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ELECTRONIC, STRUCTURAL, OPTICAL AND MECHANICAL PROPERTIES OF CUBIC STRUCTURED Ln_2X_3 (Ln = La→Lu & X=O,S): AN EMPIRICAL INVESTIGATION

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In this publication, we have examined the structural, optical, and mechanical features of cubic structured lanthanide Ln_2X_3 (Ln = La→ Lu and X = O, S) series using the valence electron plasma oscillation theory of solids. Using the Chemical bond theory of solids, which was created by Phillips and Van-Vechten, we have further confirmed our findings. Unfortunately, it has been discovered that the Phillips and Van-Vechten (PVV) dielectric description is applicable exclusively to semiconductors and insulators. It is shown that an empirical relationship previously presented by Yadav and Bhati [D.S. Yadav, J. Alloys and Comp. 537, 250 (2012); D.S. Yadav, and D.V. Singh, Phys. Scr. 85, 015701 (2012); D.S. Yadav, J. Mater. Phys. Chem. 3(1), 6-10 (2015); R. Bhati, et al., Mater. Phys. Mech. 51, 90 (2023); R. Bhati, et al., East Eur. J. Phys. (1), 222 (2023).] relating the plasmon energy of complex structured solids, rock salt, and zinc-blende to their electronic, mechanical, static, and dynamical properties which can be applied to the cubic structured lanthanide (Ln_2S_3 & Ln_2O_3) series with only minor modifications. Considering the well-known theory of dielectric for solids, an alternative technique has been devised to evaluate the electronic, structural, mechanical, and optical properties of these materials, including their band gap (ΔE_g in eV), optical dielectric constant, homopolar and heteropolar gaps, average energy gaps, chemical bond ionicity, and bulk muduli. An estimate was computed based on the almost inverse relationship between the plasmon energy of these compounds and their optical, mechanical, structural, and electrical characteristics. For these substances, the expected values of the aforementioned parameters form a straight line when plotted on a log-log scale against the plasmon energy ($\hbar\omega_p$). We examined the C-type Ln_2X_3 compounds using the recommended methods, and the values we estimated are in good agreement with the values obtained from modified PVV theory and other comparable experimental and theoretical data that is currently available.

Keywords: *Electronic Properties; Optical Properties; Structural Properties; Mechanical Properties; Ln_2O_3; Ln_2S_3; Plasma Energy*
PACS: 71.20.-b; 71.20.Eh; 71.20.Nr; 62.20.de

1. INTRODUCTION

Because of their numerous practical applications, lanthanide sesquioxides and sesquisulphides, which have cubic structures in Ln_2O_3 and Th_3P_4 in Ln_2S_3, respectively, have drawn physicists' interest. Because of their significant technological value in a variety of fields, including solid state lasers, electroluminescence, cathode-luminescence sources, crystals for chemical and organic reactions, high-K gate dielectrics, optical components of high power lasers, generation of ultra-short laser pulses, scintillating materials, radiation detectors, transistor application and electronic industries, oxygen ion conducting electrolyte in solid oxide fuel cells, and materials with strongly hydrophobic surfaces, numerous attempts have been made in the last few years to comprehend the electronic and optical properties of C-type Ln_2O_3 and Ln_2S_3 [1-4]. Semi-core *4f* levels which are mostly concentrated on Ln-atoms and typically do not participate in bonding or electronic conduction, govern many features of lanthanide oxides. However, *4f*-shell electrons can establish strong magnetic order and be available for optical absorption. Any O and S compound containing a rare earth atom is solid at room temperature. An atom's size and electrical arrangement in relation to O and S determine most of its solid state physics. When electrons are introduced to the 4f-orbitals in the lanthanide series of elements, the outer valence electrons ($5d^1$ and $6S^2$ electrons) are effectively protected from the growing nuclear charge. For every lanthanide in the series, this leads to a trivalent state whose energy varies gradually. Oxides related to each other in relatively predictable ways are produced when the atom's size contracts gradually with oxygen throughout the series. The oxides of lanthanides are among the most thermally stable compounds known to science because of the combination of their size and electrical structure. With a very high refractive index and low carrier mobility, lanthanide sesquioxides and sesquisulphides are n-type wide gap semiconductors [5, 6]. It is generally known that below 2000^{0C}, the sesquioxide crystal structure exists in three polymorphic forms: Hexagonal A-type (P3m1), Monoclinic B-type (C2/m), and Cubic C-type (Ia3) [7]. Reports have indicated that X and H phases arise above this temperature [8] Using the Vienna ab-initio simulation package (VASP), Hirosaki et al. [9] calculated the equilibrium crystal lattice dimension for most Ln_2O_3 (Ln = La→Lu) using first principles pseudo potential. Measurements of the optical band gap on Ln_2O_3 series single crystals were made by Prokofiev et al. [10]· Using the full potential linearized augmented plane wave [FPLAP] method with in local spin density

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approximation [LSDA] and Coulomb corrected local density approximation [LSDA+U], as implemented in the WIEN2K code, Singh et al. [11] reported the electronic structure and optical properties of rare earth sesquioxides. Rahm et al.'s CSM technique computed the equilibrium volume and bulk modulus of hexagonal and cubic structured RE_2O_3 [12]. Significant information about the electrical, optical, mechanical, and structural characteristics of RE_2O_3 and RE_2S_3 has been made public by numerous workers [4, 13–18]. The unit cell of the C-type structure (Figure 1) can be obtained by combining eight unit-cells of the fluorite structure (Fm3m) with 25% of the oxygen atoms removed and arranging the remaining oxygen in a specific way.

Over the past few decades, experimental and theoretical research has been conducted on the cohesive energy, heat of formation, bulk modulus, optical dielectric constant, and energy band gap of these materials. Thanks to a sophisticated computer technique, the structural, mechanical, and optical properties of a wide range of molecules and materials can now be investigated in great detail. Applying empirical concepts such as valence, empirical radii, ionicity, electro-negativity, and plasmon energy is therefore beneficial [19–24]. To the best of our knowledge, no one has investigated the mechanical, structural, electrical, and optical properties of C-type Ln2O3 and Ln_2S_3 using solid state plasma oscillation theory. Literature contains references to them. Since these ideas are closely related to the nature of chemical bonds, they offer a way to categorize and explain a wide range of fundamental characteristics of molecules and solids. Consequently, we believe it would be interesting to provide a different explanation for the C-type Ln_2X_3 series' homopolar gap, heteropolar gap, average gap, bond ionicity, optical dielectric constant, and band gap. In this work, we suggest a method for calculating the electrical, structural, optical, and mechanical properties of these materials that is based on the plasma oscillation theory of solids.

2. THEORY, RESULTS AND DISCUSSION

Modified Phillips and Van-Vechten dielectric theory of solids [25–29] states that the average energy gap (E_g) between bonding and anti-bonding (sp^3) hybridized orbitals can be broken down into contributions from symmetric and anti-symmetric parts by the potential inside the unit cell.

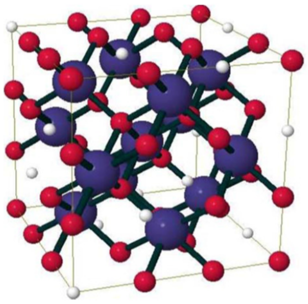

Figure 1. The unit cells of cubic C-type Ln_2O_3 and the RE atoms are shown in blue (dark gray) and oxygen are in red (light gray), vacancy positions are indicated by white spheres.

This is because the average energy gap (E_g) can be broken down into a heteropolar or part (E_c) and homopolar or covalent part (E_h). These contributions take the following form: E_c represents the heteropolar or ionic contribution, while E_h represents the homopolar or covalent contribution as-

$$E_p^2 = E_h^2 + E_c^2 . \tag{1}$$

The following is how the covalent portion E_h is dependent on the nearest neighbor separation d_{AB} -

$$E_h = A d_{AB}^{-K_1} . \tag{2}$$

where A = 40.468 eV(A°)$^{2.5}$ and the exponent $K_1 = 2.5$ are the constants, i.e., remain unchanged in different crystals. A = 39.74 and $K_1 = 2.48$ were the comparable values found by Phillips and Van-Vechten [28]. The following relation can be used to determine the ionic contribution:

$$E_c = K_2 d_0^{-1} . e^{-k_s . d_0} , \tag{3}$$

where the valence states of atoms A and B are denoted by Z_A and Z_B, respectively, and b is an adjustable quantity that is dependent upon the co-ordination number surrounding the cation [29], that is, $b = 0.089\ N_c^2$. N_c is the average coordination number, K_s is the Thomas Fermi Screening Parameter (TFSP), and $d_0=(d/2)$ (d-the nearest-neighboring distance) are the values of b for C-type RE_2O_3 and Th_3P_4 type RE_2S_3 respectively.

The effective number of free electrons in the valence band is correlated with both this screening factor and the bond length. As a result, the bond length and quantity exiting the cations determine the values of E_h and E_c. Ten electrons per molecule (four for RE and six for O & S) was taken into consideration while determining the value of ks, which is defined as:

$$k_s = 2 a_B^{-0.5} (3N / \pi V)^{0.167} . \tag{4}$$

Here -a_B is Bohr radius. The ionicity of the chemical bond is defined as

$$f_i = \frac{E_c^2}{E_g^2} . \tag{5}$$

We have determined the values of E_P, E_c, and E_h for these materials based on the relations (1) through (4) above. The values of E_h^* and E_p^* can also be determined from the Phillips and Penn model$^{26-27)}$ with the use of Eqns. (4)–(7). The optical and static dielectric constants, $\varepsilon\infty$ and $\varepsilon 0$, in these relations, are derived from several sources [6, 30-33]. For Ln_2O_3, the adjustable parameter $S_0 = 0.78$, and for Ln_2S_3, 0.80. The ionic contribution (E_c) to the average energy gap (E_g), ionicity (f_i), dielectric constant (ε_∞), band gap (ΔE_g), and plasmon energy of a chemical bond must therefore be correlated in some way with the physical process. The electronic, structural, optical and mechanical properties of these materials exhibit a linear relationship when plotted on log-log scale against ($\hbar\omega_p$) of the compounds, which are presented in the Figures 2-5.

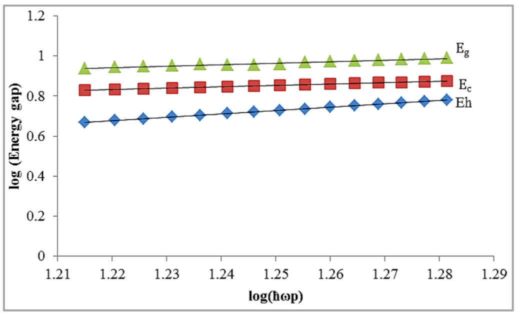

Figure 2. Plot of Energy gaps versus plasmon energy of C-type Ln_2O_3

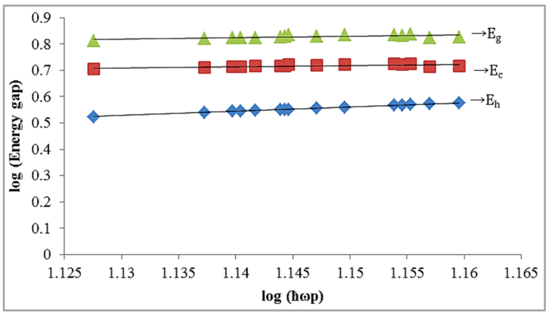

Figure 3. Plot of Energy gaps versus plasmon energy of Ln_2S_3.

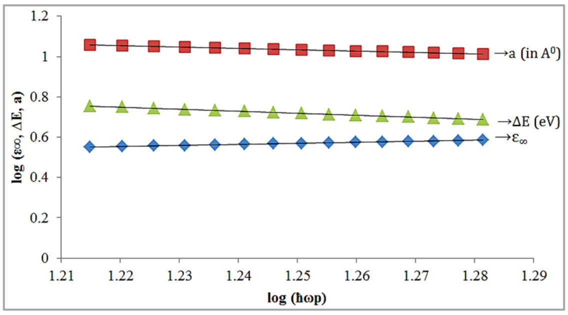

Figure 4. Plot of Dielectric constant, Optical band gap and lattice constant versus plasmon energy of C-type Ln_2O_3

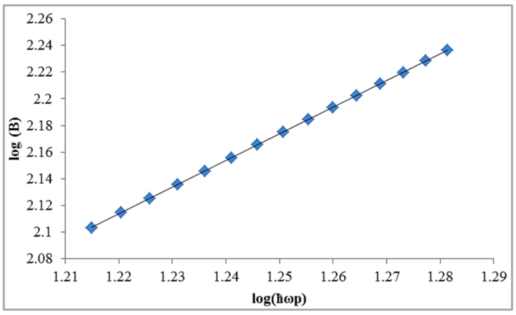

Figure 5. Plot of bulk modulus versus plasmon energy of C-type Ln_2O_3

We observe that in the plot of E_h, E_c, E_g, f_i, ε_∞, ΔE_g and lattice constant (a), versus ($\hbar\omega_p$); the lanthanide sesquioxides and sesquisulphides lies on the straight line. From Figures 2-5, it is clear that homopolar gap, heteropolar gap, average energy gap, lattice constant and optical dielectric constant trends in these materials increases with increasing plasmon energy and bond ionicity and band gap decreases on increasing this energy. We have provided empirical relations for the mechanical and electrical properties of rare earth chalcogenides and binary semiconductors in our earlier work [20–23]. Consequently, we believed it would be interesting to provide a different explanation for the optical, structural, and electrical characteristics of C-type Ln_2O_3 as follows:

$$E_h = A(\hbar\omega_p)^{1.666} . \tag{6}$$

$$E_c = B(\hbar\omega_p)^{0.666} . \tag{7}$$

$$E_g = C(\hbar\omega_p)^{0.746} . \tag{8}$$

$$f_i = D(\hbar\omega_p)^{-1.6} . \tag{9}$$

$$\varepsilon_\infty = E(\hbar\omega_p)^{0.508} . \tag{10}$$

$$\Delta E = F(\hbar\omega_p)^{-1.016} . \tag{11}$$

$$a = G(\hbar\omega_p)^{-0.666} . \tag{12}$$

$$B = H(\hbar\omega_p)^{2.0} . \tag{13}$$

The empirical constants A, B, C, D, E, F, G, and H in the aforementioned relations are listed in Table 1 and depend on the type of chemical bonds that exist between the different types of atoms. The electrical, structural, optical, and mechanical properties of these compounds have all been briefly reviewed before [2, 4, 6, 9, 25, 26–32], thus they won't be covered in length here. The values of the lattice constant (a), homopolar gap (E_h), heteropolar gap (E_c), average energy gap (E_g), bond ionicity (f_i), bulk modulus (B), optical dielectric constant (ε_∞), and band gap (ΔE) of these materials have been studied and are shown in Tables 2-4, respectively, using the proposed empirical relations (6) through (13). In this study, we have shown excellent agreement with values derived from modified PVV theory with available theoretical findings [34, 35] and experimental data. The plasmon energy is the only input parameter used in the current empirical model to estimate the electrical, structural, mechanical, and optical properties of these materials

Table 1. Values of the constants using in relations (6-12).

Constants	**A**	**B**	**C**	**D**	**E**	**F**	**G**	**H**
Ln_2O_3	0.0442	1.051	1.079	1.054	0.859	97.576	73.593	0.472
Ln_2S_3	0.0442	0.899	0.939	0.999	---	39.030	---	

Table 2. Electronic and mechanical properties of lanthanide sesquioxides (Ln_2O_3)

Ln_2O_3	**$\hbar\omega_p$ (eV)**	**Energy gaps (in eV)**								**Bond ionicity**		**Bulk modulus**	
		Homopolar gap (E_h)			**Ionic gap (E_c)**		**Penn gap (E_p)**			**f_i**		**B (in GPa)**	
		Calc. Eq. (6)	**PVV Eq. (2)**	**Philips model**	**Calc. Eq. (7)**	**PVV Eq. (3)**	**Calc. Eq.(8)**	**PVV Eq.(1)**	**Penn model**	**Calc. Eq. (9)**	**Phillips Eq. (5)**	**Calc. Eq.(13)**	**Ref. [12, 34, 35]**
La_2O_3	16.403	4.672	4.442	4.435	6.772	6.434	8.697	7.819	7.861	0.67	0.67	126.9	125.6, 123.5
Ce_2O_3	16.612	4.771	4.535	4.579	6.829	6.478	8.779	7.908	7.999	0.67	0.67	130.2	129.9, 135.8
Pr_2O_3	16.818	4.870	4.631	4.608	6.886	6.685	8.860	8.133	7.908	0.67	0.67	133.5	134.3, 137.0
Nd_2O_3	17.021	4.978	4.631	4.658	6.941	6.617	8.940	8.076	8.076	0.67	0.67	136.7	139.2, 136.9
Pm_2O_3	17.222	5.067	4.703	4.732	6.995	6.735	9.078	8.214	8.198	0.67	0.67	139.9	144.3, 136.0
Sm_2O_3	17.422	5.164	4.781	4.844	7.049	6.818	9.046	8.327	8.231	0.67	0.67	143.2	146.7, 142.3
Eu_2O_3	17.617	5.262	4.989	4.919	7.102	7.215	9.012	8.772	8.084	0.66	0.67	146.4	145.0, 143.1
Gd_2O_3	17.812	5.359	5.044	4.992	7.154	7.288	9.098	8.863	8.172	0.66	0.68	149.7	154.9, 144.7
Tb_2O_3	18.004	5.456	5.329	5.014	7.205	7.822	9.322	9.465	8.158	0.66	0.67	152.9	150.0, 158.6
Dy_2O_3	18.194	5.552	5.329	5.178	7.256	7.762	9.395	9.415	8.376	0.66	0.67	156.2	159.9, 150.0
Ho_2O_3	18.382	5.648	5.329	5.246	7.306	7.702	9.468	9.366	8.444	0.66	0.67	159.4	161.6, 178.0
Er_2O_3	18.568	5.744	5.389	5.321	7.355	7.774	9.539	9.459	8.528	0.65	0.65	162.7	161.2, 155.0
Tm_2O_3	18.753	5.839	4.989	5.406	7.404	6.865	9.610	8.446	8.642	0.66	0.65	165.9	161.6, 162.0
Yb_2O_3	18.935	5.934	4.989	5.487	7.451	6.816	9.679	8.447	8.757	0.66	0.66	169.2	161.6, 181.0
Lu_2O_3	19.116	6.028	5.574	5.557	7.499	6.779	9.748	8.776	8.878	0.66	0.67	172.4	175.3, 179.4

Table 3. Electronic properties of lanthanide sesquisulphides (Ln_2S_3)

Ln_2S_3	**$\hbar\omega_p$**	**Energy gaps (in eV)**								**Bond ionicity**		**Dielectric constant**	
		E_h			**E_c**		**E_p**			**f_i**		**ε_∞**	
		Calc. Eq. (6)	**PVV Eq. (2)**	**Philips model**	**Calc. Eq. (7)**	**PVV Eq. (3)**	**Calc. Eq. (8)**	**PVV Eq. (1)**	**Penn model**	**Calc. Eq. (9)**	**Phillips Eq. (5)**	**Calc. Eq. (11)**	**Ref. [10]**
La_2S_3	13.414	3.341	3.347	3.244	5.066	4.865	6.513	5.958	6.039	0.66	0.66	2.78	2.8
Ce_2S_3	13.717	3.468	3.474	3.072	5.142	4.844	6.623	5.961	5.688	0.66	0.66	2.72	2.7
Pr_2S_3	13.795	3.501	3.507	3.611	5.162	5.138	6.651	6.221	5.714	0.65	0.68	2.71	2.6
Nd_2S_3	13.818	3.511	3.517	3.429	5.167	5.072	6.659	6.166	6.666	0.65	0.67	2.70	2.4
Pm_2S_3	13.859	3.540	3.564	---	5.195	5.155	6.669	6.259	---	0.65	0.67	2.69	---
Sm_2S_3	13.929	3.558	3.574	3.275	5.201	5.160	6.707	6.277	6.956	0.65	0.67	2.68	---
Eu_2S_3	13.941	3.563	3.608	---	5.221	5.212	6.736	6.225	---	0.65	0.67	2.68	---
Gd_2S_3	13.953	3.568	3.713	3.510	5.281	5.197	6.823	6.269	5.525	0.65	0.67	2.67	---
Tb_2S_3	14.032	3.601	3.642	3.552	5.240	5.128	6.764	6.484	5.706	0.65	0.67	2.66	---
Dy_2S_3	14.275	3.706	3.704	3.461	5.275	5.317	6.815	6.346	5.709	0.65	0.67	2.61	---
Ho_2S_3	14.111	3.635	3.723	3.725	5.286	5.196	6.831	6.346	6.652	0.65	0.67	2.64	---
Er_2S_3	14.252	3.696	3.747	3.741	5.300	5.294	6.851	6.466	5.734	0.65	0.67	2.62	---
Tm_2S_3	14.299	3.716	3.785	3.754	5.321	5.513	6.882	6.646	6.724	0.65	0.68	2.61	---
Yb_2S_3	14.354	3.740	3.540	3.754	5.185	5.362	6.684	6.541	5.805	0.65	0.67	2.60	---
Lu_2S_3	14.441	3.778	3.563	4.077	5.198	5.423	6.703	6.613	5.831	0.65	0.67	2.58	---

Table 4. Values of Optical dielectric constant (ε_∞), Optical band gap (ΔE_g, in eV) and lattice parameter (a in A^0) of C-type lanthanide (Ln_2O_3) sesquioxides.

Ln_2O_3	**$\hbar\omega_p$**	**ε_∞**		**Optical band gap (ΔE_g)**					**Lattice constant (a)**		
		Calc.	**Expt$^{\#}$**	**Calc.**	**Theo‡**	**$GW_0^{\$}$**	**$G_0W_0^{\$}$**	**Expt$^{\$}$**	**Calc.**	**Expt†.**	**Theo$^{\pm}$**
La_2O_3	16.403	3.557	3.667	5.68	5.60	5.24	4.95	5.55, 5.34, 5.30	11.42	11.38	11.39
Ce_2O_3	16.612	3.580	3.712	5.61	--	1.29	1.50	2.40	11.32	11.16	11.41
Pr_2O_3	16.818	3.603	3.775	5.54	5.56	2.82	2.86	3.90, 3.50	11.23	11.14	11.28
Nd_2O_3	17.021	3.625	3.686	5.47	4.00	4.70	4.50	4.70, 4.80	11.14	11.07	11.17
Pm_2O_3	17.222	3.646	--	5.41	--	5.41	5.25	--	11.05	10.99	11.06
Sm_2O_3	17.422	3.668	3.725	5.35	5.04	5.22	4.38	5.00	10.97	10.90	10.99
Eu_2O_3	17.617	3.689	3.877	5.28	4.48	3.48	2.77	4.40	10.89	10.82	10.81
Gd_2O_3	17.812	3.709	3.861	5.23	5.45	5.30	4.89	5.40	10.81	10.79	--
Tb_2O_3	18.004	3.730	3.857	5.17	4.77	3.74	3.81	3.80	10.73	10.73	10.66
Dy_2O_3	18.194	3.750	3.853	5.11	4.86	4.24	4.41	4.90	10.66	10.67	10.60
Ho_2O_3	18.382	3.769	3.842	5.06	5.27	5.12	4.68	5.30	10.59	10.60	10.54
Er_2O_3	18.568	3.789	3.826	5.01	5.21	5.22	4.78	5.30, 5.49	10.51	10.55	10.54
Tm_2O_3	18.753	3.808	3.803	4.96	5.25	5.15	4.73	5.40, 5.48	10.44	10.48	10.47
Yb_2O_3	18.935	3.826	3.771	4.91	5.30	4.70	3.23	4.90, 5.05	10.38	10.42	--
Lu_2O_3	19.116	3.845	3.725	4.86	5.52	4.99	4.66	4.89, 5.79, 5.50	10.31	10.38	10.35

$^{\$}$Ref. [2], $^{\#}$Ref. [6], †Ref. [4], $^{\pm}$Ref. [9], ‡Ref. [15]

3. CONCLUSIONS

Investigations into the electrical, structural, optical, and mechanical characteristics of C-type Ln_2X_3 compounds have been conducted using the suggested empirical method. Based on the findings, we draw the conclusion that a compound's plasmon energy is a crucial factor to consider when determining the electrical, structural, and optical characteristics of these materials. Notably, the values are in excellent agreement with published experimental data compared to numerous academics' theoretical findings, and the suggested approach is straightforward and broadly applicable. The current study presents empirical relationships between the valence electron plasmon energy of cubic-structured Ln_2X_3 compounds and their electrical, optical, mechanical, and structural characteristics. Using the plasmon energy ($\hbar\omega_p$ in eV) as an input parameter, this can be successfully used to estimate the electric, structural, mechanical, and optical properties of these compounds. These findings demonstrate the reasonableness of our existing method and provide us with a helpful manual for estimating and forecasting the electrical, optical, and structural characteristics of these materials. Our theoretically computed data can be used to anticipate future research and wait for upcoming experimental validations.

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ЕЛЕКТРОННІ, СТРУКТУРНІ, ОПТИЧНІ ТА МЕХАНІЧНІ ВЛАСТИВОСТІ КУБІЧНОГО СТРУКТУРОВАНОГО Ln_2X_3 (Ln = La→Lu & X=O,S): ЕМПІРИЧНЕ ДОСЛІДЖЕННЯ

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У цій публікації ми розглянули структурні, оптичні та механічні характеристики серії лантаноїдів Ln_2X_3 з кубічною структурою (Ln = La→ Lu та X = O, S) за допомогою теорії коливань плазми валентних електронів твердих тіл. Використовуючи теорію хімічного зв'язку твердих тіл, яку створили Філліпс і Ван-Вехтен, ми додатково підтвердили наші висновки. На жаль, було виявлено, що опис діелектрика Філіпса та Ван-Вехтена (PVV) застосовний виключно до напівпровідників та ізоляторів. Показано, що емпіричний зв'язок, представлений раніше Ядавом і Бхаті [D.S. Yadav, J. Alloys and Comp. 537, 250 (2012); D.S. Yadav, and D.V. Singh, Phys. Scr. 85, 015701 (2012); D.S. Yadav, J. Mater. Phys. Chem. 3(1), 6-10 (2015); R. Bhati, et al., Mater. Phys. Mech. 51, 90 (2023); R. Bhati, et al., East Eur. J. Phys. (1), 222 (2023).], пов'язує плазмонну енергію твердих тіл зі складною структурою, кам'яної солі та цинкової обманки з їхніми електронними, механічними, статичними та динамічними властивостями, які можна застосувати до кубічна структурована серія лантаноїдів (Ln_2S_3 & Ln_2O_3) лише з незначними модифікаціями. Враховуючи добре відому теорію діелектрика для твердих тіл, була розроблена альтернативна методика для оцінки електронних, структурних, механічних і оптичних властивостей цих матеріалів, включаючи їх ширину забороненої зони (ΔEg в еВ), оптичну діелектричну проникність, гомополярність і гетерополярні щілини, середні енергетичні щілини, іонність хімічного зв'язку та об'ємні мудулі. Оцінка була розрахована на основі майже зворотного зв'язку між енергією плазмону цих сполук та їхніми оптичними, механічними, структурними та електричними характеристиками. Для цих речовин очікувані значення вищезазначених параметрів утворюють пряму лінію, якщо їх відобразити в логарифмічному масштабі від енергії плазмону ($\hbar\omega p$). Ми перевірили сполуки типу C Ln_2X_3 за допомогою рекомендованих методів, і оцінені нами значення добре узгоджуються зі значеннями, отриманими на основі модифікованої теорії PVV та інших порівняннних експериментальних і теоретичних даних, доступних на даний момент.

Ключові слова: *електронні властивості; оптичні властивості; структурні властивості; механічні властивості;* Ln_2O_3*;* Ln_2S_3*; енергія плазми*