

Electronic and Optical Properties of Rare-earth Chalcogenides and Pnictides

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The dielectric description of crystal ionicity developed by Phillips and Van Vechten has been successfully employed in a wide range of semi-conductors and insulators. However, the applicability of this Phillips and Van Vechten (P.V.V) dielectric analysis has been limited to only simple $A^N B^{8-N}$ compounds. An empirical relationship previously introduced by the authors, relating the electronic properties of zinc blende and complex structured solids to their product of ionic charges, is shown to be applicable with minor modifications to the rock salt structured solids. An alternative approach to the well-known P.V.V. theory has been evolved in order to understand the electronic and optical properties such as heteropolar gap (E_c), average energy gap (E_g), crystal ionicity (f_i) and optical dielectric constants (ϵ_∞) of REX (RE = rare earth metals, X = S, Se, Te, P, As and Sb). The estimation is based on the approximate inverse relationship between the electronic properties and the product of ionic charges of these compounds. The evaluated values are in better agreement with the modified P.V.V. theory.

1. Introduction

Electronic and optical properties of rare earth monochalcogenides and pnictides have long been a challenge to investigators; the chalcogenides and pnictides are difficult to fabricate into single-phase crystals and the experimental picture of their electronic structure is far from clear. During the last few years, frequent attempts have been made to understand the electronic properties of rare earth compounds. This is because of their interesting semi conducting properties and various practical applications in the field of non-linear optics, electro-optic components, glass-making, grinding alloys, composites lasers, phosphors lasers, and electronics [1-6]. Crystal ionicity is one of the key parameter of semi conducting materials in discussing problems in the field of elastic constants, cohesive energy, heats of formation, bulk modulus and crystal structure [7]. Phillips [8, 9], Van Vechten [9,10], Levine [7] and several other researchers [11,12] have developed various theories and calculated crystal ionicity for the case of simple compounds. Phillips and Van Vechten have calculated the homopolar and heteropolar contribution to the chemical bond in the binary $A^N B^{8-N}$ crystals. This theory is based on the simple one-electron model originally suggested by Penn [11] and the model has used to separate the average energy gap into homopolar and heteropolar parts. The homopolar energy gap is taken to be a function of the nearest-neighbor distance only. Levine [7]

has extended the Phillips and Van Vechten (PVV) theory for ternary compounds considering also the effect of d core electrons. Singh and Gupta [12] have introduced the justification of Levine's theory. It is clear from the Levine's modifications as well as PVV theory that the value of homopolar energy gaps (E_h) depends upon the nearest-neighbor distance, while heteropolar energy gaps (E_c) is a function of nearest-neighbor distance and valence number of electrons taking part in the bond formation. Kumar et al. [13-15] have calculated the homopolar and heteropolar energy gaps in terms of plasmon energy because plasmon energy depends directly on the effective number of valence electrons in a compound. We, therefore, explore in the current work a new method for correlating ionic charge and the electronic properties of rare earth monochalcogenides and pnictides. In the proposed approach, only the nearest-neighbor distance and ionic charge are required as input for the computation of electronic and optical properties such as average energy gaps (E_g), heteropolar energy gaps (E_c), crystal ionicity (f_i), and dielectric constant (ϵ_∞) of rare earth monochalcogenides and pnictides. Recently, the author [16-22] has shown that the ionic charge of a metal changes when it undergoes a chemical combination and forms a compound. This is due to the fact that the ionic charge depends on the number of valence electrons, which changes when a metal forms a compound. Previously [16], we have successfully employed the present method for evaluating various parameters related to electronic and optical

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properties of zinc blende and complex structured solids.

2. Theoretical concept

Several researchers present clear picture on ionicity and covalency. The ionic picture involves electron transfer from one atom to another giving rise to two closed-shell ions which interact mainly by Coulomb force and short-range repulsion, while the covalent picture involves sharing of electrons between the atoms instead of charge transfer. In order to determine the crystal ionicity first major approach was given by Pauling [23] based on the thermo-chemical effect. Penn [11] has proposed a theory based on the one-electron model. According to Penn, the average energy gaps ($E_g = E_p$) can be evaluated as,

$$E_p = \hbar\omega_p S_o / \sqrt{(\epsilon_\infty - 1)} \quad (1)$$

$$\hbar\omega_p = 28.8 \sqrt{(N D / M)} \quad (2)$$

where, N is the number of valence electrons contributing towards the transitions, ϵ_∞ is the optical dielectric constant, $\hbar\omega_p$ is the valence electron plasmon energy, D and M are density and molecular weight, respectively, and $S_o = 1$. The average energy gaps E_g can be decomposed into a heteropolar (E_c) and a homopolar part (E_h) according to the relation [8-10,12],

$$E_g^2 = E_h^2 + E_c^2 \quad (3)$$

and the crystal ionicity as

$$f_i = E_c^2 / E_g^2 \quad (4)$$

The homopolar part E_h depends simply on the nearest-neighbour distance d as,

$$E_h = 40.468 / d^{2.5} \quad (5)$$

The heteropolar part of E_g is related to the ionic binding and represents the dielectrically screened potential difference between the fields produced by the ion cores of the two atoms participating in a given bond at the bond center [24]. According to modified Phillips-Van Vechten (PVV) theory [12], E_c may be given by the following relation,

$$E_c = be^2 \{(Z_A - Z_B) / d_0\} \exp(-K_S d_0) \quad (6)$$

Z_A and Z_B are valence state of atoms A and B, respectively. K_S is Thomas fermi screening

parameter, d_0 is $d / 2$ (d is nearest-neighbour distance), and b is the adjustable parameter that depends on co-ordination number [7] around the cation, i.e., $b = 0.089 N_c^2$, where N_c is average co-ordination number. For NaCl type crystal structure $N_c = 6$ and $b = 3.204$.

Recently, Kumar et al. [13-15] have shown that the homopolar and heteropolar energy gaps of rock salt structured solids can be expressed in terms of plasmon energy by the following relations,

$$E_h = K_1 (\hbar\omega_p)^{1.6533} \text{ eV}, \quad (7)$$

$$E_c = K_2 b (\hbar\omega_p)^{2/3} \times \exp[-K_3 (\hbar\omega_p)^{-1/3}] \text{ eV} \quad (8)$$

In the above equations, b is the prescreening factor and K_1, K_2, K_3 are constants depending upon the structure elements.

The physical meaning of equation (6) is that E_c is given by the difference between the screened Coulomb potentials of atoms A and B having core charges Z_A and Z_B . These potentials are to be evaluated at the covalent radii d_0 . Only a small part of the electrons are in the bond, the rest screen the ion cores, reducing their charge by the Thomas-Fermi screening factor $\exp(-K_S d_0)$, which affects the chemical trend in a compound. This screening factor, as well as the bond length, is related to the effective number of free electrons in the valence band. The ionic charge also depends directly on the effective number of free electrons in the valence band. Thus, there must be some correlation between the physical process, which involves the ionic contribution E_c to the average energy gap E_g and the product of ionic charge of a compound ($Z_1 Z_2$), where Z_1 and Z_2 are the ionic charges on cation and anion, respectively.

Krishnan-Roy theory [25], Jayaraman et al. [26] and Sirdeshmukh et al. [27] found that substantially reduced ionic charges must be used to get better agreement with experimental values. The crystal ionicity of rare earth monochalcogenides and pnictides exhibits a linear relationship when plotted against nearest-neighbour distance, but fall on three different straight lines according to the ionic charge product of the compounds, which is presented in Fig. 1. From Fig. 1, one can easily predict that the values of crystal ionicity can be presented in terms of nearest-neighbour distance and the product of ionic charges. For the better agreement with modified PVV theory, we have been able to evolve the following relations for the heteropolar (E_c) and average energy (E_g) gaps determination.

$$E_c = A / (Z_1 Z_2)^{0.7} d^2 \text{ eV}, \quad (9)$$

$$E_g = S / (Z_1 Z_2)^{0.5} d^{2.12} \text{ eV} \quad (10)$$

Where, Z_1 and Z_2 are ionic charges, d is nearest-neighbour distance in Å, and A and S are constants. The values of these constants depend upon the crystal structure of the compounds. For rock salt structured solids the values of these constants have been calculated $A = 130$ and $S = 125$. On solving equations (4), (9) and (10) the crystal ionicity may be expressed by the following relations,

$$f_i = 1.0816 \times d^{0.24} / (Z_1 Z_2)^{0.4} \text{ eV}, \quad (11)$$

The values of the powers, raised on d and $Z_1 Z_2$, are so chosen so as to reflect a systematic trend in the values of crystal ionicity obtained by the proposed approach for the entire class of rock salt structure solids. In order to justify the values of E_c and E_g evaluated by the proposed approach, we have calculated the values of dielectric constants by using the well known relation given by [7, 11],

$$\epsilon_\infty = 1 + \{(\hbar\omega_p)^2 / (E_g)^2\} \quad (12)$$

The electronic polarizability has also been calculated using the well-known phenomenological approach of Clausius and Mossotti. Thus,

$$\alpha = \{(n^2 - 1) M \times 10^{-24}\} / \{(n^2 + 2) D \times 2.53\} \quad (13)$$

Where, M is the molecular weight, D is the density, n^2 is refractive index and where $n^2 = \epsilon_\infty$ (optical dielectric constant of the material).

3. Results and discussion

The solid state physics of an atom in combination with anion as S, Se, Te, P, As and Sb depends primarily upon its electronic configuration. Any change in crystallographic environment of an atom is related to core electrons via the valence electrons.

The change in the wave function that occurs for the outer electrons usually means a displacement of electric charge in the valence shell so that the interaction between valence, shell and core electrons is changed. This leads to a change in the binding energy of the inner electron and to a shift in the position of the absorption edge. Ionic charge depends on the effective number of valence electrons, which changes when a metal forms a compound. We have calculated electronic and optical properties such as average energy gaps (E_g), heteropolar energy gaps (E_c), crystal ionicity (f_i), dielectric constant (ϵ_∞), and electronic polarizability (α) of rare earth monochalcogenides

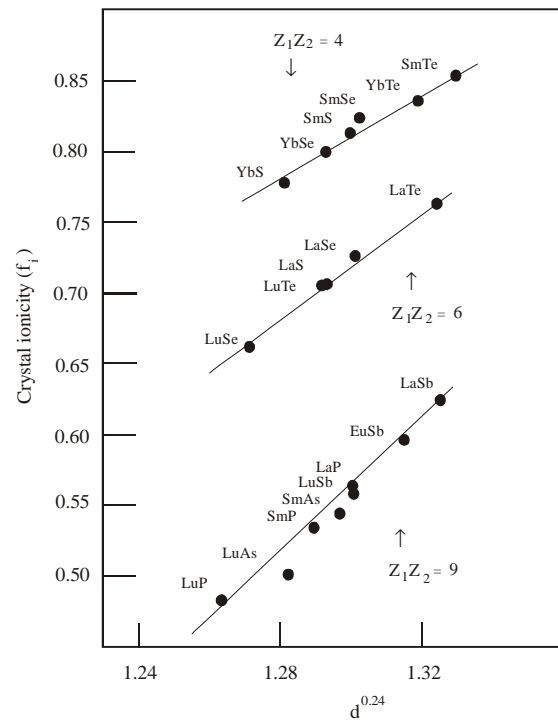


Fig.1: Plot of crystal ionicity (f_i) and nearest-neighbour distance (d) for rare earth monochalcogenides and pnictides. In this figure, the crystal ionicity of divalent ($Z_1 Z_2 = 4$) and trivalent ($Z_1 Z_2 = 6$) rare earth monochalcogenides lie on the lines nearly parallel to the line for the rare earth pnictides ($Z_1 Z_2 = 9$). In this figure all data are taken from calculated values of modified PVV theory, which is presented in table 1.

and pnictides using this idea. Rare-earth monochalcogenides are prepared by the reaction between rare-earth metals and VIB elements of the periodic table at high temperatures. Rare-earth monochalcogenides and pnictides have the rock salt structure at room temperature and at normal pressure [3]. Several of these compounds exhibit non-integer valence at high pressure and display numerous allotropic structures and properties, which can be in general, interpreted in terms of mixed valences or valence fluctuations, arising from unstable f -orbitals.

The rare earth ions in pnictides and chalcogenides are usually in the trivalent state. In the rare earth series of elements, the outer valence electrons (the $5d^1$ and $6s^2$ electrons) are effectively shielded from the increasing nuclear charge as electrons are added to the $4f$ orbitals. Rare-earth elements are transitional in their chemical properties between the alkaline-earth elements, especially Ba and the $5d$ transition elements Hf. With certain exceptions they behave like transition elements of the Sc group with additional f electrons in discrete levels. The exceptions are mainly due to

the high stability of empty, half or completely filled 4f shell. Certain compounds formed by Eu and Yb, in some cases also Sm and Tm chalcogenides, show close similarities, therefore, with corresponding alkaline earth chalcogenides (i.e., Eu, Yb, Sm and Tm chalcogenides are divalent) [5,6,28,29]. Yb pnictides are trivalent at room temperature and change to heavy fermion behaviour at low temperatures [30]. We realize that divalency in rare earth compounds is encountered in chalcogenides only. Rare-earth monochalcogenides are semi conducting if the rare-earth ion is in divalent state and metallic if trivalent [26].

Divalent rare earth has the outer electronic structure $4f^{14}5d^06s^2$ and the two s electrons contribute the valence electrons. In the monochalcogenides of rare earth, these two electrons fill the valence band derived from the p state of the anion. In the valence transition toward the trivalent state, the outer electronic structure of rare-earth changes from $4f^{14}5d^06s^2$ to $4f^{(14-x)}5d^x6s^2$, i.e., the fraction x of one 4f electron per formula, is expected to go into the 5d conduction band state. This should result in a semiconductor to metal transition. The more ionic crystals exhibit larger energy gaps between the valence and conduction bands. Because of this the more ionic crystals are less polarizable and they have correspondingly smaller dielectric constants.

Using equations (9)–(13), the ionic gaps (E_c), average energy gaps (E_g), crystal ionicity (f_i), dielectric constant (ϵ), electronic polarizability (α in \AA^3), and plasmon energy are evaluated for rare earth monochalcogenides and pnictides, except for ($\hbar\omega_p$) where equation (2) is used. The results are presented in Table 1 and Table 2. The calculated values are in better agreement with the values calculated by modified PVV theory. In the present model the ionic gaps (E_c), average energy gaps (E_g) and crystal ionicity (f_i) can be calculated without having any knowledge of the experimental value of the dielectric constant while the earlier models require this value in their calculation.

For the further support of the proposed relations, we have evaluated electronic and optical properties of Pb and Mg monochalcogenides, having the rock-salt structure. These values are presented in Table 3 and Table 4.

4. Conclusion

From the results presented in tables 1 to 4, we came to conclusion that the product of ionic charges of rock salt crystal structured solids is the key information for an understanding of the electronic and optical properties of these compounds. The ionic gap (E_c) and average energy gap (E_g) of these materials is inversely related to inter atomic distance and the product of ionic charges, and dielectric constants (ϵ_∞) of these materials is directly related to inter atomic distance and the product of ionic charges. The calculated values are presented in Table 1 and Table 2. The values evaluated show a systematic trend and are consistent with the modified P. V. V. theory, which proves the validity of the approach. It is also note worthy that the proposed relations are simpler and widely applicable. This work is in support of earlier research papers [16-22] in which we have already reported electronic and optical properties of zinc blende and complex structured solids using the proposed approach. Simply, we are of the view that the proposed approach is one of the best approaches in order to explain the electronic and optical properties of entire range of crystalline solids.

Table 1: In this table we have presented the calculated values of ionic gaps (E_c) and average energy gaps (E_g) from modified PVV theory and proposed approach for the rare earth monochalcogenides and pnictides. The value of ionic charge of anion (Z_2) for S, Se and Te is 2 and for P, As and Sb is 3.

Solids	Z_1	d	E_h [PVV]	E_c [PV.V]	E_c [this work]	E_g [PVV]	E_g [this work]
LaS	3	2.927	2.761	4.303	4.329	5.113	5.236
CeS	3	2.887	2.858	4.386	4.450	5.236	5.391
PrS	3	2.872	2.895	4.394	4.496	5.262	5.451
NdS	3	2.846	2.962	4.187	4.579	5.129	5.557
SmS	2	2.985	2.629	5.470	5.533	6.070	6.152
EuS	2	2.984	2.631	5.420	5.537	6.025	6.156
GdS	3	2.787	3.121	4.460	4.775	5.444	5.810
TbS	3	2.759	3.201	4.520	4.872	5.538	5.935
DyS	3	2.745	3.242	4.530	4.922	5.570	6.000
HoS	3	2.733	3.277	4.543	4.965	5.602	6.056
ErS	3	2.715	3.332	4.558	5.032	5.646	6.141
TmS	2	2.710	3.347	6.353	6.713	7.181	7.551
YbS	2	2.829	3.010	5.721	6.160	6.465	6.893
LuS	3	2.685	3.513	4.464	5.145	5.681	6.287
LaSe	3	3.030	2.532	4.125	4.040	4.840	4.866
CeSe	3	2.994	2.609	4.200	4.137	4.936	4.991
PrSe	3	2.975	2.651	4.204	4.190	4.970	5.059
NdSe	3	2.950	2.707	4.247	4.262	5.037	5.150
SmSe	2	3.100	2.373	5.209	5.130	5.724	5.678
EuSe	2	3.098	2.396	5.164	5.137	5.693	5.686
GdSe	3	2.886	2.860	4.282	4.453	5.150	5.395
TbSe	3	2.863	2.918	4.324	4.525	5.217	5.488
DySe	3	2.856	2.936	4.307	4.547	5.213	5.516
HoSe	3	2.840	2.977	4.323	4.598	5.249	5.582
ErSe	3	2.831	3.001	4.309	4.628	5.251	5.620
TmSe	2	2.920	2.778	5.587	5.782	6.239	6.446
YbSe	2	2.930	2.754	5.498	5.743	6.149	6.339
LuSe	3	2.730	3.286	4.569	4.976	5.628	6.070
LaTe	3	3.240	2.142	3.902	3.533	4.451	4.222
CeTe	3	2.944	2.609	4.589	4.137	5.279	4.991
PrTe	3	3.161	2.278	4.036	3.712	4.635	4.448
NdTe	3	3.131	2.333	4.080	3.783	4.701	4.539
SmTe	2	3.299	2.047	4.993	4.530	5.396	4.976
EuTe	2	3.299	2.047	4.952	4.530	5.358	4.976
GdTe	3	3.070	2.450	4.116	3.935	4.790	4.733
TbTe	3	3.051	2.489	4.146	3.984	4.836	4.795
DyTe	3	3.038	2.516	4.150	4.018	4.854	4.839
HoTe	3	3.025	2.540	4.160	4.053	4.874	4.883
ErTe	3	3.011	2.570	4.163	4.091	4.893	4.931
TmTe	2	3.110	2.373	5.415	5.097	5.912	5.639
YbTe	2	3.170	2.262	5.110	4.906	5.588	5.416

Table 1: Continued.

Solids	Z_1	d	E_h [PVV]	E_c [PVV]	E_c [this work]	E_g [PVV]	E_g [this work]
LuTe	3	2.920	2.780	4.354	4.350	5.166	5.263
LaP	3	3.013	2.568	2.926	3.076	3.894	4.021
CeP	3	2.971	2.660	2.987	3.164	3.996	4.142
PrP	3	2.953	2.701	3.002	3.202	4.039	4.196
NdP	3	2.932	2.749	3.020	3.248	4.084	4.260
SmP	3	2.890	2.850	3.052	3.343	4.176	4.392
EuP	3	2.875	2.890	3.056	3.378	4.206	4.441
GdP	3	2.862	2.920	3.062	3.409	4.231	4.484
TbP	3	2.843	2.969	3.086	3.455	4.283	4.548
DyP	3	2.827	3.010	3.086	3.494	4.311	4.602
HoP	3	2.814	3.047	3.096	3.526	4.344	4.648
ErP	3	2.800	3.085	3.119	3.562	4.387	4.697
TmP	3	2.786	3.124	3.113	3.598	4.410	4.747
YbP	3	2.775	3.155	3.111	3.626	4.431	4.787
LuP	3	2.650	3.540	3.422	3.976	4.923	5.279
LaAs	3	3.079	2.449	2.741	2.946	3.676	3.840
CeAs	3	3.040	2.511	2.885	3.022	3.825	3.946
PrAs	3	3.011	2.572	2.862	3.080	3.848	4.027
NdAs	3	2.997	2.603	2.903	3.109	3.899	4.067
SmAs	3	2.955	2.696	2.946	3.198	3.994	4.190
EuAs	3	2.945	2.719	2.944	3.220	4.008	4.220
GdAs	3	2.925	2.766	2.964	3.264	4.055	4.282
TbAs	3	2.910	2.801	2.970	3.298	4.083	4.329
DyAs	3	2.896	2.835	2.974	3.330	4.109	4.373
HoAs	3	2.883	2.867	2.982	3.360	4.137	4.415
ErAs	3	2.870	2.900	2.984	3.390	4.162	4.457
TmAs	3	2.858	2.931	2.988	3.419	4.190	4.497
YbAs	3	2.843	2.969	2.996	3.455	4.218	4.548
LuAs	3	2.830	3.004	3.004	3.487	4.249	4.592
LaSb	3	3.244	2.135	2.751	2.653	3.482	3.438
CeSb	3	3.206	2.20	2.796	2.717	3.558	3.525
PrSb	3	3.183	2.24	2.809	2.756	3.593	3.579
NdSb	3	3.161	2.28	2.826	2.795	3.630	3.632
SmSb	3	3.140	2.14	2.816	2.832	3.535	3.684
EuSb	3	3.125	2.34	2.823	2.859	3.667	3.721
GdSb	3	3.105	2.38	2.840	2.896	3.705	3.772
TbSb	3	3.085	2.42	2.861	2.934	3.747	3.825
DySb	3	3.070	2.45	2.868	2.963	3.772	3.864
HoSb	3	3.060	2.47	2.866	2.982	3.783	3.891
ErSb	3	3.048	2.50	2.867	3.006	3.804	3.924
TmSb	3	3.040	2.51	2.864	3.022	3.808	3.946
YbSb	3	3.034	2.52	2.858	3.034	3.811	3.962
LuSb	3	3.020	2.55	2.875	3.062	3.843	4.001

Table 2: In this table we have presented the calculated values of crystal ionicity (f_i), plasmon energy ($\hbar\omega_p$ in eV), optical dielectric constant (ϵ_∞) and electronic polarizability (α in \AA^3) of rare earth monochalcogenides and pnictides.

Solids	f_i [PVV]	f_i [this work]	$\hbar\omega_p$	ϵ_∞	α
LaS	0.708	0.684	15.72	10.01	8.96
CeS	0.702	0.681	16.05	9.86	8.55
PrS	0.697	0.680	16.18	9.81	8.41
NdS	0.666	0.679	16.41	9.71	8.15
SmS	0.812	0.809	14.40	6.48	8.18
EuS	0.809	0.809	14.40	6.47	8.17
GdS	0.671	0.676	16.92	9.48	7.61
TbS	0.666	0.674	17.18	9.38	7.36
DyS	0.661	0.673	17.31	9.32	7.24
HoS	0.658	0.672	17.42	9.27	7.13
ErS	0.652	0.671	17.60	9.21	6.98
TmS	0.783	0.790	16.64	5.86	5.86
YbS	0.783	0.799	15.60	6.12	6.80
LuS	0.618	0.670	17.89	9.10	6.73
LaSe	0.726	0.689	14.94	10.43	10.05
CeSe	0.724	0.687	15.21	10.30	9.66
PrSe	0.716	0.686	15.35	10.21	9.46
NdSe	0.711	0.685	15.54	10.11	9.20
SmSe	0.828	0.816	13.60	6.74	9.32
EuSe	0.823	0.816	13.63	6.75	9.27
GdSe	0.691	0.681	16.10	9.91	8.56
TbSe	0.687	0.680	16.24	9.76	8.32
DySe	0.683	0.680	16.32	9.75	8.26
HoSe	0.678	0.679	16.44	9.67	8.10
ErSe	0.673	0.678	16.52	9.64	8.02
TmSe	0.802	0.805	14.89	6.34	7.59
YbSe	0.800	0.821	14.73	6.40	7.78
LuSe	0.659	0.672	17.45	9.26	7.11
LaTe	0.767	0.700	13.69	11.51	12.27
CeTe	0.756	0.687	13.87	8.72	11.02
PrTe	0.758	0.696	14.02	10.94	11.55
NdTe	0.753	0.695	14.20	10.79	11.19
SmTe	0.856	0.829	12.39	7.20	11.49
EuTe	0.854	0.829	12.42	7.23	11.46
GdTe	0.738	0.691	14.63	10.56	10.48
TbTe	0.735	0.690	14.77	10.48	10.27
DyTe	0.731	0.690	14.88	10.46	10.13
HoTe	0.729	0.689	14.97	10.40	9.99
ErTe	0.724	0.688	15.08	10.35	9.84
TmTe	0.839	0.817	13.54	6.77	9.42
YbTe	0.836	0.821	13.10	6.85	10.09
LuTe	0.710	0.683	15.77	9.98	8.89
LaP	0.565	0.585	14.57	14.13	10.06
CeP	0.559	0.584	15.03	14.17	9.45

Table 2: Continued.

Solids	f_i [PVV]	f_i [this work]	$\hbar\omega_p$	ϵ_∞	α
PrP	0.552	0.582	15.13	14.00	9.30
NdP	0.547	0.581	15.26	13.83	9.13
SmP	0.534	0.579	15.56	13.55	8.74
EuP	0.528	0.579	14.94	12.32	8.95
GdP	0.524	0.578	15.33	12.69	8.88
TbP	0.519	0.577	15.49	12.60	8.69
DyP	0.512	0.576	15.61	12.51	8.54
HoP	0.508	0.576	15.71	12.42	8.42
ErP	0.506	0.575	15.85	12.39	8.27
TmP	0.498	0.575	15.96	12.30	8.14
YbP	0.493	0.574	16.04	12.23	8.03
LuP	0.483	0.567	17.20	11.62	6.91
LaAs	0.556	0.589	13.62	13.58	11.42
CeAs	0.569	0.587	14.03	13.64	10.77
PrAs	0.553	0.585	14.25	13.52	10.43
NdAs	0.554	0.584	14.39	13.52	10.22
SmAs	0.544	0.583	14.57	13.09	9.90
EuAs	0.540	0.582	14.69	13.12	9.75
GdAs	0.534	0.581	14.84	13.01	9.54
TbAs	0.529	0.580	14.95	12.93	9.38
DyAs	0.524	0.580	15.06	12.86	9.23
HoAs	0.520	0.579	15.16	12.79	9.10
ErAs	0.514	0.579	15.26	12.72	8.96
TmAs	0.509	0.578	15.38	12.70	8.85
YbAs	0.505	0.577	15.48	12.59	8.69
LuAs	0.500	0.577	15.59	12.53	8.56
LaSb	0.624	0.596	12.70	14.65	13.33
CeSb	0.618	0.594	12.93	14.46	12.83
PrSb	0.611	0.593	13.07	14.34	12.84
NdSb	0.606	0.592	13.20	14.21	12.25
SmSb	0.635	0.591	13.39	14.21	11.96
EuSb	0.593	0.590	13.44	14.05	11.82
GdSb	0.588	0.590	13.57	13.94	11.57
TbSb	0.583	0.588	13.70	13.83	11.33
DySb	0.578	0.588	13.80	13.76	11.16
HoSb	0.574	0.587	13.87	13.71	11.04
ErSb	0.568	0.587	13.96	13.66	10.89
TmSb	0.565	0.587	14.00	13.59	10.80
YbSb	0.562	0.586	14.05	13.58	10.44
LuSb	0.560	0.586	14.14	13.49	10.58

Table 3: In this table we have presented theoretical and calculated values of ionic gaps (E_c) and average energy gaps (E_g) by proposed approach for the Pb and Mg monochalcogenides. The value of ionic charge of anion (Z_2) for O, S, Se and Te is 2.

Solids	Z_1 [15,17]	d	E_c [15,17]	E_c [9]	E_c [this work]	E_g [15,17]	E_g [9]	E_g [this work]
PbS	4	2.96	3.24	3.51	3.46	4.19	4.42	4.43
PbSe	4	3.07	2.97	3.08	3.22	3.84	3.95	4.10
PbTe	4	3.24	2.61	2.41	2.89	3.38	3.24	3.66
MgO	2	2.105	14.3	14.3	11.2	15.6	15.6	12.9
MgS	2	2.54	7.54	7.2	7.64	8.10	8.10	8.66
MgSe	2	2.72	6.4	6.4	6.66	7.16	7.2	7.49

Table 4: In this table we have presented theoretical and calculated values of crystal ionicity (f_i) and optical dielectric constant (ϵ_∞) of Pb and Mg monochalcogenides.

Solids	f_i [15,17]	f_i [9]	f_i [our]	$\hbar\omega_p$ [15,17]	ϵ_∞ [15]	ϵ_∞ [9]	ϵ_∞ [this work]
PbS	0.603	0.633	0.61	16.124	15.84	18.8	14.25
PbSe	0.60	0.61	0.62	15.322	16.94	21.1	14.97
PbTe	0.60	0.55	0.62	14.218	18.68	28.6	16.1
MgO	0.84	0.84	0.74	24.27		3.0	4.54
MgS	0.87	0.79	0.78	18.28		5.1	5.46
MgSe	0.79	0.79	0.79	16.45		5.9	5.82

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