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Research paper

Optical and Electronic Properties of II-VI Group Semiconductor Nanomaterials from Energy Gaps

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Abstract

A simple relation between the energy gap and refractive index is given for II-VI group semiconductors. Optical and electronic properties are evaluated by proposing a relation between energy gap and refractive index. The computed values are in fair agreement with the experimental values and earlier researches. This work emphasizes the understanding of interrelation between these parameters.

Keywords: *Electronic Polarisability, Energy Gap, Fermi Energy, Ionocity and Refractive Index.*

1. Introduction

The formation of various solid-state electronic device starts with a semiconductor substantial of the supreme quality. Semiconductors are substantial whose conductivity lies between that of conductors and insulators. Compound semiconductors are useful in certain electronic circuit operations as well as in applications that involve light like LEDs. Semiconductors abundant in optoelectronic characteristics have produced ample research and industrial curiosity in current era through their modernistic applications in various apparatus like laser diodes(LDs), photo detectors, integrated circuits, light emitting diodes (LEDs), nanotechnology [1,2].
The II-VI compounds are being greatly used in optical fiber communications, infrared detectors, and advanced microwave equipments. These materials have the useful direct band gap to make LEDs and lasers from blue to red span [3,4]. Wide band gap II-VI semiconductors are needed in optoelectronic devices like laser diodes and light emitting diodes performing in blue-green spectral span [5-7].
In semiconductors, two essential characteristics specifically refractive index and energy gap determine their electronic and optical function. There have been several efforts to connect these two quantities with a relevent relation [8-10]. In the current work, we have used Tripathy relation [11] and modified this relation to examine some of the electronic and optical characteristics of II-VI group semiconductors. We have computed the refractive indices from their energy gap using refractive index-energy gap relations. We have computed characteristics like Refractive index, Dielectric constant, Reflectivity, Electronic polarizability, Fermi energy and Plasmon energy.

2. Optical Properties

Optical measurement comprises the paramount methods of deciding the band structures of semiconductors. Photon-induced electronic transitions may occur between different bands or within a single band. [2,12].

2.1. Refractive Index

The refractive index (RI) is one of the elemental characteristics of a material as this is linked to the electronic polarisability of ions and the local field inside the material. The RI in semiconductors is a strength of its transparency to incident spectral radiation. The RI decides how much light is bent, or reflected when entering a material [2,10].
In the current work, we have used Tripathy relation [11] and proposed RJ relation to calculate refractive index of II-VI group of semiconductors for a wide range of energy gaps. As per the Tripathy relation, the RI of a semiconductor with energy gap E_g is stated as

$$n = n_o[1 + \alpha e^{-\beta E_g}] \quad (1)$$

Here, $\alpha = 1.9017$, $n_0 = 1.73$, $\beta = 0.539$/eV are the constant parameters for a specified pressure and temperature. According to proposed RJ relation, the RI of a semiconductor with energy gap E_g is stated as

$$n = 2 + \alpha e^{-\beta E_g} \quad (2)$$

Here, $\beta = 0.539$/eV, $\alpha = 1.9017$ are the constant parameters for a specified pressure and temperature. In the current work, we have used the values of refractive indices computed from these formulations to examine some of their electronic and optical and characteristics.

2.2. Dielectric Constant

This is a macroscopic quantity that evaluates how effective an electric field is in polarizing the material. The term dielectric is used to store the energy storing capacity of the material. The static limit dielectric constant E_∞ is linked to the RI n along a simplified expression $E_\infty = n^2$, where the magnetic permeability of the medium is close to 1. The paramount characteristics of dielectrics is

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their strength to become polarized under the action of an external electric field [2,10].

2.3. Reflectivity

Reflectivity is an optical characteristics of material, which defines how much light is reflected from the material in relation to an amount of light incident on the material. It can be calculated as

$$R = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \quad (3)$$

Here, n is refractive index and k is extinction coefficient. For very high frequencies K→ 0. We will use the formula $R = \frac{(n-1)^2}{(n+1)^2}$ to calculate the reflectivity of II-VI group semiconductor nanomaterials [2].

3. Electronic Properties

3.1. Electronic Polarisability

Electronic polarization occurs due to displacement of the center of the negatively charged electron cloud relative to the positive nucleus of an atom by the electric field. It decides the dynamical response of a bound system to external fields, and imparts insight into a molecule's internal structure. It can be determined using the Lorentz-Lorenz formula as [13,14].

$$\alpha = 0.3965\left(\frac{n^2-1}{n^2+2}\right)\frac{M}{\rho} \quad (4)$$

3.2. Plasmon Energy

Plasmons are used as transmitting information on computer chips, high-resolution lithography and microscopy due to their extremely small wavelength[15,16]. The valence electron Plasmon energy can be calculated as

$$\hbar\omega_p = k_1 e^{-k_2 n} \quad (5)$$

Where k_1= 22.079 , k_2= 0.1779 and n is refractive index[17,18].

3.3. Fermi Energy

The highest energy level that an electron can occupy at the absolute zero temperature is known as the Fermi level. The Fermi energy can be calculated as [18]

$$E_F = 0.2947(\hbar\omega_p)^{\frac{4}{3}} \quad (6)$$

3.4. Ionicity

The ionicity of a bond is described as the fraction F_i of ionic or heteropolar character compared to the covalent or homopolar fraction F_h so that $F_i + F_h = 1$ where $0 \le F_i \le 1$. It can be calculated as

$$f_i^T = \sqrt{\left[\frac{1-\frac{E_g}{4*E_F}}{E_\infty - 1}\right]} \quad (7)$$

Where, Eg, E_F and E∞ are the energy gap, fermi energy and dielectric constant respectively [19,20].

4. Results

The calculated values of refractive index, reflectivity, dielectric constant, electronic polarisability, plasmon energy, fermi energy and ionicity using Tripathy relation and proposed RJ relation are shown in Table1 and Table2 respectively. It can be observed from the table that the refractive index and reflectivity decreases with the energy gap. Whereas plasmon energy, fermi energy, E-polarisability and ionicity increase with the increase in energy gap. Using these values, graphs are plotted as a function of energy gap. This is interesting to note that our calculations are in fair agreement with the known values.

Table 1: Refractive index, Reflectivity, Dielectric constant, Electronic polarisability, Plasmon energy, Fermi energy and Ionicity of some II-VI group semiconductors calculated from Tripathy relation.

Compounds	Eg (eV)	n	R	E_∞	α	$\hbar\omega_p$ (eV)	E_F (eV)	f_i^T
CdSe	1.73	3.0249	0.3485	9.1498	37.4972	12.8907	8.9073	0.3418
HgS	2.1	2.7907	0.3332	7.7882	32.7042	13.4389	9.4160	0.3732
ZnTe	2.26	2.7031	0.3278	7.3067	34.5602	13.6501	9.6138	0.3866
CdS	2.42	2.6227	0.3230	6.8785	33.8807	13.8467	9.7989	0.3998
MgTe	2.6	2.5402	0.3183	6.4524	44.5082	14.0516	9.9926	0.4144
ZnSe	2.7	2.4976	0.3160	6.2382	30.8405	14.1582	10.0939	0.4224
PbS	2.9	2.4192	0.3119	5.8525	35.3204	14.3572	10.2835	0.4381
C	3.08	2.3541	0.3087	5.5416	9.0576	14.5245	10.4436	0.4520
ZnO	3.3	2.2855	0.3056	5.2237	16.1596	14.7027	10.6147	0.4678
ZnS	3.66	2.1875	0.3018	4.7854	26.3738	14.9612	10.8643	0.4925
MgS	3.9	2.1320	0.2999	4.5455	21.8824	15.1097	11.0084	0.5077

Table 2: Refractive index, Reflectivity, Dielectric constant, Electronic polarisability, Plasmon energy, Fermi energy and Ionicity of some II-VI group semiconductors calculated from proposed RJ relation.

Compounds	Eg (eV)	n	R	E_∞	α	$\hbar\omega_p$ (eV)	E_F (eV)	f_i^T
CdSe	1.73	2.7485	0.2176	7.5541	48.8800	17.7618	13.9029	0.3845
HgS	2.1	2.6131	0.1993	6.8285	42.5924	18.0888	14.2452	0.4065
ZnTe	2.26	2.5625	0.1924	6.5663	45.0001	18.2153	14.3782	0.4154
CdS	2.42	2.5160	0.1859	6.3303	44.1110	18.3333	14.5024	0.4240
MgTe	2.6	2.4683	0.1792	6.0925	57.9484	18.4562	14.6323	0.4332
ZnSe	2.7	2.4437	0.1758	5.9718	40.1561	18.5203	14.7001	0.4381
PbS	2.9	2.3984	0.1693	5.7522	45.9999	18.6400	14.8268	0.4474
C	3.08	2.3615	0.1639	5.5769	11.8009	18.7406	14.9336	0.4552
ZnO	3.3	2.3211	0.1582	5.3876	21.0632	18.8476	15.0475	0.4641
ZnS	3.66	2.2645	0.1500	5.1279	34.4136	19.0029	15.2130	0.4772
MgS	3.9	2.2324	0.1454	4.9836	28.5766	19.0919	15.3081	0.4848

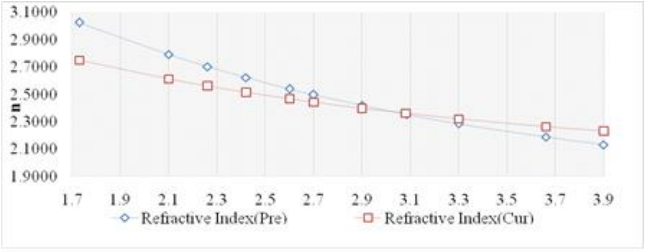


Fig. 1: Refractive index as a function of energy gap

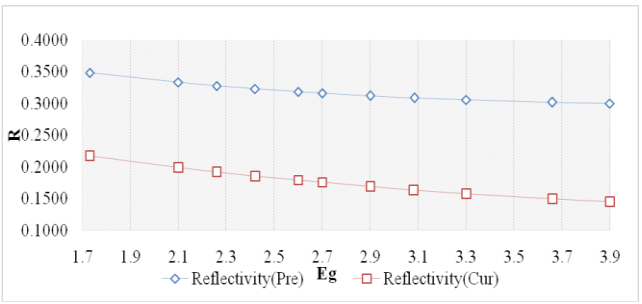


Fig. 2: Reflectivity as a function of energy gap

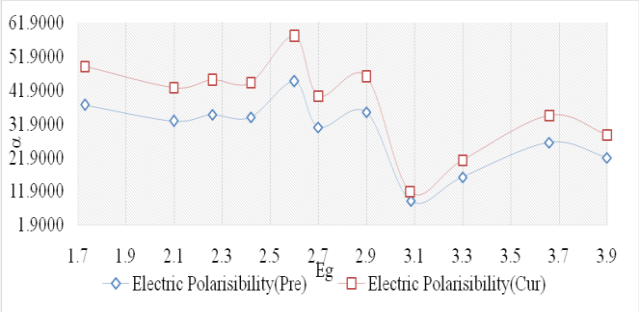


Fig. 3: E-Polarisibility as a function of energy gap

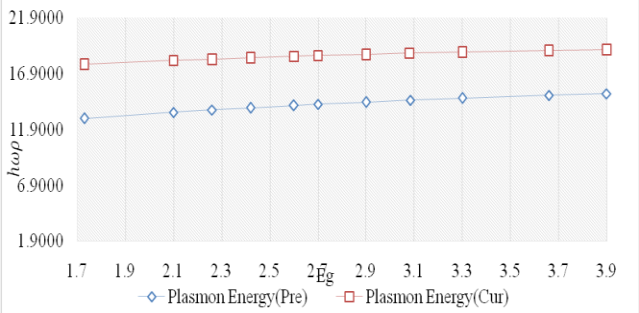


Fig. 4: Plasmon energy as a function of energy gap

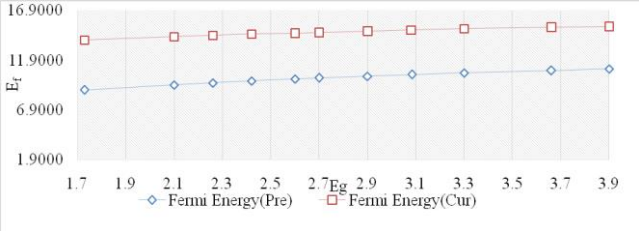


Fig. 5: Fermi energy as a function of energy gap

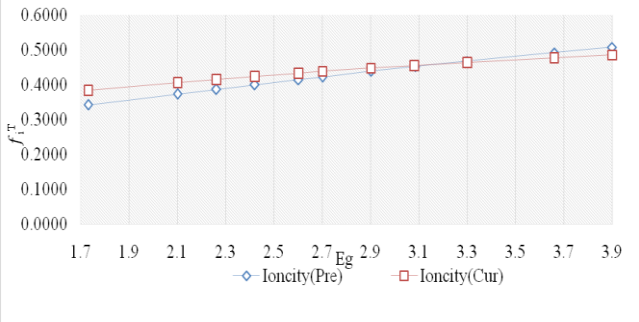


Fig. 6: Ionicity as a function of energy gap

5. Conclusion

In this work, we have calculated some of the electronic and optical characteristics of II-VI group binary semiconductor nanomaterials with respect to their operational calculation from energy gaps. Here, we have determined the refractive indices from their energy gaps using Tripathy relation and proposed RJ relation. Various optical and electronic properties are evaluated from their respective refractive indices. Even the computations of RI from proposed RJ relation and Tripathy relation are quite different but match with the familiar values at more number of data points then the previous equations. We have introduced an empirical relation for its computation and the computed values are in fair agreement with the familiar values. Even though the empirical relationship is a simple one; we believe that it can utilize to a broad range of binary as well as ternary semiconductors.

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