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Simplistic Theoretical Model for Optoelectronic Properties of Compound Semiconductors

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Abstract In order to enhance the viability of this paper for that issue, we suggest adding this to the beginning of the abstract: "Binary semiconductors with ($A^{II}B^{VI}$ and $A^{III}B^{V}$) composition and ternary semiconductors ($A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) composition, owing to their devices such as photonic crystals, wave guides, solar cells and detectors, are technologically important materials. The recent successful fabrication of the blue-green laser diode based on these compounds has renewed interest in their opto-electronic properties. In this paper we present a relationship to evaluate opto-electronic properties such as electronic polarizability (α), refractive index (n), band gap (Eg) and optical electronegativity ($\Delta\chi$*) in terms of product of ionic charges (PIC) and average atomic number of constituent atoms (Z_{av}) for zinc blende ($A^{II}B^{VI}$ and $A^{III}B^{V}$) and chalcopyrites ($A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) structured solids. The electronic polarizability (α), refractive index (n), band gap (E_g) and optical electronegativity ($\Delta\chi$) of these solids exhibit a linear relationship when plotted against the average atomic number constituent atoms (Z_{av}), but fall on different lines due to the region of product of the ionic charges (PIC) of the compounds. We have applied the proposed relation on these solids and found a better agreement with the experimental data as compared to the values evaluated by earlier researchers so far.

Keywords: *referactive index, band gap, optical electronegativity, chalcopyrites*

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1. Introduction

One of the properties of semiconductors, which are very important for device applications, is the band gap. The best values of the band gap are obtained by optical absorption. If the band gap is sufficiently small, thermal excitation can promote an electron from the valence band to the conduction band. If impurities are present in the band gap, thermal excitation can also be used to excite an electron from an impurity level to the conduction band [1,2,3]. Thus, the measurements of electrical resistance of the specimen as a function of temperature can be used to determine the band gap of the specimen. The refractive index of a material is one of the key parameter for device design in nearly all fields of modern electronics. Furthermore, it is of fundamental importance for the behaviour of charge carriers, dopants, defects and impurities in insulators and semiconductors. Electronegativity is one of the useful parameter in explaining and even predicting many properties related to the energy and charge distribution in chemical bonds. The properties include the ionic character, the charge distribution, the degree of polarity of the bond dissociation energies, the bond moments and the force constants [4].

Tetrahedrally coordinated semiconductors of the chemical formula $A^{N}B^{8-N}$ have been extensively studied because of their technical and scientific importance and have the zinc blende crystallographic structure. Chalcogenide and pnictide semiconductors with the formula $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ have been widely studied because of their possible technological applications as photo-voltaic detectors, solar cells, light emitting diodes, modulators, filters and their use in nonlinear optics [5,6,7,8].

Recently [9,10,11]' numerous attempts have been made to understand the electronic, mechanical, elastic and optical properties of these semiconductors. There is a great deal of interest, both experimental and theoretical in the solid state properties of semiconductors. Experimental and also theoretical methods for calculating these material properties have been well understood and established for binary and ternary semiconductors. Due to the difficulties of the experimental process and its cost as well as difficulties of getting accurate values of optoelectronic properties and due to the long process as well as complicated computational methods and a series of approximations, such a method has always been the complicated one, researchers moved to calculate these parameter through theoretical methods.

Theoretical calculations based on empirical relations have become an essential part of material research. These relations do not give highly accurate results for each specific material, but they still can be extremely useful. In particular, the simplicity of empirical relations allows a broader class of researchers to calculate useful properties, and often trends become more evident. Empirical concepts such as valence, empirical radii, ionicity and plasmon energy are directly associated with the character of the chemical bond and thus provide means for explaining and classifying many basic properties of molecules and solids [12,13,14].

Recently, Verma and co-authors [15,16,17,18] have been evaluated the structural, electronic, mechanical and ground state properties of binary and ternary crystals with the help of ionic charge theory of solids. Therefore we thought it would be of interest to give an alternative explanation for electronic polarizability (α in $Å^3$), band gap (E_G in eV), refractive index (n) and optical electronegativity ($\Delta\chi^*$) of compound semiconductors.

2. Previous Theories for the Analysis of Optoelectronic Properties of Solids

Some simplistic theoretical methods were established that can predict electronic polarizability, band gap, refractive index and optical electronegativity of binary and complex structured solids from selected atomic properties of their constituent elements. First, Chemla [19] has defined a simplistic relation for the average bond polarizability {$\alpha_{(XY)}$, (XY = AC and BC bonds)} of a tetrahedrally coordinated compound in terms of average energy gap or Penn gap (E_p) as follows:

$$\alpha_{XY} = \frac{(2a_o)^3 E_o^2 D_{XY}}{(E_p)^2_{XY}} \quad (1)$$

where $a_o = \hbar^2/me^2$ and $E_o = me^4/2\hbar^2$. The correction term D_{XY} has been introduced to take into consideration the contribution of the core electrons [20]. Using equation (1) the bond polarizabilities have been investigated for individual bonds in a molecule. The total polarizability has been evaluated by summing the polarizabilities of two bonds in the molecule.

$$\alpha_{\text{Total}}(ABC_2) = \alpha(AC) + \alpha(BC) \quad (2)$$

Based on the Clausius–Mossotti equation [21], a relation has been developed by Ravindra and Srivastava [22,23] for the calculation of electronic polarizability of binary crystals from their plasmon energy ($\hbar\omega_p$) and Penn gap (E_p), and later on used by Reddy et al [24], in the case of some AIIBVI semiconductors.

Recently, Reddy *et al [25]*, have proposed a relation between the bulk modulus (B) and electronic polarizability as follows:

$$\alpha = 0.395\times10^{-24}\times\frac{(5.563-0.33B)^2-1}{(5.563-0.33B)^2+2}\times\frac{M}{\sigma}cm^3 \quad (3)$$

where *M* is the molecular weight, is the density of the substance. Kumar *et al [26]*, have developed a relation based on the plasma oscillations theory of solids for the calculation of electronic polarizability of $A^{II}B^{VI}$ and $A^{III}B^{V}$ semiconductors and electronic polarizability of these semiconductors may be expressed as,

$$\alpha = ae^{-bh\omega p} \quad (4)$$

where 'a' and 'b' are constants. The numerical values of the constants 'a' and 'b' are, respectively, 46.470 and 0.124 for $A^{II}B^{VI}$ group and 61.586 and 0.129 for $A^{III}B^{V}$ group of semiconductors. The energy of a quantum of plasma oscillations of the valence electrons in both metal and compound is given by the relation [26],

$$h\omega_p = 28.8\sqrt{\frac{Z\sigma}{M}} \quad (5)$$

where Z is the effective number of valence electrons taking part in the plasma oscillations. Equation (5) is valid for free electrons but it is also applicable for semiconductors and insulators, up to a first approximation.

For the band gap, Moss [27,28], has proposed a general relationship based on the concept that in a dielectric energy, levels are scaled by a factor ε_∞^2, (where $\varepsilon_\infty = n^2$ is the optical dielectric constant) i. e.

$$E_g = \frac{95}{n^4}eV \quad (6)$$

Ravindra et. al. [29,30], have proposed another linear relationship,

$$n = 4.084 - 0.62E_g \quad (7)$$

Based on the oscillatory theory, Herve and Vandamme [31], have proposed the following for the refractive index,

$$n = \sqrt{1+\left(\frac{A}{E_g}+B\right)^2} \text{ where } A = 13.6 \text{ and } B = 3.4 \text{ eV} \quad (8)$$

Recently, Anani et al [32], have proposed an empirical relationship between referative index(n) and band gap (E_g) of solids and is as follows,

$$E_g = 17 - 5neV \quad (9)$$

Optical electronegativity is one of the most important parameter in understanding the nature of chemical bonding, and several important physical parameters can be predicted by using it. The correlation between band gap (E_g) and optical electronegativity has been enlightened by Duffy [33,34] in various binary systems. Duffy [33,34] has made an attempt to describe the metallic character of chemical bonding for compounds that are inadequately described in a solely "ionic/covalent" framework from the point of view of band gap electronegativity. Optical absorptions for a semiconductor or insulator arise through electron transfers from the valence band to the conduction band. The transfer of electrons from an anion to a cation and the associated optical absorption is known as "electron transfer" or "charge transfer absorption". Duffy [33,34] has well established the above concept and introduced it in terms of the "optical electronegativity" and may be determine by the following relation,

$$\Delta\chi^* = 0.2688\ E_g \quad (10)$$

Where $\Delta\chi^* = \chi^*_{anion} - \chi^*_{cation}$ with χ^*_{anion} and χ^*_{cation} being the optical electronegativities of the anion and cation resepectively.

Salem [2] has studied refractive index of compound semiconductors by the following relation,

$$n = \frac{(2.5)^m}{(\Delta\chi^* - D)^{1/4}} \quad (11)$$

where m and D are numerical constants, which depends group of semiconductors.

Reddy et al [3], have studied band gap in terms of optical electronegativity by the following relation,

$$E_g = 1 + \frac{97}{\left[\ln\left(\frac{9.76}{\Delta\chi^*}\right)\right]} \quad (12)$$

Recently, Reddy et al [1], have proposed an empirical relationship between refrative index (n) and optical electronegetivity ($\Delta\chi^*$) of solids and is as follows,

$$\Delta\chi^* = 9.8e^{-n} \quad (13)$$

where n is refractive index.

The energy gap (E_g) of semiconducting or insulating compounds, involves transference of an electron from the valence band to the conduction band. Since, usually, the valence band involves primarily orbitals of the anion, while the conduction band involves primarily orbitals of cation, it seems reasonable to expect some numerical parameter, e.g. ionisation energy, electronegativity, etc, of cation and anion to be correlatable with E_g. The problem has been discussed in detail [27,28,29,30], but correlations which have been made are restricted to small groups of compounds and no overall correlation has yet been found to operate for ternary compounds generally.

3. Concept of Ionic Charge Theory and Proposed Relations

Any change in the crystallographic environment of an atom is related to core electrons via the valence electrons. The change in wave function that occurs for the outer electrons usually means a displacement of electric charge in the valence shell so that the interaction between valence, shell and core electrons is changed. This leads to a change in binding energy of the inner electron and to a shift in the position of the absorption edge. A chemical bond is formed when the atoms with incomplete valence shells combine. There are following main types of bonds:

1. Ionic or electrovalent bond
2. Covalent bond
3. Coordinate bond
4. Metallic bond

The valence electrons refer to the electrons that take part in chemical bonding. These electrons reside in the outer most electron shell of the atom. The participation of valence shell electrons in chemical bonding may be explained on the basis of following grounds.

(i) The outermost-shell electrons are farthest away from the nucleus and therefore, are not very firmly bound to the nucleus. As such these are easier to remove due to low ionization energy.

(ii) The outermost-shell electrons of an atom are also close to any foreign atom that may approach them and are therefore the first to be attracted by the approaching atom.

Using this idea to get better agreement with experimental and theoretical data for the electronic polarizability (α), refractive index (n), optical electronegativity ($\Delta\chi^*$) and band gap (E_g) of zinc blende and chalcopyrite crystals may be written in terms of product of ionic charges (PIC) and average atomic number of constituent atoms (Z_{av}) of the compounds as,

For binary crystals,

$$\alpha = 0.24(PIC)^{0.5} Z_{av}^{0.75} \quad (14a)$$

For ternary solids

$$\alpha = 1.13(PIC)^{0.5} Z_{av}^{0.75} \quad (14b)$$

For binary crystals,

$$\text{Refractive index(n)} = 1.79(\text{PIC})^{0.75}(Z_{av})0.01 \quad (15a)$$

For ternary crystals,

$$\text{Refractive index(n)} = 1.1(\text{PIC})^{0.15}(Z_{av})0.15 \quad (15b)$$

For zinc blende crystals,

$$\text{Optical electronegativity}(\Delta\chi^*) = \frac{25}{(PIC)^{0.65}(Z_{av})^{0.75}} \quad (16a)$$

For chalcopyrite crystals ($A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$),

$$\text{Optical electronegativity}(\Delta\chi^*) = \frac{36.4}{(PIC)^{0.4}(Z_{av})^{0.9}} \quad (16b)$$

$$\text{Band gap}(E_g) = \frac{160}{\text{PIC}(Z_{av})^{0.35}}\ \text{eV} \quad (17)$$

It is obvious that the valence structures of the compounds can be written as A+ B3+ C22- (A = Cu, Ag; B = Al, Ga, In; C = S, Se, Te) and A2+ B4+ C23- (A = Zn, Cd; B = Si, Ge, Sn; C = P, As). Therefore the product of ionic charges (PIC) is 4 for $A^{II}B^{VI}$, 9 for $A^{III}B^{V}$, 12 for $A^IB^{II}IC_2^{VI}$ and 48 for $A^{II}B^{IV}C_2^{V}$.

4. Curves between the Optoelectronic Properties and Average Atomic Number of the Compounds

We have plotted $\Delta\chi^*$ Vs Z_{av} and n Vs Z_{av} curve for $A^{II}B^{VI}$ and $A^{III}B^{V}$ semiconductors, which are presented in figure 1 and figure 2; we observe that in the plot of optical electronegativity and average atomic number of

compounds and refractive index and average atomic number of compounds, the group $A^{III}B^{V}$ semiconductors lie on line nearly parallel to the group $A^{II}B^{VI}$ semiconductors. Similarly, we have plotted Eg Vs Z_{av}, $\Delta\chi^*$ Vs Z_{av}, n Vs Z_{av} and Vs Z_{av} curves for $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrites, which are presented in the following figure 3, figure 4, figure 5 and figure 6. We observed that in the plot of optical electronegativity, band gap and refractive index value increase or decrease with two distinct lines like as the group $A^{III}B^{V}$ semiconductors lie on line nearly parallel to the group $A^{II}B^{VI}$ semiconductors and the $A^{I}B^{III}C_2^{VI}$ chalcopyrites lie on line nearly parallel to the line for the $A^{II}B^{IV}C_2^{V}$ chalcopyrites. If we plot all values with product of ionic charges (PIC) and average atomic number (Z_{av}) of the compounds, these are presented in figure 7 and figure 8. We found all values close on a single line and found a single relation by curve fitting method.

5. Results and Discussions

The refractive index, optical electronegativity and band gap are important optoelectronic properties of a material. The band gap determines the threshold for absorption of photons in semiconductors. The refractive index in the semiconductor is a measure of its transparency to incident spectral radiation. T. S. Moss [27,28], suggest a basic relationship between these two properties using the common theory of photoconductivity, which was based on the photo effect studies of Mott and Gurney [35], Smekal [36], Zwicky [37], Gudden and Pohl [38] and Pearson and Bardeen [39]. Pauling [13], was the primary to launch the nature of chemical bonding using the electronegativity model. It may be examined from the tables that as the ($\Delta\chi^*$) values for the collection of semiconductors with the widespread cation decreases, their refractive index increases. The tendency is pretty repeal in the case of ionic molecules. Most of the chalcopyrites energy gap (Eg) and optical electronegativity ($\Delta\chi^*$) values lie between 0.95 and 3.00 eV and 0.2 and 0.9 respectively. According to Pauling [13], the nature of crystal composition can also be understood with the help of the ionicity. Electronegativity disparity of the compound elements will give a thought of degree of ionicity. The magnitude of optical electronegativity indicates the nature of the bonding in the materials. If $\Delta\chi^*$ is high, the material is considered as ionic in nature and if its magnitude is fewer, the materials are said to be covalent in nature. Further relations were expanded as a alteration or addition to the Moss and Ravindra relations. While the Moss formula is limited by the structure of the material, the Ravindra relation is controlled by the refractive index. From the Ravindra relation, the refractive index cannot be greater than a value of 4.1, which corresponds to an energy gap of 6.587 eV. In an effort to broaden the application of these two concepts; several authors [40,41], have presented variations of the Moss and Ravindra relations. Although the properties of the $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors have been widely examined and several of these compounds have attracted awareness for practical applications [42], the knowledge of their electronic and optical properties such as band gap (E_g), refractive index (n) and optical electronegativity ($\Delta\chi^*$) are rather incomplete. Experimental data are available for few compounds for chalcopyrite series $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ so there are many properties of the solid solution, which have not been investigated. Therefore we thought it would be of attention to provide an option description for refractive index, band gap and optical electronegativity of zinc blende ($A^{II}B^{VI}$ and $A^{II}B^{V}$) and chalcopyrite ($A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$) semiconductors.

The physical concept behind the Eq. (6) is that the refractive index is related to the high frequency dielectric constant of the crystals [27,28]. The dielectric constant also depends on the product of ionic charge and average atomic number of constituent atoms [18]. Thus, there must be a correlation between refractive index and product of ionic charge and average atomic number of constituent atoms. Moss [27,28] and Reddy et al [41], band gap and optical electronegativity depends on the refractive index. So according to above description there must be a correlation between product of ionic charge and band gap and optical electronegativity. The proposed empirical relations (14)-(17) have been applied to evaluate refractive index, optical electronegativity values for $A^{III}B^{V}$, $A^{II}B^{VI}$, $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ semiconductors and band gap for $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ semiconductors. The values so obtained are presented in the following Table 1 and Table 2 compared with the experimental and theoretical data reported so far. We note that the evaluated values of refractive index, optical electronegativity and band gap by the proposed relations are in close agreement with the experimental data as compared to the values reported by previous researchers so far. Using the present model, we can calculate these material properties of other new compounds without the knowledge of the experimental data except the nearest neighbour distance very easily.

6. Summary and Conclusions

There are several methods in determining optoelectronic properties in semiconductors, but due to the small changes of the unit cell dimensions, the accuracy of determining these parameters always have been unpredictable. Furthermore, we found that in the compounds investigated here, the electronic polarizability, band gap, optical electronegativity and refractive index exhibit a linear relationship when plotted against the average atomic number of the constituent atoms, but fall on different straight lines according to the product of ionic charges of the compounds, which are presented in figure 1 - figure 6. From the results and discussion obtained by using the proposed empirical relation, it is quite obvious that the electronic polarizability, band gap, optical electronegativity and refractive index reflecting the optoelectronic properties can be expressed in terms of product of ionic charges and average atomic number of the constituent atoms of these materials. The calculated values are presented in Table 1 - Table 2. According to this idea we may evaluate all-important properties of binary and ternary solids using their product of ionic charges and average atomic number of the constituent atoms, which are basic parameters. An

excellent agreement between the author's calculated values of these material properties and the values reported by different researchers has been found. It is also to be note worthy that proposed empirical relation is simpler, widely applicable and values obtained are in better agreement with experiment data as compared to the empirical relations proposed by previous researchers. The method presented in this work will be helpful to material scientists for finding new materials with desired electronic polarizability, refractive index, optical electronegativity and band gap among a series of structurally similar materials.

Table 1. Values of optical electronegativity (Δχ*), refractive index (n) and electronic polarizability α (Å3) for binary (Product of ionic charges (PIC) = 4 for $A^{II}B^{VI}$ and PIC = 9 for $A^{III}B^{V}$) tetrahedral semiconductors

Solids	PIC	Z_{av}	Δχ* [40]	Δχ* Duffy's [33,34]	Δχ* This work	n (Exp.) [41]	n (Moss) [41]	n (Ravindra) [41]	This work	α(Å3) [22]	α(Å3) [21]	α(Å3) [25,26]	α(Å3) This work
ZnS	4	23	0.948	1.05	0.967	2.27	2.28	1.89	2.27	5.69	5.46 , 5.65	5.35	5.04
ZnSe	4	32	0.691	0.8	0.755	2.43	2.47	2.49	2.50	6.5	6.54 , 6.81	6.16	6.46
ZnTe	4	41	0.605	0.7	0.627	2.7	2.55	2.68	2.74	8.11	8.16 , 8.00	7.26	7.78
CdS	4	32	0.643	0.7	0.755	2.38	2.51	2.6	2.50	7.05	7.22 , 7.78	7.12	6.46
CdSe	4	41	0.455	0.45	0.627	2.49	2.74	3.03	2.74	7.91	8.27 , 9.12	8.25	7.78
CdTe	4	50	0.385	0.035	0.540	2.7	2.85	3.19	3.01	10.15	10.36 , 11.0	9.73	9.03
HgS	4	48			0.557				2.95				8.75
HgSe	4	57	0.568		0.489	2.72	2.59	2.77	3.24				9.96
HgTe	4	66			0.438				3.56				11.11
AlP	9	14	0.804	0.8	0.828	2.75	2.37	2.23	2.25	7.08	6.50 , 5.92	6.88, 6.27, 6.04	5.21
AlAs	9	23	0.578	0.6	0.571	3	2.58	2.75	2.61	8.33	8.16, 7.51	7.83, 7.62	7.56
AlSb	9	32	0.428	0.4	0.445	3.19	2.78	3.09	3.03	10.1	10.23, 9.59	10.75, 10.54	9.69
GaP	9	23	0.6	0.6	0.571	2.9	2.55	2.7	2.61			7.03, 6.70	7.56
GaAs	9	32	0.361	0.4	0.445	3.3	2.9	3.25	3.03			8.31, 8.18	9.69
GaSb	9	41	0.217	0.2	0.370	3.79	3.29	3.58	3.52			11.38, 10.64	11.67
InP	9	32	0.34	0.3	0.445	3.1	2.94	3.3	3.03			9.06, 9.33	9.69
InAs	9	41			0.370				3.52			9.72, 10.48	11.67
InSb	9	51	0.048	0.1	0.314	3.95	4.8	3.97	4.15			12.74, 13.20	13.74

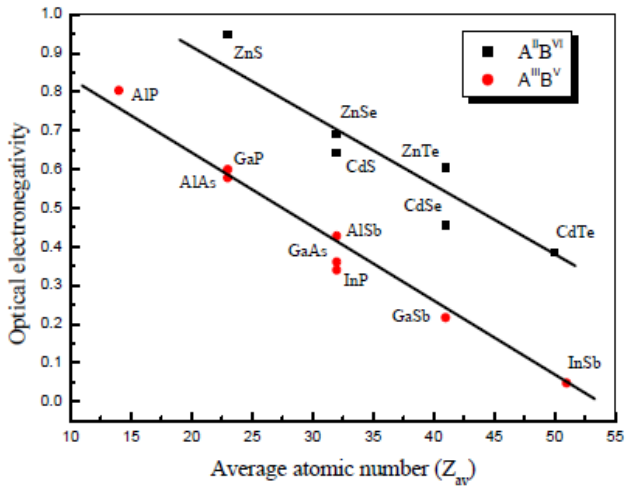

Figure 1. Plot of Δχ* (optical electronegativity) against Z_{av} (Z_{av} = average atomic number of compounds) for IIIBV and AIIBVI semiconductors. In the plots of Δχ* and Z_{av}, AIIIBV semiconductors lie on line nearly parallel o the line for AIIBVI semiconductors. In this plot all data are taken from reference [40]

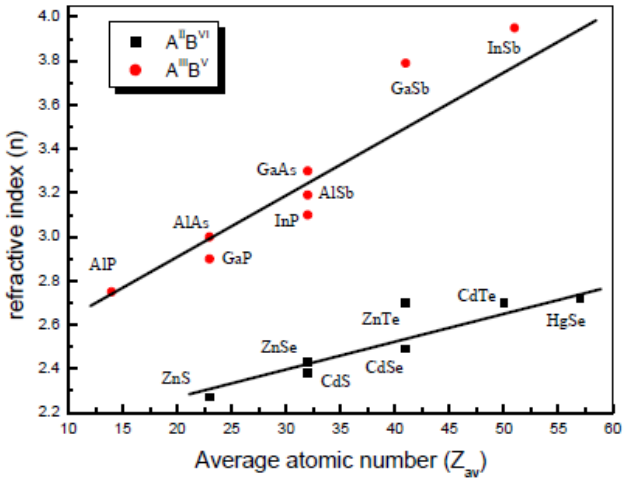

Figure 2. Plot of n (refractive index) against Z_{av} (Z_{av} = average atomic number of compounds) for $A^{III}B^{V}$ and $A^{II}B^{VI}$ semiconductors. In the plots of n and Z_{av}, $A^{III}B^{V}$ semiconductors lie on line nearly parallel to the line for $A^{II}B^{VI}$ semiconductors. In this plot all experimental data are taken from reference [41]

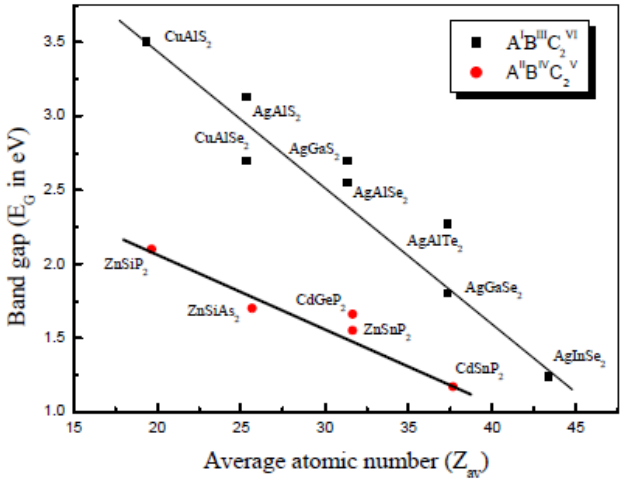

Figure 3. Plot of E_g (band gap) against Z_{av} (Z_{av} = average atomic number of compounds) for $A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors. In the plots of E_g and Z_{av}, $A^IB^{III}C_2^{VI}$ chalcopyrites lie on line nearly parallel to the line for $A^{II}B^{IV}C_2^{V}$ chalcopyrites. In this plot all data are taken from reference [40,41]

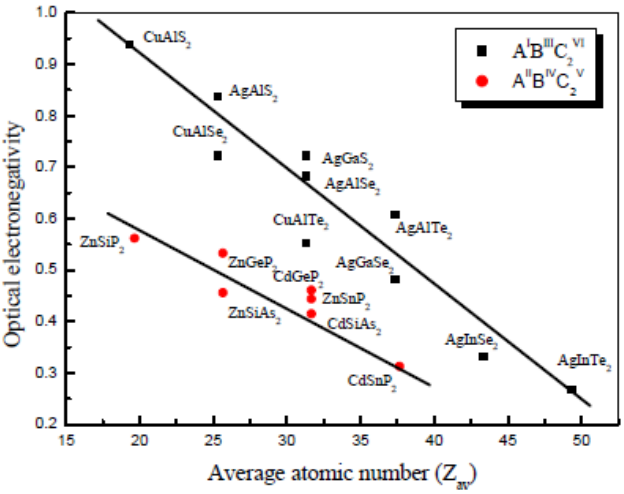

Figure 4. Plot of $\Delta\chi^*$ (optical electronegativity) against Z_{av} (Z_{av} = average atomic number of compounds) for $A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors. In the plots of $\Delta\chi^*$ and Z_{av}, $A^IB^{III}C_2^{VI}$ chalcopyrites lie on line nearly parallel to the line for $A^{II}B^{IV}C_2^{V}$ chalcopyrites. In this plot all data are taken from reference [40,41]

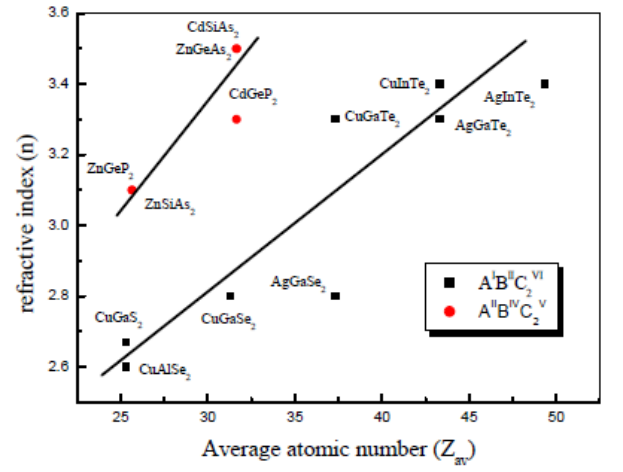

Figure 5. Plot of n (refractive index) against Z_{av} (Z_{av} = average atomic number of compounds) for $A^IB^{III}C_2V^I$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors. In the plots of n and Z_{av}, $A^IB^{III}C_2^{VI}$ chalcopyrites lie on line nearly parallel to the line for $A^{II}B^{IV}C_2^{V}$ chalcopyrites. In this plot all experimental data are taken from reference [41]

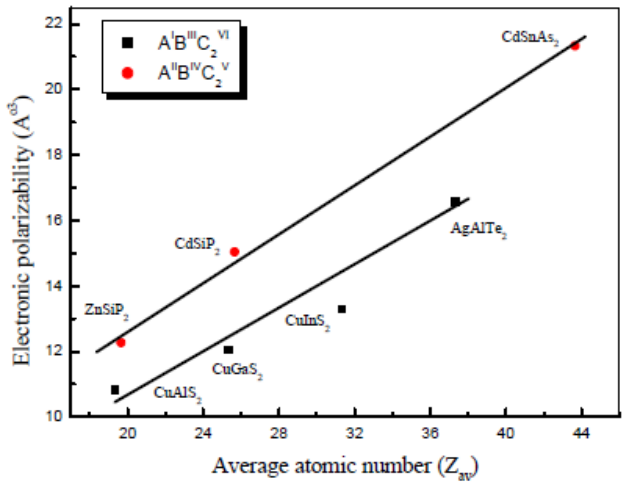

Figure 6. Plot of a (electronic polarizability in Å3) against Z_{av} (Z_{av} = average atomic number of compounds) for $A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors. In the plots of a and Z_{av}, $A^IB^{III}C_2^{VI}$ chalcopyrites lie on line nearly parallel to the line for $A^{II}B^{IV}C_2^{V}$ chalcopyrites. In this plot all data are taken from reference [25]

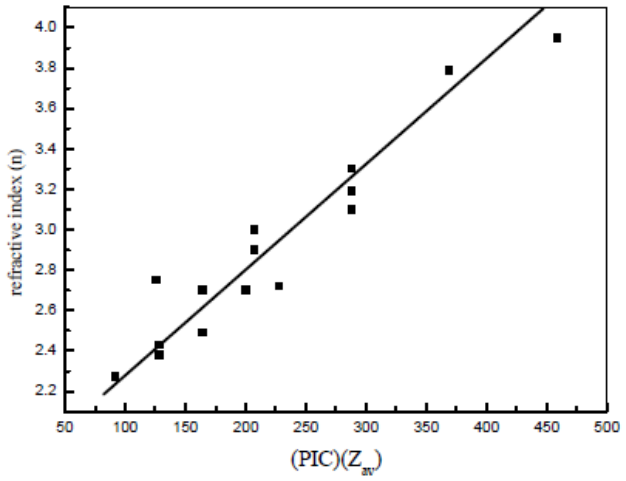

Figure 7. Plot of n (refractive index) against (PIC Z_{av}) (PIC = product of ionic charges; Z_{av} = average atomic number of compounds) for $A^{III}B^{V}$ and $A^{II}B^{VI}$ semiconductors. In this plot we found all values close on a single line. In this plot all experimental data are taken from reference [41]

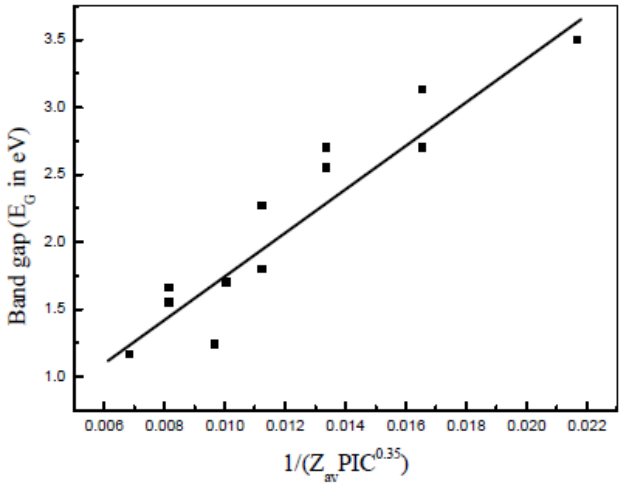

Figure 8. Plot of E_g (band gap in eV) against 1/(PIC)0.35(Z_{av}) (PIC = product of ionic charges; Z_{av} = average atomic number of compounds) for $A^IB^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ chalcopyrite semiconductors. In this plot we found all values close on a single line. In this plot all data are taken from reference [40,41]

Table 2. Values of electronic polarizability α(Å3), band gap E_G (eV), optical electronegativity (Δχ*) and refractive index (n) and for ternary (Product of ionic charges (PIC) = 12 for $A^IB^{III}C_2^{VI}$ and PIC = 48 for $A^{II}B^{IV}C_2^V$) tetrahedral semiconductors

Solids	Z_{av}	α(Å3) [43]	α(Å3) [43]	α(Å3) [25]	α(Å3) [This work]	E_G (eV) [40,41]	E_G (eV)[This work]	Δχ* [40,41]	Δχ* [This work]	n (Exp.) [41]	n (Moss) [41]	n (Ravindra) [41]	n (this work)
$CuAlS_2$	19.3	6.73	11.06	10.82	10.814	3.5	3.47	0.938	0.937				2.49
$CuAlSe_2$	25.3	10.09	13.7	13.76	13.244	2.7	2.65	0.723	0.735	2.6	2.44	2.41	2.59
$CuAlTe_2$	31.3	17.17		19.1	15.534	2.06	2.14	0.552	0.607	3.3	2.61	2.81	2.68
$CuGaS_2$	25.3	7.25	12.04	12.06	13.244	2.4	2.65	0.643	0.735	2.67	2.51	2.6	2.59
$CuGaSe_2$	31.3	10.91	14.24	15.27	15.534	1.7	2.14	0.455	0.607	2.8	2.74	3.03	2.68
$CuGaTe_2$	37.3	19.2		19.7	17.715	1	1.80	0.268	0.518	3.3	3.12	3.46	2.75
$CuInS_2$	31.3	8.42	13.1	13.29	15.534		2.14		0.607				2.68
$CuInSe_2$	37.3	12.47		16.42	17.715		1.80		0.518				2.75
$CuInTe_2$	43.3	20.86		22.63	19.810	0.95	1.55	0.254	0.453	3.4	3.17	3.49	2.81
$AgAlS_2$	25.3	9.02			13.244	3.13	2.65	0.838	0.735		2.35	2.15	2.59
AgAlSe2	31.3	11.31		13.68	15.534	2.55	2.14	0.683	0.607		2.47	2.5	2.68
$AgAlTe_2$	37.3	19.35		16.07	17.715	2.27	1.80	0.608	0.518		2.55	2.68	2.75
$AgGaS_2$	31.3	8.22	12.47	14.43	15.534	2.7	2.14	0.723	0.607	2.4	2.44	2.41	2.68
$AgGaSe_2$	37.3	12.13	14.79	16.57	17.715	1.8	1.80	0.482	0.518	2.8	2.7	2.97	2.75
$AgGaTe_2$	43.3	20.79		21.73	19.810	1.1	1.55	0.294	0.453	3.3	3.05	3.4	2.81
$AgInS_2$	37.3	9.04		14.45	17.715		1.80		0.518				2.75
$AgInSe_2$	43.3	13.51	13.96	20.08	19.810	1.24	1.55	0.332	0.453		2.96	3.31	2.81
$AgInTe_2$	49.3	23.23		24.08	21.833	1	1.36	0.268	0.403	3.4	3.12	3.46	2.87
$ZnSiP_2$	19.7	12.45	13.4	13.15, 12.27	11.184	2.1	2.10	0.562	0.530	3.1	2.6	2.78	3.07
$ZnGeP_2$	25.7	14.24	14.27	14.18, 13.54	13.656	1.98	1.61	0.533	0.417	3.1	2.63	2.85	3.20
$ZnSnP_2$	31.7	16.36	13.95	14.54	15.986	1.66	1.30	0.444	0.345	2.9	2.75	3.06	3.30
$ZnSiAs_2$	25.7	18.12	15.2	15.67, 15.04	13.656	1.7	1.61	0.456	0.417	3.1	2.74	3.03	3.20
$ZnGeAs_2$	31.7	20.52		16.83, 16.82	15.986	1.15	1.30	0.308	0.345	3.5	3.02	3.37	3.30
$ZnSnAs_2$	37.7	23.84		19.11, 19.10	18.208		1.10		0.295				3.39
$CdSiP_2$	25.7	14.34	14.84	14.98, 13.58	13.656	2.45	1.61	0.656	0.417	3.1	2.5	2.56	3.20
$CdGeP_2$	31.7	15.95	17.4	16.75, 16.05	15.986	1.72	1.30	0.461	0.345	3.3	2.73	3.02	3.30
$CdSnP_2$	37.7	18.4	17.7		18.208	1.17	1.10	0.313	0.295	3.1	3.01	3.36	3.39
$CdSiAs_2$	31.7	20.71			15.986	1.55	1.30	0.415	0.345	3.5	2.8	3.12	3.30
$CdGeAs_2$	37.7	23.16	18.4	18.99, 18.43	18.208		1.10		0.295				3.39
$CdSnAs_2$	43.7	26.68	21.36	21.47, 21.33	20.343		0.95		0.259				3.46

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