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Optical Dielectric and Electronic Properties of Rare Earth Solids

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***Abstract** – An overview of the understanding of correlation between valence electron plasmon energy and the optical properties such as optical dielectric constant (ε_∞) of ternary $A^{I}B^{III}C^{VI}_{2}$ and $A^{II}B^{IV}C^{V}_{2}$ semiconductors is presented here. We have presented an expression relating the optical dielectric constant of ternary ($A^{I}B^{III}C^{VI}_{2}$ and $A^{II}B^{IV}C^{V}_{2}$) chalcopyrites with the plasmon energy ($\hbar\omega_p$). The dielectric constant of these solids exhibit a linear relationship when plotted on a log–log scale against the plasmon energy $\hbar\omega_p$ (in eV) and the data points are lies on the straight line. We have applied the proposed relation on these semiconductors and found a better agreement with the values evaluated by earlier researchers.*

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1. INTRODUCTION

Compound semiconductors with a dynamic structure of the form $A^{I}B^{III}C^{VI}_{2}$ & $A^{II}B^{IV}C^{V}_{2}$ have attracted considerable attention because of their interesting semiconducting, mechanical, electrical, structural and optical properties. Contrasted with the twofold analogs these mixtures have higher energy holes and lower dissolving focuses as a result of which they are viewed as significant in precious stone development examines gadget applications. The ternary mixtures are immediate hole semiconductors with tetragonal chalcopyrite precious stone design. These groups of fabric are important in numerous fields including non-straight optoelectronic, optics and photograph voltaic gadgets. The composition of chalcopyrite this is appeared in figure- 1, is normal to the mixtures of substance recipe $A^{I}B^{III}C^{VI}_{2}$ and $A^{II}B^{IV}C^{V}_{2}$. Structurally these compounds are gotten in comparison to the paired sphalerite structure (III-V and II-VI) with a slight distortion. Consequently, similar to twofold mixtures They own a high non-straight powerlessness. Nevertheless, by virtue of the occurrence of two sorts of bonds in chalcopyrites they become anisotropic. This anisotropy prompts high birefringence. High non-straight defense lessness combined with high birefringence in these mixtures makes them exceptionally valuable for effective second symphonious age and stage coordinating. Aside from it the other significant mechanical uses of these material are in light radiating diodes, infrared locators, infrared motions, lasers etc. [1-9].

Owing to the troubles related with exploratory cycles and their expense, just as challenges in getting exact estimations of actual properties, scientists moved to computing the actual properties of solids through hypothetical techniques. However, regardless of the lengthy process and the complicated computational methods involving series of approximations, such a method has always been complicated [10]. During the last few years, There has been a lot of analytical work done [11–14], on strong state properties of materials. Condensed matter theorists can predict crystal structures, lattice constants, phase diagrams and related properties very accurately. Recently, many workers [11–17] there were a couple significant breakthrough in the forecast of solid-state property of solids. These upgrades rely vigorously upon new improvements in observational procedures, and positively on the experiences acquired through close coordinated efforts among scholars and experimentalists doing explore on strong state property of materials. Experimental ideas like valence electron, exact radii, electronegativity, ionicity & plasmon energy are then useful11-14. These ideas are straightforwardly connected with the personality of the substance bond and consequently give intends to clarifying and arranging numerous essential properties of atoms and solids.

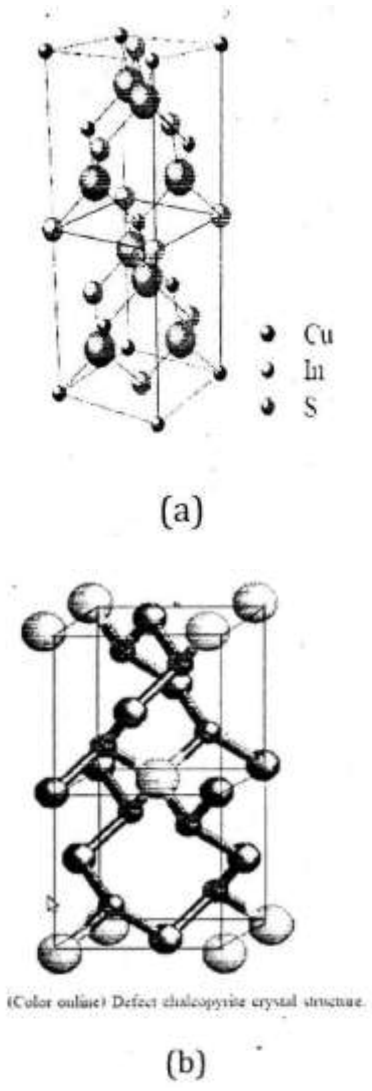


Figure 1: Crystal construction of (a) chalcopyrite lattice and (b) defect chalcopyrite crystals

Recently, Yadav and co-authors [18,19] have created exact relatives for optical, electronic, & zinc blende mechanical properties & rock-salt organized paired solids utilizing the plasmon motions hypothesis of solids. By and large, experimental specific, the straightforwardness of observational relations permit a more extensive class of scientists to ascertain valuable properties, and regularly drifts become more obvious. It is currently grounded that the A metal's plasmon energy shifts. when it go through a synthetic blend and structures a compound. This is attributed to the reality that it is real that the plasmon energy relies upon the quantity semiconductors' valence electrons, When a metal structures a compound, this shifts As a consequence, we felt it would be interesting to give a different interpretation for the optical dielectric. constant for $A^{I}B^{III}C^{VI}_{2}$ and $A^{II}B^{IV}C^{V}_{2}$ semiconductors.

Using the plasma motions theory, the aim of this project is to achieve strong plasma motions. The current examinations are coordinated as follows: the hypothetical idea is given in Section 2 & present the conversation and reenactment results for complex optical properties organized semiconductors in this Section moreover. Finally, the conclusion is given in last Section 3.

2. THEORY, RESULTS AND DISCUSSION

In almost all fields in modern electronics, the dielectric constant of a substrate is one of the most important criteria for system design. Moreover, it is of crucial significance for the conduct of charge transporters, dopants, imperfections and pollutions in protectors and semiconductors. The dielectric constants are constrained by the polarizability of the particles. which are predicted to increase with atomic number [20]. Besides, it is of principal significance for the conduct of charge transporters, dopants, imperfections and pollutants in protectors and semiconductors. The polarizability of molecules determines the dielectric constant, which would rise with the nuclear number of a powerful might be transmitted about the polarizability of its constituent particles α_e

$$\varepsilon_e = 1 + \left[(N_i\alpha_i/\varepsilon_0) \middle/ (1 - \sum \gamma N_i\alpha_i/\varepsilon_0) \right] \qquad (1)$$

Where N_i is the numeral of the atoms of species i per unit volume, ε_0 is the free space permitivity & γ is the Lorentz factor. Nag [21] considered the high-recurrence & dielectric constants at rest of cubic semiconductors and proposed an adjustment in condition (1). The dielectric consistent might be communicated as far as the normal nuclear number of constituent particles (Zav) by the accompanying connection:

$$\varepsilon = (a - bZ_{av})^{-1} \qquad (2)$$

Where a & b are constants, on the basis of the compound group.

Xue et al [22] proposed a modification in equation (2) furthermore, have demonstrated that the high-recurrence dielectric steady may likewise be communicated regarding the The cation's nuclear number (Z_A) by the follow relation:

$$\varepsilon_\infty\ (a'' - b''Z_A) \qquad (3)$$

Here a'' & b'' are constants. Srivastava [7] The sum has been measured optical dielectric constant of the X-Y bond using the well-known relation [23,24];

$$\varepsilon_\infty = 1 + (\hbar\omega_{p,xy} / E_{g,XY})^2 \qquad (4)$$

In this eq. the meaning of the material's dielectric constant depends upon the plasmon energy ($\hbar\omega_{p,XY}$), which is dependent on conduction electron density and the viable numbers of the center electrons through as the valence electrons shift metal structures a compound. Srivastava theory[7, 25,26], Kumar et al [27] found that substantially reduced plasmon energy must be used to get better concurrence with the test and hypothetical qualities. The numbers of valence electron in a substance determines its plasmon capacity. Used this definition [10,18,19] we have recently presented the optical, electronic also, mechanical properties, for example, energy hole (E_g), bulk modulus (B), heteropolar gap (E_c), ionicity (f_i), cohesive energy (E_{coh}), electronic polarizability (α_e) and optical susceptibility (χ) of zinc blende & rock-salt structured binary solids in term of plasmon energy $\hbar\omega_p$ (in eV) are given as follows;

$$E_g = M\,(\hbar\omega_p)^{1.413} \tag{5}$$

$$\alpha_e = N(\hbar\omega_p)^{-2.82} \tag{6}$$

Where M and N are constants and on the basis of various types of bonds in crystal structures.

Any adjustment in the crystallographic climate of a particle is identified with center electrons through the valence electrons. The adjustment in wave work that happens for the external electrons as a rule implies a dislodging of electric charge in the valence shell so the association between valence, shell and center electrons is changed. This causes the inner electron's binding energy to alter, in parallel to the absorption edge's rotation. The dielectric steady of various types of bonds (A-C and B-C) for $A^{I}B^{III}C^{VI}$ 2 and $A^{II}B^{IV}C^{V}$ 2 The impact of ternary chalcopyrite semiconductors right away can be seen. As seen in Figs. 2-5, A single line separates the data points as plotted against the energy of plasmons (p).

Fig. 2: Plot of dielectric constant versus plasmon energy of A-C bond in $A^{I}B^{III}C^{VI}_{2}$ chalcopyrites

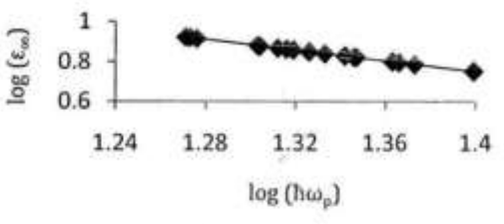


Fig. 3: Plot of dielectric constant versus plasmon energy of B-C bonds in $A^{I}B^{III}C^{VI}_{2}$ chalcopyrites

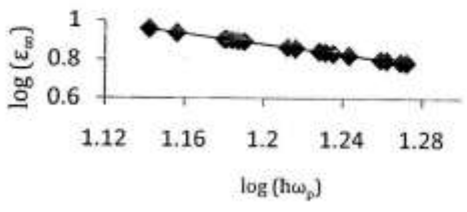


Fig. 4: Plot of dielectric constant versus plasmon energy of A-C bond in $A^{II}B^{IV}C^{V}_{2}$ chalcopyrites

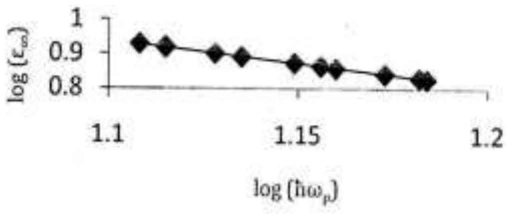
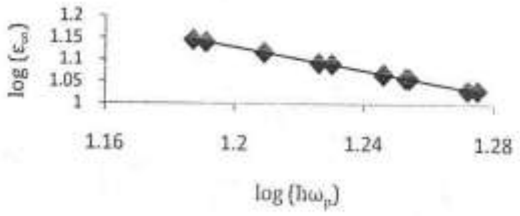


Fig. 5: Plot of dielectric constant versus plasmon energy of B-C bond in $A^{II}B^{IV}C^{V}_{2}$ chalcopyrites



From Figure, It is self-evident that the value of the dielectric constant of these substances reduces if the weather gets hotter in power of plasmons Similarly, based on above expressions & discussion, We believe that the dielectric constants of different types of bonds are linked (A-C and B-C) for $A^{I}B^{III}C^{VI}$ 2 and $A^{II}B^{IV}C^{V}$ 2 semiconductors ternary chalcopyrite is used to make this pendant can be evaluated using their plasmon energies can be calculated using the formula below;

$$\varepsilon_\infty,_{XY} = D(\hbar\omega_p,_{XY})^{-1.333} \tag{7}$$

Where D is the constant and has values 414.67 & 302.89 for A-C and B-C bonds, respectively, in $A^{I}B^{III}C^{VI}$ 2 and 255.56 and 537.55 for these bonds in $A^{II}B^{IV}C^{V}$ 2 semiconductors made of ternary chalcopyrite In this relation, Plasmon energy of the chemical bonds A-C & B-C in $A^{I}B^{III}C^{VI}$ 2 & $A^{II}B^{IV}C^{V}$ 2 References There has been a discovery of ternary chalcopyrite semiconductors. [7,27]. These materials' optical properties have been extensively explored elsewhere [1,6,7,9,23,24] & will not be discussed here. Using Eq. (7), the value of the dielectric constant (ε_∞,) It's been a while measured for these products. The results are shown in Table-1 & 2. These parameters' estimated the ideals are in fine condition alignment with Verma's recorded values[9]., Levine [23] and Kumar [27].

3. CONCLUSION

From the above results and discussions obtained by using the proposed approach, it is quite obvious that the parameters such as dielectric constant (ε_{∞},) and electronic susceptibility (χ_e) of the chemical bonds in complex structured $A^{I}B^{III}C^{VI}$ 2 and $A^{II}B^{IV}C^{V}$ 2 ternary chalcopyrite semiconductors reflecting the optical properties and can be expressed in terms of plasmon energies of these materials, which is definitely a surprising phenomenon and need further investigation of the reason. The calculated values of these parameters are presented in Table 1 & 2. From Figs. 2-5, we observe that the dielectric constant for the chemical bonds A-C and B-C in $A^{I}B^{III}C^{VI}$ 2 and $A^{II}B^{IV}C^{V}$ 2 ternary chalcopyrite semiconductors are inversly related to the plasmon energy. We note that the investigated values of these parameters by our proposed empirical relations are in close agreement with available theoretical values reported by previous researchers. The various evaluated parameters show a systemic trend and are consistent with the available theoretical values reported so far, which proves the validity of the proposed approach. It is also note worthy that the proposed empirical relation is simpler and widely applicable since we have been reasonably successful in calculating these parameters using the plasmon energy of the materials. It is natural to say that this model can easily be extended to rock-salt and zinc-blende structured crystals for which the work is in progress and will be appearing in forthcoming papers. Hence it is possible to predict the order of electronic properties of ternary chalcopyrite compounds from their plasmon energies.

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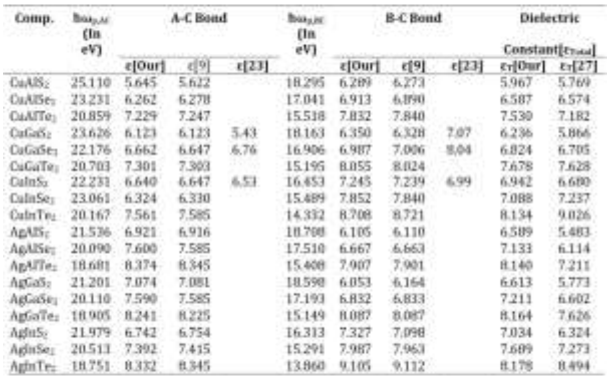
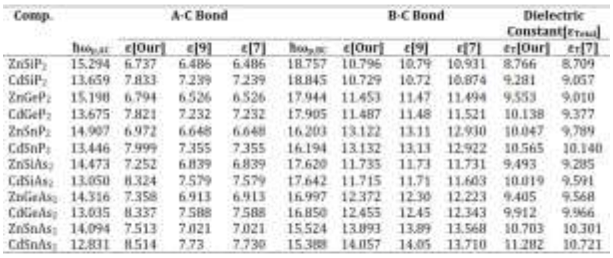
Table -1: In this table we present the dielectric constant of $A^{I}B^{III}C^{VI}_2$ class ternary chalcopyrites



Comp.	$\hbar\omega_{p,AC}$ (In eV)	A-C Bond			$\hbar\omega_{p,BC}$ (In eV)	B-C Bond			Dielectric Constant[ε_{Total}]	
		ε[Our]	ε[9]	ε[23]		ε[Our]	ε[9]	ε[23]	ε_T[Our]	ε_T[27]
$CuAlS_2$	25.110	5.645	5.622		18.295	6.289	6.273		5.967	5.769
$CuAlSe_2$	23.231	6.262	6.278		17.041	6.913	6.890		6.587	6.574
$CuAlTe_2$	20.859	7.229	7.247		15.518	7.832	7.840		7.530	7.182
$CuGaS_2$	23.626	6.123	6.123	5.43	18.163	6.350	6.328	7.07	6.236	5.866
$CuGaSe_2$	22.176	6.662	6.647	6.76	16.906	6.987	7.006	8.04	6.824	6.705
$CuGaTe_2$	20.703	7.301	7.303		15.195	8.055	8.024		7.678	7.628
$CuInS_2$	22.231	6.640	6.647	6.53	16.453	7.245	7.239	6.99	6.942	6.680
$CuInSe_2$	23.061	6.324	6.330		15.489	7.852	7.840		7.088	7.237
$CuInTe_2$	20.167	7.561	7.585		14.332	8.708	8.721		8.134	9.026
$AgAlS_2$	21.536	6.921	6.916		18.708	6.105	6.110		6.589	5.483
$AgAlSe_2$	20.090	7.600	7.585		17.510	6.667	6.663		7.133	6.114
$AgAlTe_2$	18.681	8.374	8.345		15.408	7.907	7.901		8.140	7.211
$AgGaS_2$	21.201	7.074	7.081		18.598	6.053	6.164		6.613	5.773
$AgGaSe_2$	20.110	7.590	7.585		17.193	6.832	6.833		7.211	6.602
$AgGaTe_2$	18.905	8.241	8.225		15.149	8.087	8.087		8.164	7.626
$AgInS_2$	21.979	6.742	6.754		16.313	7.327	7.098		7.034	6.324
$AgInSe_2$	20.513	7.392	7.415		15.291	7.987	7.963		7.689	7.273
$AgInTe_2$	18.751	8.332	8.345		13.860	9.105	9.112		8.178	8.494

Table -2: In this table we present the dielectric constant of $A^{II}B^{IV}C^{V}_2$ class ternary chalcopyrites



Comp.	A-C Bond				B-C Bond				Dielectric Constant[ε_{Total}]	
	$\hbar\omega_{p,AC}$	ε[Our]	ε[9]	ε[7]	$\hbar\omega_{p,BC}$	ε[Our]	ε[9]	ε[7]	ε_T[Our]	ε_T[7]
$ZnSiP_2$	15.294	6.737	6.486	6.486	18.757	10.796	10.79	10.931	8.766	8.709
$CdSiP_2$	13.659	7.833	7.239	7.239	18.845	10.729	10.72	10.874	9.281	9.057
$ZnGeP_2$	15.198	6.794	6.526	6.526	17.944	11.453	11.47	11.494	9.553	9.010
$CdGeP_2$	13.675	7.821	7.232	7.232	17.905	11.487	11.48	11.521	10.138	9.377
$ZnSnP_2$	14.907	6.972	6.648	6.648	16.203	13.122	13.11	12.930	10.047	9.789
$CdSnP_2$	13.446	7.999	7.355	7.355	16.194	13.132	13.13	12.922	10.565	10.140
$ZnSiAs_2$	14.473	7.252	6.839	6.839	17.620	11.735	11.73	11.731	9.493	9.285
$CdSiAs_2$	13.050	8.324	7.579	7.579	17.642	11.715	11.71	11.603	10.019	9.591
$ZnGeAs_2$	14.316	7.358	6.913	6.913	16.997	12.372	12.30	12.223	9.405	9.568
$CdGeAs_2$	13.035	8.337	7.588	7.588	16.850	12.455	12.45	12.343	9.912	9.966
$ZnSnAs_2$	14.094	7.513	7.021	7.021	15.524	13.893	13.89	13.568	10.703	10.301
$CdSnAs_2$	12.831	8.514	7.73	7.730	15.388	14.057	14.05	13.710	11.282	10.721

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