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RESEARCH ARTICLE - PHYSICS

Electronic and Optical Properties of Semiconductor and Alkali Halides

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Abstract A simple model based on optical electronegativity difference has been proposed for calculating the energy gap, refractive index and electronic polarizability of different semiconductors and alkali halides. Correlation between energy gap, refractive index and electronic polarizability are given for II–VI, III–V semiconductors and alkali halides. The calculated values of electronic polarizability are in fair agreement with the values obtained from Lorentz–Lorentz relation. This work highlights the significance of interrelation between energy gap, refractive index and electronic polarizability. The estimated values are then compared with the literature values. There is fair agreement between estimated values and literature values.

Keywords Electronegativity · Energy gap · Refractive index · Electronic polarizability · Semiconductors

الخلاصة

اقتُرحَ - في هذا البحث - أنموذج بسيط معتمد على الفرق في الكهروسالبية البصرية لحساب فجوة الطاقة، ومعامل الانكسار والاستقطاب الإلكتروني لأشباه الموصلات المختلفة وهاليدات القلويات، وتم إعطاء الارتباط بين فجوة الطاقة، ومعامل الانكسار والاستقطاب الإلكتروني لأشباه الموصلات II-VI و II-VI وهاليدات القلويات. إن القيم المحسوبة للاستقطاب الإلكتروني هي في اتفاق عادل مع القيم التي تم الحصول عليها من علاقة لورنتز- لورنتز. يسلط هذا العمل الضوء على أهمية الترابط بين فجوة الطاقة، ومعامل الانكسار والاستقطاب الإلكتروني. وقد تم بعد ذلك مقارنة القيم بالقيم المقدرة في الأدب، وهناك اتفاق عادل بين القيم المقدرة وقيم الأدب.

1 Introduction

Electronic and optical property of semiconductors and alkali halides has been a challenge to the investigators. During the last few years, frequent attempts have been made to understand the electronic and optical properties of these compounds. In view of much importance of semiconductors and alkali halides, theoretical prediction of their different physical properties has attracted much attention [1]. The evaluation of refractive indices of semiconductors is of considerable importance for potential applications in integrated optical devices such as switches, filters and modulators, whereas the refractive index of materials is the key parameter for designing various devices. The refractive index is closely related to the electron polarizability of ions and local field inside the material. Among the various parameters controlling the refractive index, energy band gap may be the most important one. Thus, it is of great interest to develop a correlation between refractive index and energy gap in solid materials. These materials, particularly semiconductors, have potential applications in the field of light emitting diodes (LEDs), photo-detectors (PDs), laser diodes (LDs) opto-electronic devices and integrated circuit, nanotechnology and

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biotechnology [1–5]. Moss [6–8] has proposed that all energy levels in a solid are scaled down by a factor $1/\varepsilon_{\text{opt}}^2$, where ε_{opt} is the optical dielectric constant. Ravindra et al. [9–11] have proposed a linear relation between the energy gap and the refractive index for some semiconductor materials. Ravindra and Shrivastava [12] have modified the Moss [6–8] formula for solar cells, where one has to evaluate the refractive loss in order to improve the conversion efficiency of semiconductors. Reddy et al. [3] correlated refractive index and plasmon energy and calculated the values of various physical parameters like bond length, microhardness, bulk modulus, interatomic force constant and lattice energy for II–VI and III–V semiconductors using earlier models in which these parameters are calculated from their plasmon energy [13–15]. Anani et al. [16] have proposed a model for calculated the refractive index of III–V semiconductors from their energy gaps. Singh et al. [17] have proposed a relationship between fractional ionic character and electro negativities for estimating the refractive index of the materials. Recently, Kumar et al. [18] presented a model based on the energy gap data for calculating the refractive index of different semiconductor.

The optical electronegativity is very useful parameter in understanding the nature of chemical bonding and several other important physical parameters can be predicted. It is suggested that a simple model based on the concept of optical electronegativity and some other parameters should be good enough to study the main properties of ionic crystals and semiconductors with use of only few numerical constants. The present study is an attempt to study some simple correlations between electronegativity difference, energy gap, refractive index and electronic polarizability of different semiconductors and alkali halides.

2 Theory

Moss [6,7] has proposed a general relationship between refractive index (n) and energy gap (E_g).

$$n^4 E_g = 95 \tag{1}$$

Ravindra et al. [9] proposed the following linear relation between refractive index and energy gap.

$$n = 4.084 - 0.62\, E_g \tag{2}$$

Gopal [19] modified the Penn model [20] for the high-frequency dielectric constant of semiconductors to obtain a general formula relating (n) and (E_g). The formula is as follows:

$$n^2 = 1 + \frac{A}{(E_g + B)^2} \tag{3}$$

where A and B are numerical constants.

Reddy et al. [21] have proposed an empirical relation between the refractive index (n) and band gap (E_g) for different compounds.

$$(n^2 + 2)^2 (E_g - 0.365) = 154 \tag{4}$$

Anani et al. [16] have proposed the following relation for the refractive index of III–V semiconductors.

$$n^4 = 1 + \frac{A}{E_g^2} \tag{5}$$

where $A = 40.8$ eV is constant.

Based on the oscillatory theory, Herve and Vandamme [22] have proposed the following relation for refractive index.

$$n = \left\{1 + \left(\frac{A}{E_g + B}\right)^2\right\}^{\frac{1}{2}} \tag{6}$$

where $A = 13.6$ eV and $B = 3.4$ eV are constants

Reddy et al. [2] have recently proposed the following relation between refractive index and optical electronegativity (Δx).

$$n = \left\{1 + \left(\frac{A}{3.72\Delta x + B}\right)^2\right\}^{\frac{1}{2}} \tag{7}$$

where A and B are numerical constants.

Singh et al. [17] proposed the following relation between refractive index and optical electronegativity.

$$n = \frac{f}{\Delta x^{0.5}} \tag{8}$$

where (f) is constant having values I–VII ($f = 2.35$), II–VI ($f = 2.5$) and III–V ($f = 2.0$) compounds.

Kumar and Singh [18] obtained the following relation between n and E_g:

$$n = K E_g^c \tag{9}$$

where $K = 3.3668$ and $c = 0.32234$ are constants.

Based on the above correlations, the concept of optical electronegativity and its use in estimating many physico-chemical parameters and the following expression have been obtained between optical electronegativity (Δx) and energy gap (E_g) for different semiconductors and alkali halides.

$$E_g = A\Delta x^B \tag{10}$$

where $A = 3$ for (II–IV, III–V) semiconductors, 4 for alkali halides and $B = 0.8$ are numerical constants.

Accordingly, the following may be suggested for refractive index (n).

$$n = C - \ln E_g \tag{11}$$

where $C = 3.6$ eV is a numerical constant.

Table 1 Energy gap (E_g), refractive index (n), and electronic polarizability (α) of II–VI semiconductors

II–VI group semiconductors	Electronegativity difference (Δx)	Energy gap (E_g)		Refractive index (n)		Electronic polarizability (α) $\times 10^{-24}$ cm^3		
		Present study (Eq. 10)	Refs. [6,8,23]	Present study (Eq. 11)	Refs. [9,10,23]	Present study (Eq. 12)	Present study (Eq.13)	Refs. [24,25]
MgO	2.93	7.09	7.20	1.64	1.74	1.60	1.65	1.80
MgS	1.27	3.63	3.90	2.31	2.26	4.62	4.40	4.53
MgSe	1.20	3.47	2.98	2.35	2.43	5.83	5.57	6.00
MgTe	0.79	2.48	2.60	2.69	2.65	8.93	8.58	8.82
CaO	2.50	6.24	6.15	1.76	1.82	2.74	2.76	2.90
CaS	1.50	4.15	5.40	2.18	2.12	6.33	6.03	6.13
CaSe	1.90	5.01	5.00	1.99	2.26	6.54	6.30	7.62
SrO	2.50	6.24	5.80	1.76	1.80	3.58	3.60	3.72
SrS	1.50	4.15	4.80	2.18	2.10	7.10	6.77	6.80
SrSe	1.40	3.92	4.60	2.23	2.21	9.90	9.45	8.47
SrTe	1.10	3.23	4.00	2.42	2.41	10.89	10.41	10.84
BaO	2.05	5.32	5.20	1.93	1.98	504	4.89	5.22
BaS	1.60	4.36	4.00	2.12	2.15	8.45	8.11	8.61
BaSe	1.50	4.15	3.35	2.17	2.27	9.41	9.02	9.88
ZnO	1.10	3.23	3.20	2.42	2.00	3.54	3.38	2.86
ZnS	0.90	2.75	3.70	2.59	2.39	6.33	6.05	5.91
ZnSe	0.80	2.51	2.58	2.68	2.43	7.07	6.78	6.53
ZnTe	0.60	1.99	2.10	2.91	2.70	8.57	8.32	8.14
CdO	0.67	2.18	2.60	2.82	2.68	5.10	4.92	5.18
CdS	0.90	2.76	2.40	2.58	2.38	7.72	7.40	7.57
CdSe	0.56	1.88	1.70	2.96	2.44	9.89	9.63	9.13
CdTe	0.38	1.38	1.44	3.28	3.23	11.69	11.56	11.41

Table 2 Energy gap (E_g), refractive index (n), and electronic polarizability (α) of III–V semiconductors

III–V group semiconductors	Electronegativity difference (Δx)	Energy gap (E_g)		Refractive index (n)		Electronic polarizability (α) $\times 10^{-24}$ cm^3		
		Present study (Eq. 10)	Refs. [6,8,23]	Present study (Eq. 11)	Refs. [9,10,23]	Present study (Eq.12)	Present study (Eq. 13)	Refs. [24,25]
AlN	1.43	3.99	3.80	2.21	2.20	2.80	2.68	2.79
AlP	0.80	2.51	3.00	2.67	2.75	5.39	5.19	5.51
AlAs	0.58	1.94	2.40	2.93	2.92	7.57	7.36	7.55
AlSb	0.43	1.52	1.50	3.17	3.19	10.45	10.30	10.49
GaN	1.20	3.47	3.40	2.35	2.40	3.26	3.11	3.10
GaP	0.70	2.25	2.24	2.79	2.90	6.68	6.43	6.85
GaAs	0.37	1.35	1.40	3.30	3.30	8.24	8.16	8.24
GaSb	0.21	0.86	0.81	3.74	3.75	10.94	11.16	10.94
InN	0.76	2.40	2.40	2.72	2.35	5.03	4.84	4.45
InP	0.41	1.47	1.25	3.21	3.10	9.09	8.97	8.92
InAs	0.10	0.47	0.36	2.85	3.51	12.20	12.25	10.47
InSb	0.13	0.58	0.18	3.06	3.96	14.35	11.90	13.42

Table 3 Energy gap (E_g), refractive index (n), and electronic polarizability (α) of alkali halides

Alkalihalides	Electronegativity difference (Δx)	Energy gap (E_g)		Refractive index (n)		Electronic polarizability (α) $\times 10^{-24}$ cm^3		
		Present study (Eq.10)	Refs. [6,8,23]	Present study (Eq.11)	Refs. [9,10,23]	Present study (Eq. 12)	Present study (Eq. 13)	Ref. [26]
LiF	3.0	8.84	9.49	1.33	1.39	0.99	0.76	0.89
LiCl	2.0	6.96	7.02	1.66	1.66	3.06	2.98	2.98
LiBr	1.6	5.82	5.91	1.83	1.78	4.31	4.35	4.12
LiI	1.2	4.62	4.38	2.06	1.95	7.58	7.84	6.15
NaF	3.1	9.88	9.99	1.31	1.34	1.64	1.24	1.15
NaCl	2.4	8.06	8.13	1.51	1.54	3.51	3.19	3.24
NaBr	2.1	7.24	7.21	1.62	1.64	4.64	4.45	4.38
NaI	1.6	5.82	6.00	1.83	1.77	7.02	7.09	6.41
KF	3.1	9.88	9.77	1.31	1.36	2.35	1.78	1.99
KCl	2.2	7.52	8.59	1.58	1.49	5.24	4.94	4.08
KBr	2.0	6.96	7.96	1.66	1.56	6.48	6.30	5.22
KI	1.9	6.88	6.88	1.70	1.68	8.02	8.10	7.25
RbF	3.2	10.14	9.43	1.28	1.40	2.83	2.03	2.54
RbCl	2.2	7.52	8.56	1.58	1.49	6.03	5.68	4.63
RbBr	2.0	6.96	8.02	1.66	1.55	7.39	7.20	5.77
RbI	1.7	6.11	7.15	1.79	1.65	9.94	10.00	7.80
CsF	3.3	10.40	8.65	1.26	1.48	3.41	3.39	3.60
CsCl	2.1	7.24	7.50	1.62	1.61	6.10	5.85	5.69
CsBr	2.0	6.96	6.95	1.65	1.67	7.18	6.90	6.83
CsI	1.7	6.11	5.88	1.78	1.79	9.57	9.55	8.86
CuF	2.1	7.24	–	1.62	1.58	2.82	2.71	2.57
CuCl	1.1	4.32	3.31	2.14	1.93	4.90	5.14	6.79
CuBr	0.9	3.68	2.94	2.30	2.10	6.37	6.69	7.13
CuI	0.6	2.66	2.60	2.62	2.35	8.48	8.86	8.55
AgF	2.0	6.96	–	1.66	1.70	4.01	3.16	3.31
AgCl	1.0	4.0	3.10	2.21	2.00	5.49	5.74	5.50
AgBr	0.7	3.00	2.85	2.50	2.15	6.97	7.30	7.00
AgI	0.6	2.66	2.80	2.62	2.22	9.80	10.22	11.36

According to the classical theory of dielectric constant, electron polarizability (α) for a material can be calculated with the help of Lorentz–Lorentz relation which is given by:

$$\alpha = \left(\frac{n^2-1}{n^2+2}\right)\frac{M}{d} \times 0.395 \times 10^{-24}\,\mathrm{cm}^3 \tag{12}$$

where E_g, M and d are energy gap (eV), molecular weight (g/cm^3) of the substances, respectively. Estimated refractive index values from Eq. (11) are employed in Eq. (12) and electronic polarizability values are estimated. It is interesting to investigate the relationship between energy gap (E_g) and electron polarizability (α). The following expression has been obtained between energy (E_g) and electronic polarizability (α) for II–VI, III–V semiconductors and alkali halides.

$$\alpha = \left[\frac{12.41-3\sqrt{E_g-0.365}}{12.41}\right]\frac{M}{d} \times 0.395 \times 10^{-24}\,\mathrm{cm}^3 \tag{13}$$

where E_g, M and d are energy gap (eV), molecular weight (g/mol) and density (g/cm^3) of the substances, respectively. The estimated energy gap (E_g) values from Eq. (10) are employed in Eq. (13) and electronic polarizability values are estimated.

3 Results and Discussion

The present study is an attempt to correlate electronegativity difference, energy gap, refractive index and electronic polarizability of II–VI, III–V semiconductors and alkali halides. These physical parameters are computed using Eqs. (10–13) and are listed in Tables 1, 2, 3. An excellent agreement has

been observed between the calculated and the values reported by different workers [6,8–10,23–26] as well as the available experimental values. The accuracy of estimated physical parameters energy gap, refractive index and electronic polarizability mainly depends on the reliability and precision of the electronegativity difference (input data). The proposed relationships between optical electronegativity, energy gap, refractive index and electronic polarizability give an access to study the nature of chemical bonding using the electronegativity concept. It can be observed from the tables that as the electronegativity difference for the groups of semiconductors with common cation decreases with the energy gap, refractive index and electronic polarizability increases. The ionic character can be understood from the proposed relations. Electronegativity difference of the atoms forming a compound and band gap is interrelated. Compounds with the ionic bonding have the largest band gaps and covalent bond have the smallest ones. Electronegativity describes the predisposition of an atom to absorb electrons, its units are the square root of bond strength. Thus an atom with higher electronegativity will be more reactive chemically than one with lower electronegativity. When the electronegativities of atoms engaged in covalent bonding are similar, this factor has little influence on bonding. However, when the electronegativity difference of the two species is equal or more than about 0.2 Units, small amounts of ionic bonding may take place along with the covalent bonding.

Larger electronegativity difference involves higher degree of ionicity in the bonding. It is probable that perfectly pure covalent bonding normally does not exist in compounds because no two atoms have identical electronegativity; small degree of ionicity is present. After careful examination of crystal structure, it is known that the wurtzite structure is more favorable for crystals with larger difference of electronegativity between the two kinds of atoms. Thus the general tendency is that the wurtzite structure is more proven in comparison to zinc blende structure having a higher degree of ionicity. The nature of bonding is clearly evident from this discussion.

Estimated physical parameters in the present study are in good agreement with the values reported by different investigators. Several other workers have also estimated these parameters with distinct ideas. But all the methods enumerated in the literature involve many experimental parameters. The main advantage of the present model is the simplicity of the formula, which does not require any experimental data except electronegativity difference of the materials. The empirical relationship proposed in the present study will stimulate basic research in describing the physical characterization of compounds. In most of the cases, the values coincide with that of others. Hence, it is possible to predict the above parameters of the compounds with the knowledge of only one parameter, the electronegativity difference.

4 Conclusion

A simple relationship for the study of energy gap, refractive index and electronic polarizability for II–VI, III–V semiconductors and alkali halides has been presented. It is observed from the table that the energy gap values for the group semiconductors with common cation decreases while refractive index and electronic polarizability increases. Fair agreement between calculated and experimental electronic polarizability indicates the correctness of estimated refractive indices in the present work. It is found that the behavior of different materials within a group of compounds is almost similar but significantly different from the compounds of other groups. Even in I–VII compounds the behavior of Cu halides and Ag halides is different from those alkali halides. Similarly in II–VI group of compounds the behavior of Zn chalcogenides and Cd chalcogenides is also different from that of alkali earth chalcogenides. This is mainly because of different nature of chemical bond of these compounds. It is pertinent to mention here that the inclusion of electronegativity has direct bearing on the concept of chemical bond. Highest electronegativity for a material indicates its strength of ionicity, whereas low electronegativity represents its covalency. From this study, it is possible to correlate electronegativity difference, energy gap, refractive index, electronic polarizability and nature of chemical bonding. The present approach in computing the above-mentioned parameters for semiconductors and alkali halides is a step forward in finding suitable relationship between electronegativity difference, energy gap, refractive index and electronic polarizability.

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