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Thermodynamic Properties of Tetrahedral Semiconductors

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Abstract – This research paper focuses on, thermodynamic properties such as heat of formation of tetrahedral semiconductors were evaluated. An interesting empirical relationship it was proposed as a method of calculating the heat of formation for $A^{II} B^{VI}$, $A^{III} B^{V}$, $A^{I} B^{III} C^{VI}_{2}$ and semiconductors with tetrahedral structure using their lattice constant. We used the proposed model to quantify the heat of formation on binary and ternary chalcopyrite semiconductors. The formation's heat (- H_f in KJ/mol) for these compounds exhibits As compared to the lattice constant, the relationship is linear (in A^{o}), which lies on the straight line. The available test and hypothetical qualities recorded by past analysts were discovered to be in fantastic arrangement.

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1. INTRODUCTION

In the recent past much attention has been given towards the investigation of numerous optical, electronic, elastic & thermal property of group $A^{II} B^{VI}$, $A^{III} B^{V}$, $A^{I} B^{III} C^{VI}_{2}$ & $A^{II} B^{IV} C^{V}_{2}$ semiconductors. The $A^{I} B^{III} C^{VI}_{2}$ and $A^{II} B^{IV} C^{V}_{2}$ compounds crystallize in the chalcopyrite structure with a tetrahedral space group $I\bar{4}2d\left(D_{2d}^{12}\right)$ having four formula units in each unit cell & are the ternary analogues of the II-VI & III-V semiconductors, respectively. The composition of chalcopyrite is essentially as upper lattice of the zinc blendes structure obtained by doubling its unit cube along the Z-axis that becomes the c-axis of the chalcopyrite structure. These binary and ternary semiconductors have potential applications in the fields of light emitting diodes (LEDs), laser diodes (Ms), photo detectors (PDs), non-linear optical (NL0) devices, frequency conversion applications, integrated optics and nano-electronics [1]. Recently, a new magnetic material, MnGeP2 with tetrahedral The structure The crystal's composition has been established synthesized by doping Mn in ZnGeP2 & CdGeP2 by Medvedkin, et. Al. [2, 3] & several other researchers [4-6]. These ferromagnetic materials are also having wide Magneto-optical applications, spin dependent and magnetically control able non linear optical devices [2]. The CuInSe2 (CIS) [7,8] and CuInGaSe2 (CIGS) [9] materials reports have been made as most usable energy materials for solar cells and photo-voltaic applications. Despite their potential uses, The heat produced during the creation of these semiconductors has received insufficient attention.

There is a significant number of empirical job has been carried out in recent years [10-13], on solid land of the state materials. Crystal shapes, lattice constants, phase diagrams, and other property of condensed matter it is possible to forecast very specifically by condensed matter theories. As of late, some huge forward leaps things also been completed in the expectation in strong land of the state solids [10-16]. These advancements are largely dependent on recent advance in empirical methods, in addition insights obtained from near partnerships between theorists and experimentalists working on solid-state solids' properties. Valence electrons, plasmon, electronegativity, ionicity, & empirical radii capacity are also valuable terms [10-13]. These ideas are linked to the chemical bond's character, and they can be used to describe and characterise a variety of fundamental molecular and solid properties.

Semiconductors of tetrahedral coordination of the chemical formula $A^{N} B^{8-N}$ Because of their technological and science significance, they have been thoroughly researched. zincblende crystallographic structure. Zinc is utilized in everything from crude iron and zinc precious stones to man-made GaN and BN semiconductors. Instead of this their future mechanical applications as photovoltaic indicators, sunlight based cells, light emanating diodes, modulators, channels, and nonlinear optics, photovoltaic identifiers, sun powered cells, light discharging diodes, modulators, channels, and nonlinear optics chalcogenide and pnictide semiconductors containing the recipe $A^{I} B^{III} C^{VI}_{2}$ and Both $B^{IV} C^{V}_{2}$ are well-known contemplated [17-20]. These semiconductors solidify in the chalcopyrite structure, which is The zinc blende structure is the base of this term. by substituting two separate atomic species for the cationic

sublattice. This causes the cell of the unit to double in size in a position known as c, in addition a tetragonal distortion. This distortion is characterized [1] by the parameter π = c/2a, where a & c are the the lattice parameters, and by the anion displacement u = 0.25+ $[d^2_{A-C}+d^2_{B-C}]/a2$ from its position in the cubic cell, Where d_{A-C} & d_{B-C} are the cation-anion distances. Because of the added structural [n;u] and chemical $[d_{A-C} \neq d_{B-C}]$ degrees of freedom in contrast to their binary equivalents, the ternary semiconductors exhibits a large number of interesting physical and chemical property [21-25].

Many researches [26-29] attempt have been designed to comprehend the electronic, mechanical, elastic & visual zinc blende properties ($A^{II} B^{VI}$ and $A^{III} B^{V}$) and chalcopyrite ($A^{I} B^{III} C^{VI}_2$ and $A^{II} B^{IV} C^{V}_2$) semiconductors. together experimentally and theoretically, the solid state properties of semiconductors are extremely important. new and theoretical methods for measuring these material properties in binary & ternary semiconductors have been around for a long time well established and established. Theoretical approaches are used when the experimental procedure is complex and expensive. a broad variety of theoretical equations focused on observational Relationships have certainly played a major role in my life substance science in the last few years. Empirical relationships do not often provide extremely reliable findings for each particular content, but they may also be quite helpful. The versatility of analytical relations, in particular, helps a larger a party of scientists to quantify valuable properties, and patterns often emerge. empirical radii, Valence, ionicity, & plasmon capacity are also useful empirical terms [10, 13, 30]. These ideas are linked in comparison to the chemical bond's character, and they can be a term used to classify and characterise a variety of fundamental property of molecules & solids.

Recently, the author [31-34] has calculated the static and dynamic, electronic, Zinc blende, mechanical &optical qualities of wurtzite and rock salt structured binary solids using the solids principle of plasma oscillations. This is since A compound's plasmon energy is the same as compound's efficient amount of valence electrons. While observational relationships do not often have particularly reliable findings for each individual material, they can also be quite helpful. The straightforwardness of observational relationships, in particular, helps a larger a party of scientists to quantify valuable properties, and sometimes trends emerge. Therefore, we thought it would be a matter of considerable concern to give an alternative explanation for the heat produced during the phase of wurtzite forming and zinc blende ($A^{II} B^{VI}$ and $A^{III} B^{V}$) and chalcopyrite ($A^{I}B^{III} C^{VI}_2$ and $A^{II} B^{IV} C^{V}_2$) structured semiconductors with their lattice constant.

The aim of this project is to is to obtain heat produced during the creation of group $A^{II}B^{VI}$, $A^{III}B^{V}$, $A^{I}B^{III}C^{VI}_2$ and $A^{II}B^{IV}C^{V}_2$ semiconductors using their lattice constant a (in A^0). The theoretical background is given in Section -2. We present and discuss the simulation Section-3 contains the information on binary semiconductors' thermal properties. Finally, the conclusion is given in the last Section-4.

2. THEORETICAL BACKGROUNDS

The heat of forming is a significant thermal feature of materials, and some researchers [10, 35] have explored it When it comes to electro-negativity contrast between the atoms that make up the system. The energy of bond forming between atom A & B, according to Pauling [10], is provided by making use of the following formula:

$$D(A-B)=\frac{1}{2}\left[D(A-A)+D(B-B)+23\sum(X_A-X_B)\right] \quad (1)$$

Where D (A-B), D(A-A) and D(B-B) are the energies of A-B heteropolar bonds and homopolar A-A and B-B bonds respectively. X_A and X_B are the electro-negativities of atoms A and B. The third term on the right hand side of the equation (1) gives the cost of standard heat of formation:

$$-\Delta H_f = 23\sum (X_A - X_B)^2 \quad (2)$$

Where Σ is taken over all the bond in the compound. Phillips [35] The heat a few compound semiconductors are developed was studied, and the following updated relationship was proposed:

$$-\Delta H_f = \frac{2}{3}\times 23\sum (X_A - X_B)^2 \quad (3)$$

Mulokozi [36] The heat of creation was studied. The formation's heat relationship when it comes to nearest-neighboring distance d_{RX} was suggested for rare earth compounds. The following partnership, according to him, can be put to work express the formation's heat:

$$-\Delta H_f = \frac{Ae^2(\Delta X)^2}{d_{RX}} + C \quad (4)$$

In a sequence of rare earth compounds (where the cation X does not change), the partial charge X would remain stable is the elementary charge. A is a constant, whereas C is a covalent contribution. According to Mulokozi [36], Ae^2 $(X)^2$ and C are cation based. According to Phillips and Van-Vectan [37], the temperature at which binary

compounds are formed is proportional to the distance between their closest neighbours:

$$\Delta H_f = \Delta H_0 \left(\frac{d_{Ge}}{d_{AB}} \right)^s D(AB) f_{iAB} \quad (5)$$

Where d_{Ge} and d_{AB} are the distances between germanium and the binary compound AB, respectively, $f_{i, AB}$ is a substance's ionicity bond [33] and D(AB) is provided by the relation [38,39]

$$D(XY) = 1 - b\left[\frac{E_1(XY)}{E(XY)}\right]^2 = 1 - b\left[\frac{2E_1(XY)}{E_0(XY) + E_1(XY)}\right]^2 \quad (6)$$

Where $E_0[XY]$ is the smallest direct energy difference, $E_1[XY]$ are the compound's essential energies that are higher, E(XY) is the average of $E_0[XY]$ and $E_1[XY]$, and b=0.0467. The worth of $E_0[XY]$, $E_1[XY]$, and $E_2[XY]$ can be found out statistically or based on reflectivity data obtained from experiments using Van Vechten [40] and Neumann [39] equations. Phillips & Van Vechten [37] determine the ideals of scaling factor X_0 & the exponent s in Eq. [5] for two separate sets of H0 and s. X_0 = -300 KJ/mol for s=4 and -287 KJ/mol for s=3. Later, Neumann [39] measured new analytical values of X_0=-304 KJ/mol and s=3.575 by integrating new values of Xf for binary (II-VI and III-V) compounds published in different literatures [41-43] with Van Vechten's ionicities, essential point powers, and bond lengths [38, 40] in Eqs. [5] and [6]. Neumann [39] found an outstanding agreement between the measured and new values of $-X_f$ derived from these values of X_0 and s.

The ternary analogues of the II-VI & III-V semiconductors, respectively, are the $A^IB^{III}CV^I_2$ & $A^{II}B^{IV}CV_2$ semiconductors, which also show tetrahedral coordination [44]. Consequently, it's fair to assume that Eq. [5] may also be applied to the scorching sun of forming of ABC_2 style semiconductors. Taking into consideration the actual ABC_2 semiconductors are made up of two [AB]1/2-C groups, the formation heat can be written as[45].

$$\Delta H_f(ABC_2) = 2\Delta H_0 \left(\frac{d_{Ge}}{d} \right)^s D(ABC_2) f_i(ABC_2) \quad (7)$$

Where $^{\Delta}X_0$=-304 Kj/mol and s=3.575 have the same values as When it comes to binary semiconductors,, d_{Ge}=2.45 A^0, d= $(d_{AC}+d_{BC})/2$ is the total length of a bond ABC_2 compounds and fi[ABC_2] =[$f_{i,AC}$+ $f_{i,BC}$]/2is the typical bond ionicity is a term that refers to the capacity to and D [ABC_2]is again defined by Eq. [6] but now the energies E_0, E_1 & E_2 are the characteristics of ABC_2 compound itself. Since all the $A^IB^{III}C^{VI}_2$ Compounds are straightforward gap semiconductors the energies E_0, E_1 & E_2 can be taken from data from tests for the fundamental energy gap in these resources. However, difficulties arise in the procedure for determining the results of the experiment of E_1 & E_2 In principle E_1 &E_2 can be theoretically calculated based on equations given by Van Vechten [40] and Neumann [39]. Recently, Kumar, et. Al. [13] have developed a relationship for calculating the formation's heat of solids based on Theory of plasma oscillations. $A^{II}B^{VI}$,$A^IB^{III}C^{VI}_2$ & $A^{II}B^{IV}C^V_2$ semiconductors may be expressed as-

$$\Delta X_f = A\,(\hbar\omega_p)^B \quad (8)$$

where A & B are constants of varying meanings based on the situation form of semiconductor. We can deduce based on the preceding equations that The plasmon energy is linked to the heat of formation, the difference in electro-negativity, the ionicity of the bonds, and the difference in electro-negativity. Binary and ternary semiconductors are binary and ternary semiconductors, respectively. the free electron plasmon energy is provided by -

$$(\hbar\omega_p)^2 = \frac{4\pi N_e^2 e^2}{m} \quad (9)$$

From which we have

$$N_e^2 = \frac{m}{4\pi e^2}(\hbar\omega_p)^2 \quad (10)$$

The Plasmon energy is denoted by p. The effective amount of free electrons involved in plasma oscillations is Ne, and the charge and mass of the electron are e & m, respectively. These authors' findings differed significantly from previously published values in many instances [39, 46]. However, these findings suggest that there may be a connection between the heat of forming ($-^{\Delta}H_f$) and the plasmon energy (p) of materials. These claims point to a potential connection between plasmon energy and heat of creation. For $A^{II}B^{VI}$, $A^{III}B^V$, $A^{II}B^{III}C^{VI}_2$, & $A^IB^{III}C^{VI}_2$ semiconductors, a graph showing variance of $-^{\Delta}H_f$ with plasmon energy (p) was plotted using the stated values [33].

The plot of $-\Delta H_f$ versus $\hbar\omega_p$ for certain substances need Fig. 1-4 linear as-

$$\Delta H_f = M\,(\hbar\omega_p) - N \quad (11)$$

where M & N are numerical constants and have values 30.26 and 303.10 for $A^{II}B^{VI}$,28.53 and 334.70 for $A^{III}B^V$, 92.03 and 1092.0 for $A^IB^{III}C^{VI}_2$

and 20.73 and 45.05 for $A^{II}B^{IV}C^{V}_2$ semiconductors respectively.

To comprehend the relation between heat of formation and lattice constant a (in A^0) , it is argued that the heat of formation and the lattice constant a (in A^0) The amount of valence electrons per unit volume in a unit cell of a crystal in a solid is calculated by the existence of bonding, which is The number of valence electrons defines the structure of a material per unit volume-

$$N_e = \frac{\frac{Z_A}{N_{CA}} + \frac{Z_B}{N_{CB}}}{V_b} \quad (12)$$

Where Z_A & Z_B are the valence electron counts of atoms A & B, respectively. In AB compound N_{CA} & N_{CB} are the coordination numbers of the atoms A & B, V_b is the bond volume. For tetrahedral crystals N_{CA} = N_{CB}= 4, Z_A+Z_B= 8 and V_b = d3/3$\sqrt{3}$ .Substituting these values in Eq. [12] and using in Eq. [10], we get the following equation for the bond length (in A^0) of binary and ternary semiconductors as-

$$d = 15.30\ (\hbar\omega_p)^{-2/3} \quad (14)$$

For zinc blende and chalcopyrite structured semiconductor, the bond length in terms of lattice constant as given by [47]-

$$d = \frac{\sqrt{3}a}{4} \quad (15)$$

Combning the eqs. (11), (14) and (15), we get-

$$\Delta H_f = Da^{-1.5} - S \quad (16)$$

The numerical constants D and S for the $A^{II}B^{VI}$, $A^{III}B^{V}$, $A^{I}B^{III}C^{VI}_2$, and $A^{II}B^{IV}C^{V}_2$ groups of semiconductors are described in Table-1. Since these ($A^{II}B^{VI}$, $A^{III}B^{V}$, $A^{I}B^{III}C^{VI}_2$, and $A^{II}B^{IV}C^{V}_2$) semiconductors can be used in zinc blende, wurtzite, and chalcopyrite structures, it is thought that the same series of constants can be used for the $A^{II}B^{VI}$, $A^{III}B^{V}$, $A^{I}B^{III}C^{VI}_2$, and $A^{II}B^{IV}C^{V}_2$ community semiconductors. As the heat of forming of these semiconducting materials is plotted against the lattice constant (in A_0) of these compounds [46], as seen in figure 5-8, a linear relationship emerges. The $A^{II}B^{IV}$, $A^{III}B^{V}$, $A^{I}B^{III}C^{VI}_2$, and $A^{II}B^{IV}C^{V}_2$ semiconductors lie on the straight line in the plot of heat of forming versus lattice constant. It is clear from figs. 5-8 that the heat of forming in these compounds decreases as the lattice parameter rises. A systematic analysis of these semiconductors' thermal properties has already been published [10, 13, 35-37, 39, 45, 46, 48] and will not be repeated here.

3. RESULTS AND DISCUSSION

The present paper presents a relationship between binary semiconductors' heat of forming (-H_f, in KJ/mole) and their lattice constant (a in A_0). This method can be used to figure out how hot everything is forming using their lattice constant. Using the suggested analytical relationship, the heat of formation of these semiconductors was measured [16]. Tables [2] through [5] show the estimated values, as well as the values recorded by previous researchers. We notice that the formation heat prices measured using the future empirical relation are remarkably close to those stated by previous researchers [37, 39, 46, 48]. Closer agreement of the findings supports our hypothesis that the sequence of values of the constants in eqs. [11] and [16] remains constant for a particular crystal and may be considered a crystal structure feature since they remain constant for all substances belonging to that crystal structure. These findings demonstrate that our new method is sound and can be used to calculate and estimate the constants of inter atomic force of these products.

4. CONCLUSIONS

This paper looked at binary and ternary compound semiconductors' thermodynamic properties. These products' thermodynamic properties, such as the heat of formation, obtained from our proposed analytical relation are in line with the results of other theoretical measurements. Of the most common is interesting features of these simulations is that it shows the vital function that lattice constants play in these products. Using the lattice constant as a starting point, we suggested an analytical relationship to approximate the heat of creation.. The physical cause of the correlation has been investigated. The model that has been proposed is clear and accurate. It's important to keep in mind that the proposed relationship's constants are crystal structure properties. Their ideals are unaffected by the crystal structure.The crystal structures of zinc blended, wurtzite, and chalcopyrite have all shown this. The obtained findings are in full harmony with the hypothesis stated assumptions & support the proposed model's foundation. It's also worth mentioning that the analytical relationship we present is easy, dependable, and relevant to a large range of situations.

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Table 1: Values of the constants

Constants	$A^{II}B^{VI}$	$A^{III}B^{V}$	$A^{I}B^{III}C^{V}_{2}$	$A^{II}B^{IV}C^{V}_{2}$
D	6356.41	5991.30	19326.3	4354.54
S	303.10	334.70	1092.0	45.05

Table 2: Values of the heat of formation ($-\Delta H_f$, in KJ/mole) of $A^{II}B^{VI}$ semiconductors

$A^{II}B^{VI}$ Solids	Plasmon energy (In eV)	Lattice Constants (In Å)	Heat of Formation, $-\Delta H_f$ (in KJ/Mole) Using Eq. [11]	Using Eq. [16]	Expt. [37, 39]	Neumann [39]
ZnO	21.48	4.631	346.88	334.72	349.4	
ZnS	16.71	5.409	202.54	202.18	205.9	199.0
ZnSe	15.78	5.667	174.40	168.07	164.4	179.0
ZnTe	14.76	6.101	143.53	118.7	118.0	111.7
ZnPo	12.36	6.621	70.91	70.00		
CdO	18.46	5.059	255.49	255.51		
CdS	14.88	5.832	147.16	148.22	156.9	156.2
CdSe	14.01	6.051	120.84	123.94	136.0	135.1
CdTe	13.09	6.353	93.00	93.85	92.8	105.4
CdPo	11.43	6.975	42.77	41.96		
BeS	19.52	4.865	287.57	289.26		
BeSe	18.39	5.139	253.38	242.52		
BeTe	16.12	5.626	184.69	173.23		
BePo	14.91	5.843	148.07	146.94		
HgS	14.85	5.861	146.26	144.87		
HgSe	13.99	6.096	120.23	119.22		
HgTe	12.85	6.451	85.74	84.84		
MgTe	12.97	6.411	89.37	88.48		

Table 3: Values of the heat of formation ($-\Delta H_f$, in KJ/mole) of $A^{III}B^{V}$ semiconductors

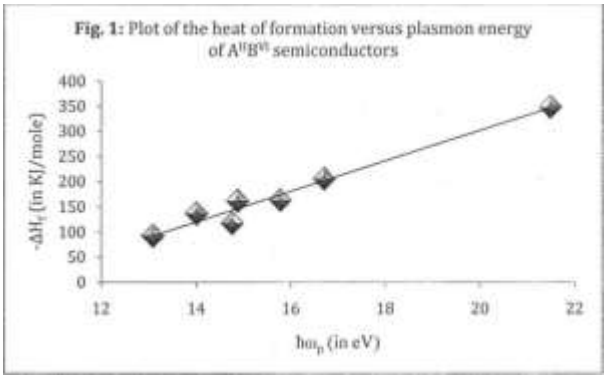
$A^{III}B^{V}$ Solids	Plasmon energy (In eV)	Lattice Constants (In Å)	Heat of Formation, $-\Delta H_f$ Using Eq. [11]	Using Eq. [16]	Expt. [37, 39]	Neumann [39]
BN	24.53	4.194	365.14	362.85		
BP	21.46	4.538	277.55	285.06		
BAs	20.12	4.777	239.32	239.13		
BSb	17.85	5.183	174.56	173.05		
BBi	16.15	5.539	126.05	124.89		
AlN	22.97	4.391	320.63	318.44		
AlP	16.65	5.451	140.32	136.06	167.2	
AlAs	15.75	5.662	114.64	109.99	116.7	
AlSb	13.72	6.135	56.73	59.57		
AlBi	12.79	6.471	30.19	29.26		
GaN	21.98	4.512	292.38	290.42		
GaP	16.50	5.490	136.04	131.06	121.8	113.7
GaAs	15.35	5.653	103.23	111.06	100.8	74.9
GaSb	13.38	6.095	47.03	45.46	44.8	44.6
GaBi	12.76	6.480	29.34	28.51		
InN	18.82	5.004	202.23	200.53		
InP	14.76	5.868	86.40	86.78	87.8	87.5
InAs	14.07	6.058	66.71	67.11	66.2	50.2
InSb	12.73	6.478	28.48	28.67	30.5	35.4
InBi	18.85	4.998	203.09	201.49		

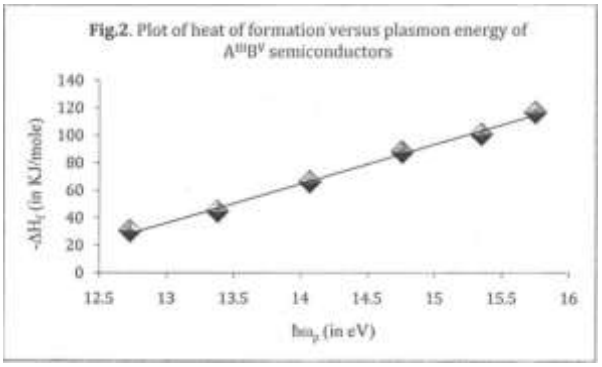
Table 4: Values of the heat of formation (-ΔH_f, in KJ/mole) of $A^IB^{III}C^{VI}_2$ Chalcopyrite semiconductors

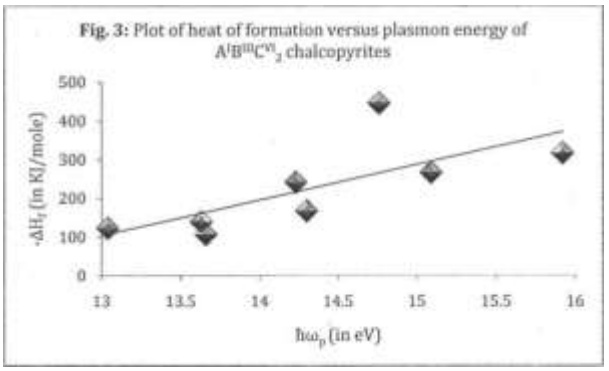
$A^IB^{III}C^{VI}_2$ Compounds	Plasmon energy (In eV)	Lattice Constants (In A^0)	Heat of Formation, -ΔH_f (in KJ/Mole) Using Eq. [11]	Using Eq. [16]	Neumann [39]	Expt. [39]	Ref. [48]
$CuAlS_2$	17.25	5.303	495.51	490.47	463.8		357.8
$CuAlSe_2$	15.86	5.608	367.59	363.08	389.9		333.5
$CuAlTe_2$	14.35	5.994	228.63	224.68	285.4		299.2
$CuGaS_2$	17.10	5.334	481.71	476.73	420.4		355.5
$CuGaSe_2$	15.92	5.594	373.11	368.58	329.5	317	329.5
$CuGaTe_2$	14.30	6.008	224.02	220.09	260.8	168	295.8
$CuInS_2$	16.12	5.548	391.52	386.91	327.7		333.5
$CuInSe_2$	15.09	5.797	296.73	292.51	263.5	267	312.0
$CuInTe_2$	13.66	6.194	165.12	161.43	228.5	107	282.7
$AgAlS_2$	16.21	5.527	399.80	395.16	417.9		333.5
$AgAlSe_2$	15.16	5.779	303.80	298.92	361.3		312.0
$AgAlTe_2$	14.50	5.953	242.43	238.43	279.9		282.7
$AgGaS_2$	16.10	5.552	389.68	385.08	394.8		329.5
$AgGaSe_2$	14.76	5.883	266.36	262.26	318.2	446	308.5
$AgGaTe_2$	13.63	6.203	162.36	158.68	252.7	140	281.1
$AgInS_2$	15.21	5.766	307.77	303.51	330.6		315.7
$AgInSe_2$	14.23	6.028	217.58	213.68	268.0	242	294.2
$AgInTe_2$	13.04	6.389	108.07	104.59	217.9	123	267.5
$AgFeS_2$	16.24	5.520	402.56	397.91			
$CuTlS_2$	15.89	5.601	370.35	365.83			
$CuTlSe_2$	14.88	5.851	277.40	273.26			
$CuFeS_2$	17.19	5.315	489.99	484.98			

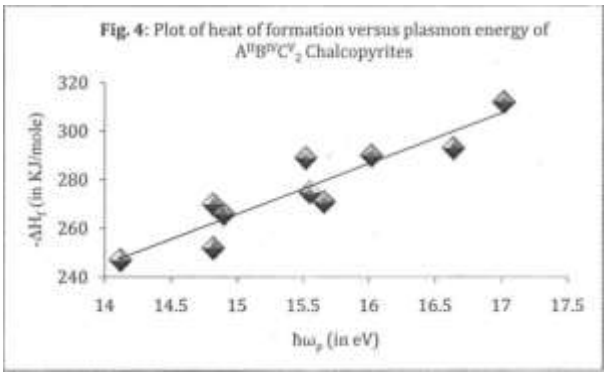
Table 5: Values of the heat of formation (-ΔH_f, in KJ/mole) of $A^{II}B^{IV}C^{V}_2$ Chalcopyrite semiconductors

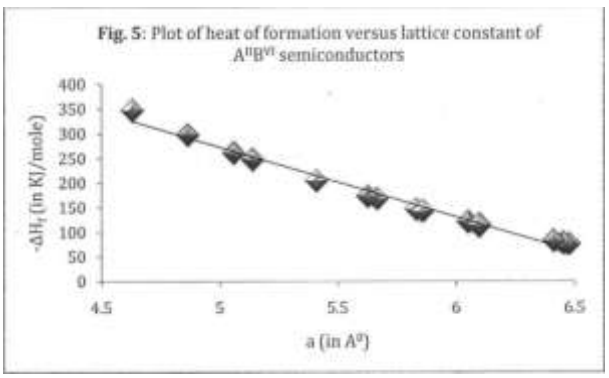
$A^{II}B^{IV}C^{V}_2$ Compounds	Plasmon energy (In eV)	Lattice Constants (In A^0)	Heat of Formation, -ΔH_f (in KJ/Mole) Using Eq. [11]	Using Eq. [16]	Expt. [46]	Ref. [48]
$ZnSiP_2$	17.02	5.40	307.77	301.96	312	303.3
$CdSiP_2$	16.19	5.67	299.56	277.47		286.5
$ZnGeP_2$	16.64	5.46	299.89	296.26	293	295.7
$CdGeP_2$	15.52	5.74	276.67	271.59	289	279.4
$ZnSnP_2$	15.55	5.65	277.30	279.19	275	277.7
$CdSnP_2$	14.82	5.75	262.16	270.77	270	262.9
$ZnSiAs_2$	16.02	5.56	287.04	287.09	290	284.5
$CdSiAs_2$	15.35	5.88	273.15	260.35		270.9
$ZnGeAs_2$	15.66	5.67	279.58	277.47	271	279.4
$CdGeAs_2$	14.90	5.81	263.82	265.89	266	264.7
$ZnSnAs_2$	14.82	5.98	262.16	252.72	252	264.7
$CdSnAs_2$	14.12	6.05	247.65	247.57	247	251.1











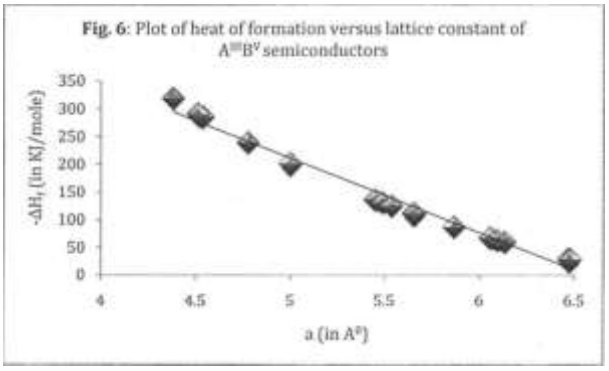


Fig. 6: Plot of heat of formation versus lattice constant of $A^{III}B^{V}$ semiconductors

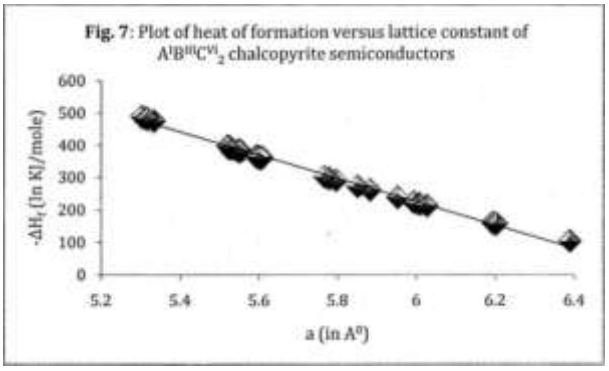


Fig. 7: Plot of heat of formation versus lattice constant of $A^{I}B^{III}C^{VI}_{2}$ chalcopyrite semiconductors

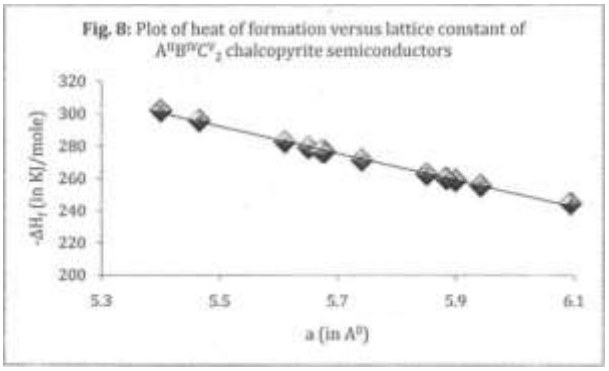


Fig. 8: Plot of heat of formation versus lattice constant of $A^{II}B^{IV}C^{V}_{2}$ chalcopyrite semiconductors

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