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Lattice Energy of II-VI and III-V Binary Solids and I-VII Ioniccrystals

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Abstract – In this paper, we'll look at, an interesting empirical relationship has been proposed to calculate the lattice energy of II-VI and III-V semiconductors and I-VII ionic crystals using their lattice constant. We have applied the proposed empirical relation for the calculation of lattice energy on the binary tetrahedral semiconductors and alkali halides. As applied to other similar theoretical results, the accessible experimental values show outstanding consensus. The lattice energy (in Kcal/mol) When these materials are plotted, they display a linear association against the tattice constant (in A), which lies at the straight line. The trial values for lattice energy vary the following quantities: Be0- 0.23%, BeS-0.639%, BeSe-0.0%, BeTe-0.78%, ZnO-1.75%, ZnS-0.10%, ZnSe-0.3496, ZnTe-1.46%. CdS-0.35%, CdSe-1.12%, CdTe-0.53%, MgTe-1.3%, BP-0.09%, BAs-0.29%, AlN-1.09%. AIP 0.80%, AlAs-0.79%, AlSb-0.16%, GaN-0.35%. GaP-0.90%, GaAs-0.39%, GaSb 0.16%, InN-0.12%, lnP-0.26%, InAs-0.13%. InSb-0.11%. LiF-4.86%, LiCl-4.06% LiBr-0.58%, LiI-2.37%, NaF-2.78%, NaCl-1.12%, NaBr-1.84%, NaI-1.07%, KF-2.01%. KCl-1.70%, KBr-2.61%, KI-2.97%, RbF-1.48%, RbCl-2.56%. RbBr-3.51% and RbI-3.82% the latest studies.

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1. INTRODUCTION

Lattice energy is a critical parameter since a measure of the powers that bind between ions in a crystal. In the recent past, increasing much attention has been given towards the study of various electronic, optical, structural & zinc blende mechanical properties Because of their rising science and technical uses, rock salt binary solids are becoming more organised. (1) to (7) However, the lattice power for these compounds has received little attention. Previously few years, a selection of theoretical possibilities calculation based on empirical relations have become an essential part of material research Empirical formula mostly establish to be simple, easy to use and it gave a batter value for physical parameters. Materials physicists will now test optical properties using empirical approaches due to developments in high-performance computing techniques. For computational solid state studies, There have been observational relationships generally established as the tool of preference. In modern high speed computer techniques, they allow researchers to investigate many structural and Materials' intrinsic attributes only by computation or simulation instead of by traditional experiments. While analytical relations do not often have particularly precise outcomes for each particular substance, their versatility enables a larger class of researchers to quantify valuable properties, and sometimes patterns emerge. The usage of mathematical terms like valence empirical radii, ionicity, and plasmon energy [8-10] becomes useful. These theories are connected to the chemical bond's character, They can also be seen to describe and define number of Molecules and solids have basic properties.

With the assistance of plasma oscillations principle of solids, Yadav et.al. (11, 12) measured the both static and dynamic, electronic & zinc blende mechanical properties, Binary solids with a structure such as wurtzite and rock-salt This is since a compound's plasmon energy is proportional to the effective number of valence electrons in the compound. Consequently, we found a new process for the lattice energy semiconductors that are binary II-VI & III-V, in addition I-VII ionic crystals, with their lattice constant (in A°), would be of great interest.

The aim of this analysis is to measure the lattice energy of binary semiconductors in the II-VI and 111-V classes, in addition I-VII ionic crystals, using their lattice constants (in A). Section -2 explains the theoretical definition In We now present the third portion. and analyse the simulation results for these materials' lattice energy. Finally, in Section 4, the conclusion is presented.

2. THEORETICAL CONCEPTS:

For calculating lattice energy Alkali halides & semiconductors of binary tetrahedral structure, many hypothetical Several methods have been written. Ladd and Lee [13] calculated the lattice energy (U) of an ionic crystal in a rock-salt configuration using the Born-Haber cycle. Several other researchers have suggested different Born-Haber-based theoretical models [14, 15], & Reddy, et. al. [4,16] used the plasma oscillation principle of solids to compute the lattice energy (U) semiconductors of binary tetrahedral structure, which was later used by Kumar, et. al. [17] When it comes to binary semiconductors, II-VI and I 1 I-V The temperature dependency of lattice energy of alkali metal nuorides and halides of Sodium, Lithium, Potassium, Rubidium, and Cesium was examined by Subrahmanyam, et. al. [18-20]. For II-VI semiconductors, Reddy and coworkers (4. 16] suggested a regular relationship between lattice energy (U in Kcal/mole) & Plasmon energy (E in eV).

$$U=381.9+24.3(\hbar\omega_p) \qquad (1)$$

Kumar, et. Al. [17) proposed a quadratic relation between lattice energy & Plasmon energy for both 11-V and III-V semiconductors with a compound structure:

$$U=421.224+27.940\ (\hbar\omega_p)-0.178\ ((\hbar\omega_p)^2 \qquad (2)$$

From both the equations we find that lattice energy & Plasmon energy is related to each other. The free electron Plasmon energy of binary semiconductors and ionic compounds is given by

$$\hbar\omega_p=\hbar\ (4\pi Ne^2/m)^{1/2} \qquad (3)$$

The letter p represents the Plasmon force. The charge and mass of the electron are e and m, respectively, and the amount of free electrons involved in plasma oscillation (per unit volume) is N. In certain instances, the authors' results were substantially different from historically reported values (14, 21, 22). These findings, on the other hand, suggest a connection between lattice energy & Plasmon energy in materials. The sum of energy used to isolate a salid's constituent ions is known as its lattice energy. In other terms, it's the same as the ion binding power of a solid. The stronger the relation between ions gets as radiation increases, and hence the Plasmon energy rises. These claims imply that lattice energy & Plasmon energy are related. To display the variation of U with Plasmon energy p for II-VI and III-V semiconductors, as well as I-VII alkali halides, a graph was plotted using the observed values. Figures 1-3 show that the plot of U versus p for these compounds is linear-

$$U=M\ (\hbar\omega_p)+N \qquad (4)$$

Where M and N are 19.5 and 511.6 for II-V1 semiconductors and 21.61 and 473.6 for III-V semiconductors, respectively, & 6.631 and 80.11 for I-VII ionic crystals.

To read more about the partnership between the two lattice energy & lattice constant, click here (in A^0), The lattice constant and binding energy are thought to be related. In terms of individual bond properties, the essence of bonding (in A^0) of a unit cell of a crystal in a solid is defined by the amount of valence electrons of the bonding atoms.

$$N=\frac{\frac{Z_A}{N_{CA}}+\frac{Z_B}{N_{CB}}}{v_b} \qquad (5)$$

Where Z_A & Z_B are the valence electron numbers of atoms A & B, respectively. In the compound AB, N_{CA} & N_{CB} are the atoms A & B's coordination numbers, Vb is the bond volume. For tetrahedral crystals $N_{CA}=N_{CB}=4$, $Z_A+Z_B=8$ &

$$v_b=\frac{4d^3}{3\sqrt{3}} \qquad (6)$$

N may be represented in the same way as single bond compounds.

$$N=\frac{\left(\frac{Z_A}{N_{CA}}+\frac{Z_B}{N_{CB}}\right)\bar{N}_c}{v_b} \qquad (7)$$

Where Z_A is the number of cation valence electrons, N_{CA} is the atom A's coordination number, N_{CB} is atom B's coordination number, N_C is the average amount of teamwork, v_b, is the unit cell volume. For rock salt crystals,

$$N_{CA}=N_{CB}=6,\ Z_A+Z_B=8, Z_M=4 \text{ and } v_b=8d^3$$

Here Z_M is the number of molecules per unit cell & using these values and taking help of Eqs. [3][5] and [7] we find the following relation between bond length and plasmon energy for these materials,

$$d=C\ (\hbar\omega_p)^{-2/3} \qquad (8)$$

where C is the constant and the values for binary semiconductors & alkali halides are 15.30 and 17.669, respectively. For these products, the relationship between bond duration and lattice constant (a in A^0) is [23|-

$$d=\frac{\sqrt{3}a}{4} \qquad \text{(Zinc-blende structure)} \qquad [9\text{-a}]$$

$$d=a/2 \qquad \text{(Rock-salt structure)} \qquad [9\text{-b}]$$

Using Eqs. [4], [8] and [9], we get-

$$U = Da^{-1.5} + S \quad [10]$$

The numerical constants D and S are determined by the arrangement of the compounds. The values of D and S for II-VI, 4538.75 and 473.6 for III-V semiconductors, and 1393 and 80.11 for I-VII ionic solids, respectively, are 4095.6 and 511.6.

These materials' lattice energy has a linear distribution relationship [in A0][21, 25], as seen in Figures 4-6 when plotted against the lattice constant. In the plot of lattice energy versus lattice constant, the zinc blende and rock-salt structured solids are on the straight side. The lattice energy patterns of these compounds decrease as the lattice parameter of these compounds increases, as seen in Figs. 4-6. The lattice energy of these materials has already been defined in detail [2, 3, 13-20, 24, 25] and will not be reiterated here.

3. RESULT AND DISCUSSION

The grid energy of double semiconductors and antacid halides is addressed as a component of their cross section steady in this article. This technique can be utilized to figure the grid power from the cross section steady. The grid energy of twofold semiconductors and soluble base halides has been estimated utilizing the recommended logical connection [10]. The assessed values, just as the qualities recorded by past specialists, are introduced in Tables 1-3, individually. just as the co-appointment amount, appear to influence grid energy. A 4:4 (tetrahedral) coordination exists in zinc blende organized precious stones of II-VI & III-V semiconductors with a compound structure, while a 6:6 coordination exists in rock salt gems of I-VII ionic mixtures. The grid energy of tetrahedral compounds is higher. This is more probable since, within the sight of countless neighbors, the iota's capacity to pull in spite of valence fee precious stone is part into more bonds, bringing about a lessening in restricting limit. Cross section energy will in general be affected by in a given class of mixtures, the scale of the anion or cation. The grid energy of a given cation diminishes as the size (sweep) of the anion increments. Likewise, the cross section power of a given anion keeps on diminishing because of the scale of the cation develops. This example remains constant for every one of the three kinds of mixtures recorded previously.

The most un-ionic III-V compound semiconductors, on the opposite side, have the biggest grid energy levels. The cross section energy of unadulterated ionic I-VII soluble base halides is low. The cross section energies of semiconductors II-VI are in the middle. Truly, sp covalent holding between molecules happens in tetrahedrally planned II-VI & III-V semiconductors with a compound structure. The idea of such a tie is horizontal, bringing about a higher holding power. The bond in I-VII compounds is non-directional and weak, resulting in lower capacity. We notice that the lattice energy values measured using the proposed empirical comparison are very close to those stated by previous researchers [2. 3, 4, 16, 21, 22, 24]. In certain ways, our measured lattice energy values for these compounds when compared to the new values by 0-486 percent For example. The result for lattice energy in comparison to the experimental values by the following amounts: BeO-0.23%, BeS-0.63%, BeSe-0.0%, BeTe-0.78%, ZnO-1.75%, ZnS-0.10%. ZnSe-0.34%, ZnTe-1.46%, CdS-0.35%, CdSe-1.12%, CdTe-0.53%, MgTe-1.3%, BP-0.09%, BAs-0.29%, AlN-1.09%, AlP 0.80%. AlAs-0.79%. AlSb-0.16%. GaN-0.35%, GaP-0.90%, GaAs-0.39% GaSb-0.16%, InN-0.12%, InP-0.26%, InAs-0.13%, InSb-0.11%, LiF-4.86%, LiCl-4.06%, LiBr-0.58%, LiI-2.37%, NaF-2.78%, NaCl-1.12%, NaBr-1.84 %, NaI-1.07%, KF-2.01%, KCl-1.70%, KBr-2.61%, KI-2.97%, RbF-1.48%, RbCl-2.56%, RbBr-3.51% and RbI-3.82% in the present study. Close harmony of the findings confirms our theory that the constants' set of potential values in Eqs. [4] & [10] remain constant for a particular crystal and may be considered as a crystalline type attribute since they are constant for all substances belonging to that crystal structure. These findings demonstrate that our current method is reasonable and can be put to work to calculate and calculate these materials' lattice energy.

4 CONCLUSIONS

The lattice energy of paired semiconductors and soluble base halides was investigated in this article. The lattice energy derived from our proposed empirical relation agrees well with other theoretical estimates for these materials. Of the most common is interesting a facet of these equations is that it highlights the critical position that these materials' lattice constants perform. Using their lattice constant, we recommended a scientific relationship to assess the Lattice limit. The correlation's physical origin has been debated. The suggested model is clear and detailed. It's worth mentioning that the constants are in the suggested relationship are crystal structure features. Their ideals remain constant for a given precious stone construction. On account of the zinc blend and the rock-salt structured complex, this has been shown. The obtained findings are in outstanding harmony with the reported principles and reinforce the proposed model's foundation. It's also It's worth remembering that methodological relationship we present is straightforward and broadly applicable.

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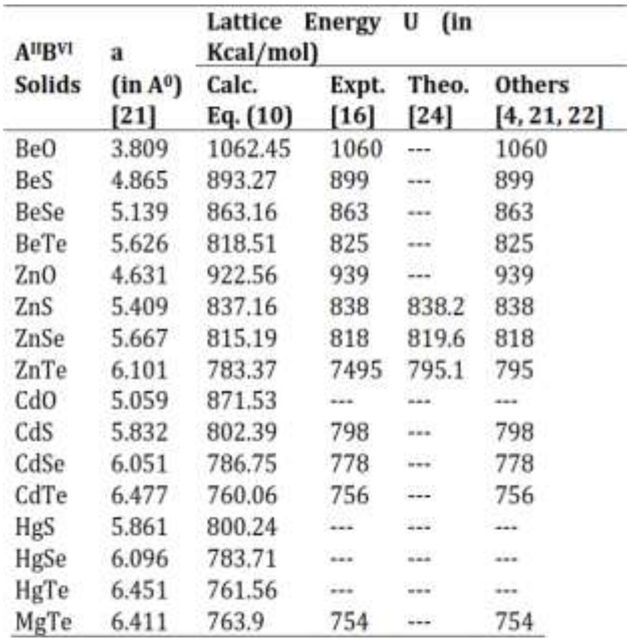
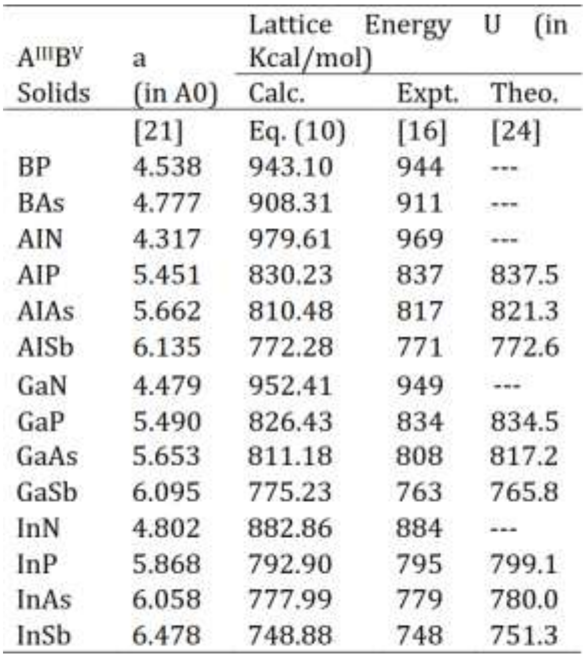
Table 1: Value of Lattice energy U (in Kcal/mol) for II-Vi group binary solids.



$A^{II}B^{VI}$ Solids	a (in A^0) [21]	Lattice Energy U (in Kcal/mol) Calc. Eq. (10)	Expt. [16]	Theo. [24]	Others [4, 21, 22]
BeO	3.809	1062.45	1060	---	1060
BeS	4.865	893.27	899	---	899
BeSe	5.139	863.16	863	---	863
BeTe	5.626	818.51	825	---	825
ZnO	4.631	922.56	939	---	939
ZnS	5.409	837.16	838	838.2	838
ZnSe	5.667	815.19	818	819.6	818
ZnTe	6.101	783.37	7495	795.1	795
CdO	5.059	871.53	---	---	---
CdS	5.832	802.39	798	---	798
CdSe	6.051	786.75	778	---	778
CdTe	6.477	760.06	756	---	756
HgS	5.861	800.24	---	---	---
HgSe	6.096	783.71	---	---	---
HgTe	6.451	761.56	---	---	---
MgTe	6.411	763.9	754	---	754

Table 2: Value of Lattice energy U (in Kcal/mol) for III-V group binary solids.



$A^{III}B^{V}$ Solids	a (in A0)	Lattice Energy U (in Kcal/mol) Calc.	Expt.	Theo.
	[21]	Eq. (10)	[16]	[24]
BP	4.538	943.10	944	---
BAs	4.777	908.31	911	---
AIN	4.317	979.61	969	---
AIP	5.451	830.23	837	837.5
AIAs	5.662	810.48	817	821.3
AISb	6.135	772.28	771	772.6
GaN	4.479	952.41	949	---
GaP	5.490	826.43	834	834.5
GaAs	5.653	811.18	808	817.2
GaSb	6.095	775.23	763	765.8
InN	4.802	882.86	884	---
InP	5.868	792.90	795	799.1
InAs	6.058	777.99	779	780.0
InSb	6.478	748.88	748	751.3

Table 3: Value of Lattice energy U (in Kcal/mol) for I-VII ionic crystals.

I-VII Ionic	a (in A⁰)	Lattice Energy U (in Kcal/mol) Calc.	Expt.	Theo.
Crystals	[25]	Eq. (10)	[2]	[3]
LiF	4.41	230.52	248.44	242.3
LiCI	5.41	190.81	197.08	198.9
LiBr	5.48	188.69	191.82	189.8
Lil	6.06	173.69	174.86	177.7
NaF	4.62	220.38	216.43	214.4
NaCl	5.62	184.66	184.91	182.6
NaBr	5.92	176.81	175.82	173.6
Nal	6.46	164.95	160.77	163.2
KF	5.32	193.63	193.51	189.8
KCI	6.28	168.62	167.71	165.8
KBr	6.58	162.64	160.71	158.5
KI	7.06	154.36	151.69	149.9
RbF	5.64	184.10	181.79	181.4
RbCl	6.54	163.39	16.16	159.3
RbBr	6.84	157.97	151.93	152.6
Rbl	7.32	150.44	150.26	144.9

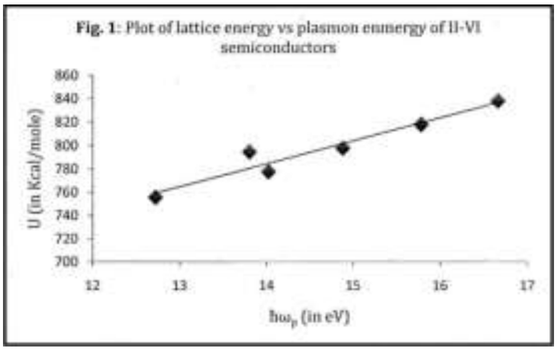


Fig. 1: Plot of lattice energy vs plasmon enmergy of II-VI semiconductors

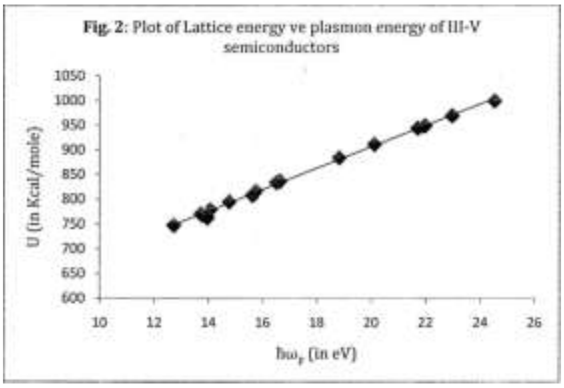


Fig. 2: Plot of Lattice energy ve plasmon energy of III-V semiconductors

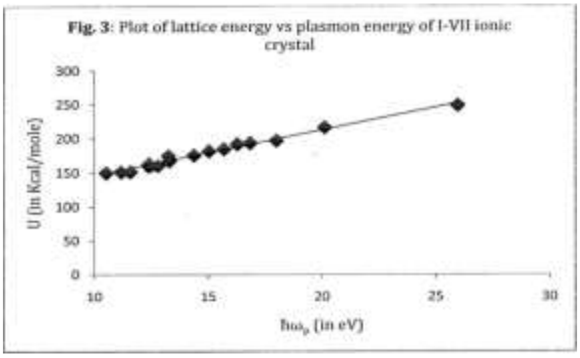


Fig. 3: Plot of lattice energy vs plasmon energy of I-VII ionic crystal

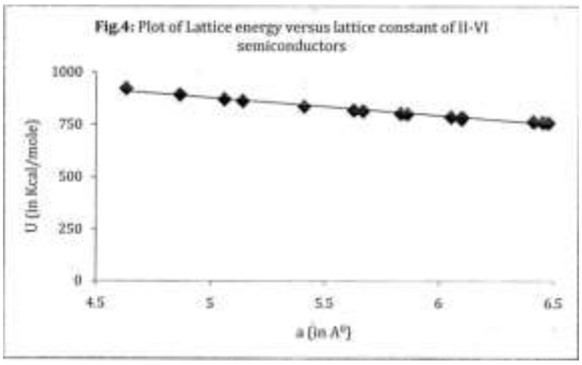


Fig.4: Plot of Lattice energy versus lattice constant of II-VI semiconductors

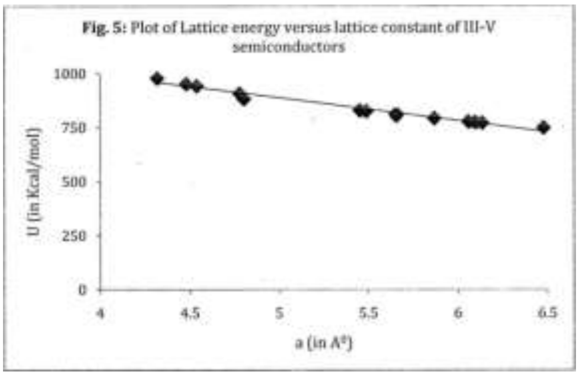


Fig. 5: Plot of Lattice energy versus lattice constant of III-V semiconductors

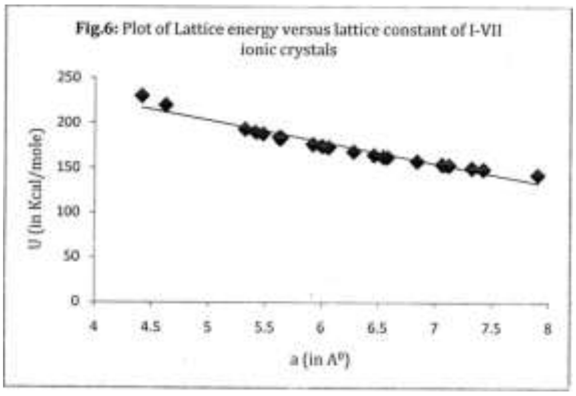


Fig.6: Plot of Lattice energy versus lattice constant of I-VII ionic crystals

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