$	3.09	3.22	3.33	3.48
$CUlnTe_2$	3.16	3.28	3.42	3.59
$AgAlSe_2$	2.47	2.50	2.49	2.58
$AgAlTe_2$	2.54	2.60	2.59	2.69
$AgGaS_2$	2.46	2.48	2.47	2.57
$AgGaSe_2$	2.68	2.79	2.77	2.89
$AgGaTe_2$	2.98	3.12	3.18	3.32
$AglnS_2$	2.70	2.80	2.79	2.90
$AglnSe_2$	2.96	3.10	3.14	3.29
$AglnTe_2$	3.12	3.25	3.37	3.53
$ZnSiP_2$	2.38	2.36	2.37	2.46
$ZnGeP_2$	2.52	2.57	2.56	2.66
$ZnSnP_2$	2.75	2.87	2.86	2.98
$ZnSiAs_2$	2.59	2.66	2.64	2.75
$ZnGeAs_2$	3.02	3.15	3.22	3.37
$ZnSnAs_2$	3.38	3.44	3.73	3.92
$CdSiP_2$	2.50	2.53	2.52	2.62
$CdGeP_2$	2.73	2.84	2.83	2.95
$CdSnP_2$	3.00	3.14	3.20	3.35
$CdSiAs_2$	2.80	2.92	2.92	3.05
$CdGeAs_2$	3.59	3.57	4.04	4.26
$CdSnAs_2$	4.37	3.85	5.20	5.53

Table 1 continued

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Ternary Compounds	S.Tripathy(n)	Ravindra(n)	Reddy et al(n)	Anani et al.(n)	Known values(n)[26-27]	E_g(ev)[28-30]
$CUAlS_2$	2.23	1.91	1.99	1.44	2.40	3.50
$CUAlSe_2$	2.51	2.43	2.32	1.61	2.60	2.67
$CUAlTe_2$	2.81	2.81	2.71	1.81	3.30	2.06
$CUGaS_2$	2.62	2.58	2.45	1.68	2.67	2.43
$CUGaSe_2$	3.06	3.04	3.07	1.98	2.80	1.68
$CUGaTe_2$	3.43	3.32	3.79	2.30	3.30	1.23
$CUlnS_2$	3.17	3.14	3.27	2.07	2.60	1.53
$CUlnSe_2$	3.61	3.44	4.29	2.50	2.90	1.04
$CUlnTe_2$	3.70	3.50	4.61	2.61	3.40	0.95
$AgAlSe_2$	2.56	2.50	2.38	1.64	2.47	2.55
$AgAlTe_2$	2.70	2.68	2.55	1.73	2.54	2.27
$AgGaS_2$	2.54	2.47	2.36	1.63	2.40	2.60
$AgGaSe_2$	2.96	2.95	2.91	1.91	2.80	1.83
$AgGaTe_2$	3.45	3.34	3.86	2.33	2.30	1.20
$AglnS_2$	2.98	2.97	2.94	1.92	2.50	1.80
$AglnSe_2$	3.42	3.32	3.77	2.29	3.32	1.24
$AglnTe_2$	3.65	3.46	4.42	2.54	3.40	1.00
$ZnSiP_2$	2.40	2.25	2.19	1.54	3.40	2.96
$ZnGeP_2$	2.66	2.63	2.51	1.71	3.10	2.34
$ZnSnP_2$	3.08	3.06	3.10	1.99	2.90	1.66
$ZnSiAs_2$	2.78	2.77	2.66	1.78	2.90	2.12
$ZnGeAs_2$	3.50	3.37	3.98	2.38	3.10	1.15
$ZnSnAs_2$	3.95	3.63	5.83	2.91	3.10	0.73
$CdSiP_2$	2.61	2.57	2.44	1.67	3.10	2.45
$CdGeP_2$	3.03	3.02	3.03	1.96	3.30	1.72
$CdSnP_2$	3.48	3.36	3.93	2.36	3.10	1.17
$CdSiAs_2$	3.16	3.12	3.24	2.06	3.50	1.55
$CdGeAs_2$	4.15	3.73	7.78	3.35	3.40	0.57
$CdSnAs_2$	4.59	3.92		4.96	3.70	0.26

Table 2: Summary of the result of comparing known values with calculated values of refractive index

S/N	NULL HYPOTHESIS	TEST	SIGNIFICANCE LEVEL(α)	P-VALUE	DECISION
1	The distributions of Moss,Herve &Vand.,Kumar &singh.,S.Ahmad & Haq.,Tripathy,Ravindra,Reddy et al.,Anani et al., and known values are the same	Related samples Friedman's Two-way Analysis of variance by Ranks	0.05	0.000	Reject the null hypothesis
2	The distributions of Moss,Herve &Vand.,Kumar &singh.,S.Ahmad & Haq.,Tripathy,Ravindra,Reddy et al.,Anani et al., and known values are the same	Related samples Kendall's coefficient of concordance	0.05	0.000	Reject the null hypothesis

Table 3: Summary of the result of comparing known values with calculated values of refractive index

S/N	NULL HYPOTHESIS	TEST	SIGNIFICANCE LEVEL(α)	P-VALUE	DECISION
1	The median of differences between Moss and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.052	Retain the null hypothesis
2	The median of differences between Herve&Vandamme and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.289	Retain the null hypothesis
3	The median of differences between Kumar & Singh and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.762	Retain the null hypothesis

4	The median of differences between S.Ahmad & Haq. and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.161	Retain the null hypothesis
5	The median of differences between Tripathy and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.088	Retain the null hypothesis
6	The median of differences between Ravindra and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.466	Retain the null hypothesis
7	The median of differences between Reddy el at and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.111	Retain the null hypothesis
8	The median of differences between Anani et al and known values equals 0	Related samples Wilcoxon signed Rank Test	0.05	0.000	Reject the null hypothesis

Table 4: Electronic Polarizability (α)($Å^3$=×$10^{-24}$$cm^3$) and known values for ternary chalcopyrite

Ternary Chalcopyrite	Moss (α)	Herve and Vand.(α)	Kumar and Singh (α)	Ahmad and Haq.(α)
$CUAlS_2$	10.32	9.97	10.16	10.51
$CUAlSe_2$	13.06	13.12	13.12	13.54
$CUAlTe_2$	16.42	16.80	16.72	17.22
$CUGaS_2$	11.45	11.60	11.56	11.92
$CUGaSe_2$	14.22	14.64	14.60	15.01
$CUGaTe_2$	9.57	19.08	19.24	19.71
$CUlnS_2$	14.10	14.52	14.52	14.91
$CUlnSe_2$	17.11	17.51	17.80	18.21
$CUlnTe_2$	21.14	21.56	22.02	22.51
$AgAlSe_2$	14.42	14.55	14.52	14.98
$AgAlTe_2$	16.16	16.45	16.38	16.88

$AgGaS_2$	12.74	12.82	12.80	13.21
$AgGaSe_2$	15.35	15.78	15.72	16.16
$AgGaTe_2$	20.56	21.12	21.32	23.65
$AglnS_2$	15.38	15.81	15.76	16.20
$AglnSe_2$	21.01	21.59	21.77	22.30
$AglnTe_2$	21.61	22.08	22.49	23.00
$ZnSiP_2$	11.06	10.98	11.03	11.40
$ZnGeP_2$	12.20	12.39	12.34	12.72
$ZnSnP_2$	21.18	21.81	21.77	22.37
$ZnSiAs_2$	13.38	13.67	13.61	14.02
$ZnGeAs_2$	15.65	16.06	16.24	16.63
$ZnSnAs_2$	18.59	18.75	19.42	19.81
$CdSiP_2$	12.75	12.91	12.87	13.27
$CdGeP_2$	14.90	15.33	15.29	15.72
$CdGeAs_2$	18.94	18.88	19.82	20.17
$CdSnAs_2$	22.65	21.69	23.68	23.98

Table 4 continued

Ternary Chalcopyrite	Tripathy (α)	Ravindra et al. (α)	Reddy et al.(α)	Anani et al.(α)	Known values (α)[31]
$CUAlS_2$	10.06	8.31	8.78	4.69	6.73
$CUAlSe_2$	13.38	13.00	12.45	7.27	10.09
$CUAlTe_2$	17.39	17.36	16.91	10.70	17.17
$CUGaS_2$	11.90	11.75	11.26	6.78	7.25
$CUGaSe_2$	15.28	15.23	15.32	10.26	10.91
$CUGaTe_2$	20.10	19.79	21.00	15.13	19.20
$CUlnS_2$	15.21	15.11	15.45	10.59	8.40
$CUlnSe_2$	18.49	18.10	19.71	14.68	12.47
$CUlnTe_2$	22.80	22.23	24.54	18.57	20.86
$AgAlSe_2$	14.88	14.59	13.96	8.27	11.31
$AgAlTe_2$	16.93	16.84	16.21	9.97	19.35
$AgGaS_2$	13.10	12.79	12.24	7.22	8.22
$AgGaSe_2$	16.42	16.39	16.26	10.64	12.13
$AgGaTe_2$	22.25	21.90	23.32	16.89	20.79
$AglnS_2$	16.46	16.44	16.34	10.75	9.04
$AglnSe_2$	22.74	22.41	23.74	17.08	13.51
$AglnTe_2$	23.33	22.80	24.98	17.01	23.23
$ZnSiP_2$	11.14	10.45	10.14	11.74	12.45
$ZnGeP_2$	12.73	12.62	12.13	5.98	14.24
$ZnSnP_2$	22.78	22.70	22.88	12.00	16.36
$ZnSiAs_2$	14.13	14.10	13.68	8.59	18.12

$ZnGeAs_2$	16.93	16.64	17.84	13.03	20.52
$ZnSnAs_2$	19.86	19.21	21.95	17.30	23.84
$CdSiP_2$	13.23	13.05	12.50	7.50	14.34
$CdGeP_2$	16.00	15.95	15.98	10.64	15.95
$CdGeAs_2$	20.01	19.24	22.57	18.34	23.16
$CdSnAs_2$	22.97	21.85		23.43	26.68

Table 5: Electronic Polarizability (α)($Å^3$=×$10^{-24}cm^3$), molecular weight(g/mol), mass density(g/cm^3), known values(α) and energy gap[E_g(ev)] for ternary chalcopyrite

Ternary Chalcopyrite	molecular weight (g/mol)	Density (g/cm^3)	model of Ahmad and Haq (α)	model of Tripathy and Anup (α)	Known values(α) [31]	E_g (ev) [26-27]
$CUAlS_2$	154.65	3.47	10.10	10.51	6.73	3.50
$CUAlSe_2$	248.45	4.70	13.27	13.46	10.09	2.67
$CUAlTe_2$	345.73	5.50	17.09	16.98	17.17	2.06
$CUGaS_2$	197.39	4.35	11.74	11.82	7.25	2.43
$CUGaSe_2$	291.19	5.56	15.02	14.70	10.91	1.68
$CUGaTe_2$	388.47	5.99	19.97	19.08	19.20	1.23
$CUlnS_2$	242.49	4.75	14.98	14.56	8.40	1.53
$CUlnSe_2$	336.29	5.77	18.57	17.50	12.47	1.04
$CUlnTe_2$	433.57	6.10	23.04	21.55	20.86	0.95
$AgAlSe_2$	292.77	5.07	14.72	14.87	11.31	2.55
$AgAlTe_2$	390.05	6.18	16.68	16.70	19.35	2.27
$AgGaS_2$	241.71	4.72	12.97	13.12	8.22	2.60
$AgGaSe_2$	335.51	5.84	16.13	15.88	12.13	1.83
$AgGaTe_2$	432.79	6.05	22.14	21.12	20.79	1.20
$AglnS_2$	286.87	5.00	16.17	15.91	9.04	1.80
$AglnSe_2$	380.61	5.18	22.59	21.60	13.51	1.24
$AglnTe_2$	447.86	6.12	23.35	22.07	23.23	1.00
$ZnSiP_2$	155.40	3.39	11.10	11.36	12.45	2.96
$ZnGeP_2$	199.90	4.17	12.55	12.60	14.24	2.34
$ZnSnP_2$	246.00	3.16	22.40	21.90	16.36	1.66
$ZnSiAs_2$	242.20	4.70	13.90	13.84	18.12	2.12
$ZnGeAs_2$	287.80	5.32	16.89	16.06	20.52	1.15
$ZnSnAs_2$	333.90	5.53	20.53	18.76	23.84	0.73
$CdSiP_2$	202.43	4.00	13.06	13.16	14.34	2.45
$CdGeP_2$	246.94	4.48	15.72	15.41	15.95	1.72
$CdGeAs_2$	334.83	5.60	21.26	18.91	23.16	0.57
$CdSnAs_2$	380.93	5.72		21.80	26.68	0.26

CIF IMPACT FACTOR: 4.465

Table 6: Anova Single Factor

SUMMARY

Groups	*Count*	*Sum*	*Average*	*Variance*
Moss	27.00	425.92	15.77	14.29
Herve and vand.	27.00	441.47	16.35	13.49
Kumar and Singh	27.00	446.57	16.54	15.31
Ahmad and Haq	27.00	460.01	17.04	16.36
Tripathy	27.00	460.50	17.06	16.24
Ravindra et al.	27.00	450.85	16.70	16.32
Reddy et al.	26.00	442.14	17.01	23.32
Anani et al.	27.00	325.05	12.04	21.50
Known values	27.00	416.32	15.42	31.87
model Ahmad and Haq	26.00	435.94	16.77	16.23
model Tripathy and Anup	27.00	445.23	16.49	12.69

ANOVA

Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
Between Groups	562.61	10.00	56.26	3.13	0.00	1.86
Within Groups	5098.33	284.00	17.95			
Total	5660.93	294.00				

Table 7: comparing mean of known values and values of electronic polarizability from the models

S/N	NULL HYPOTHESIS	TEST	SIGNIFICANCE LEVEL(α)	P-VALUE	DECISION
1	The mean of differences between Moss and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.79	Retain the null hypothesis
2	The mean of differences between Herve and Vandamme and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.48	Retain the null hypothesis
3	The mean of differences between Kumar and Singh and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.40	Retain the null hypothesis
4	The mean of	t-Test Two-Sample	0.05	0.23	Retain the null

	differences between Ahmad and Haq and known values equals 0	Assuming Unequal Variances			hypothesis
5	The mean of differences between Tripathy and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.23	Retain the null hypothesis
6	The mean of differences between Ravindra et al.and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.34	Retain the null hypothesis
7	The mean of differences between Reddy el at. and known values equals 0	t-Test Two-Sample Assuming equal Variances	0.05	0.14	Retain the null hypothesis
8	The mean of differences between Anani et al. and known values equals 0	t-Test Two-Sample Assuming equal Variances	0.05	0.01	Reject the null hypothesis

Table 8: comparing mean of known values and values electronic polarizability from the two models

S/N	NULL HYPOTHESIS	TEST	SIGNIFICANCE LEVEL(α)	P-VALUE	DECISION
1	The mean of differences between Model of Ahmad and Haq and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.32	Retain the null hypothesis
2	The mean of differences between model of Tripathy and Anup and known values equals 0	t-Test Two-Sample Assuming Unequal Variances	0.05	0.41	Retain the null hypothesis

5.0. CONCLUSION

So, using the appropriate statistical analysis tool in comparing the values of refractive index of ternary chalcopyrite semiconductors with their known values; results showed that the model of Kumar and Singh gave values closest to the known values. Also comparing the values of electronic polarizability using the calculated refractive index from the different models with the known values; results showed that the model of Moss gave the closest values of electronic polarizability to the known values of electronic polarizability. So, for ternary chalcopyrite semiconductors in the range of energy gap $0.26ev \leq E_g \geq 3.50ev$, the model of Kumar and Singh , model of Moss gave the closest values of refractive index and electronic polarizability to their known values which can be extended to other semiconductors in the range of energy gap $0.26ev \leq E_g \geq 3.50ev$.

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