

# Electronic and Mechanical Properties of Chemical Bonds (A-O & B-O) in Cubic Phase $A^{+2}B^{+4}O_3$ Perovskite Oxides

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**Abstract:** In the present manuscript, electronic and mechanical properties of a series of  $ABO_3$  ( $A \rightarrow$  alkaline earth metals,  $B \rightarrow$  transition metal) perovskites are presented. Using the plasma oscillation theory of solids, empirical relations are proposed for computation of the homopolar/ covalent gap ( $E_h$ ) and heteropolar/ ionic gap ( $E_c$ ) of the chemical bonds A-O and B-O in the cubic phase of  $ABO_3$  perovskites. To examine the validity of our calculated results, the average energy gap ( $E_g$ ), Phillips ionicity ( $f_i$ ) and covalence ( $f_c$ ) of the chemical bonds of these perovskites are investigated. The dielectric constant ( $\epsilon_\infty$ ) and refractive index ( $n$ ) are computed and the results obtained are analyzed in comparison to results obtained by different researchers and these are found in fairly good agreement. Electronic polarizability ( $\alpha_{total}$ ) was calculated through a well-known phenomenological Clausius-Mossotti relation and the values were found in accord with the results obtained from the Chemla's relation. Further, a simple Neumann scaling approach has been employed to estimate the bulk modulus of these materials using the Phillips ionicity model. Present estimations are found in excellent agreement with the available experimental reports as compared to other such previous theoretical reports. This report supports the composition of new perovskites and hereto perceives their other properties for optoelectronics, photonics, mechanical and thermoelectric devices.

**Keywords:** Perovskites, Electronic Properties, Mechanical Properties, Plasma Energy

## 1. Introduction

In the past few years, increasing attention has been given to the theoretical study of electronic and mechanical properties of cubic phase  $ABO_3$  perovskite oxide solids due to their important role in thermoelectric and optoelectronic applications. These materials have high optical, thermal efficiencies, high melting temperatures, low thermal conductivities and low cost. Perovskite materials are of great technical importance and have fundamental interest in the microelectronic industry, material science, chemistry and physics: such as capacitor, optical wave guides, acoustic transducer, high-temperature oxygen sensors, surface acoustic wave devices, non-volatile memories, second harmonic generation, laser-host crystals, frequency doublers,

piezoelectric actuators and dynamic random access memories etc. [1-8]. Many researchers have conducted experimental and theoretical studies on  $BaTiO_3$ ,  $CaTiO_3$ ,  $SrTiO_3$ ,  $BaZrO_3$ ,  $SrZrO_3$ ,  $CaZrO_3$ ,  $SnZrO_3$  and  $SnHfO_3$  structured perovskites [9-13]. Based on theoretical studies, Pikunov [14] and Saha et al. [15] reported electronic and optical properties of barium, calcium and lead titanate oxides employing the tight-binding linear muffin-tin orbital and full-potential linear muffin-tin orbital theory. Numerous researchers have attempted to determine the electronic, optical, structural, mechanical and thermal properties of cubic phase  $ABO_3$  perovskite materials using various theories such as density functional theory (DFT) [9, 16-20], Ab-initio calculations [22], first-principle studies [21, 23] and ionic charge theory (ICT) [24, 25]. In the recent past few years, empirical relations have become an essential

part of material research [25-27]. As empirical relations do not provide accurate results for each specific material in many cases, they can still be very useful. In general, the simplistic form of empirical relation is permissible to a broad class of researchers and determines the important properties of materials.

The fractional ionic characteristic ( $f_i$ ) and covalent characteristic ( $f_c$ ) of the chemical bonds in complex materials are among the most important parameters for describing problems related to the elastic constants, microhardness, bulk modulus, heat of formation, cohesive energy, and crystal structure. The dielectric theory of solids was developed by Phillips and Van-Vechten (PVV) [27, 28] and reported the ionic gap, covalent energy gap, average energy gap, and hence the ionicity and covalence of binary solids. Later, Levine [29] extended the PVV theory to ternary chalcopyrites and multi-bond crystals using the bond charge model (BCM) to investigate these parameters considering the effect of valence  $d$ -electrons. Recently, Yadav [30-33] and Verma [34] have proposed modified forms of PVV model to study the electronic, optical and mechanical properties of binary semiconducting materials. Various theoretical approaches [9, 27-47] have presented explicit focus to determine the ionicity and covalence of different types of semiconducting materials.

Authors [43-48] have recently developed simple empirical relations to calculate the static, dynamical, electronic, and mechanical properties of ternary chalcopyrite semiconductors, binary rare earth compounds, and semiconducting materials using plasma energy as a key parameter. As far as is known, no studies have been conducted on such materials based on plasma oscillation theory of solids. Herein, the electronic properties such as homopolar gap ( $E_h$ ), heteropolar gap ( $E_c$ ), ionicity ( $f_i$ ) and covalence ( $f_c$ ) for the chemical bonds A-O and B-O in  $ABO_3$  cubic perovskites, and their mechanical properties as bulk modulus are investigated considering the plasma oscillation theory of solids. The values of our estimations are in excellent agreement with the available experimental data as compared to various theoretical findings. The proposed perovskite oxide materials and the associated approaches are intended to serve as a framework for future perovskite material development as well as the creation of structural materials with desired electronic and mechanical properties.

## 2. Methodology

The modified dielectric theory of solids developed by Phillips *et al.* [27-32] defines the bond ionicity and covalence of  $\mu$ -type chemical bonds in complex materials as-

$$f_i^\mu = \frac{(E_c^\mu)^2}{(E_g^\mu)^2} \quad \& \quad f_c^\mu = \frac{(E_h^\mu)^2}{(E_g^\mu)^2} \quad (1)$$

where  $E_h^\mu$ ,  $E_c^\mu$  &  $E_g^\mu$  are homopolar or covalent part, heteropolar or ionic part and average energy gap in binary

$\mu$ -type bonds, which are defined as-

$$E_h^\mu = 40.468 / (d^\mu)^{2.5} \quad (2)$$

$$E_c^\mu = b^\mu e^2 (\Delta Z) \exp(-K_s^\mu d_0^\mu) / d_0^\mu \quad (3)$$

$$(E_h^\mu)^2 = (E_g^\mu)^2 - (E_c^\mu)^2 \quad (4)$$

In the above relations,  $E_h^\mu$  &  $E_c^\mu$  are inversely related to the chemical bond length ( $d^\mu$ ); The valence states of various types of atoms differ by a factor called  $\Delta Z$ ,  $d_0^\mu = d_{AB}^\mu / 2$  (half the length of chemical bond) and  $b$  is the prescreening factor depending upon the co-ordination number around the cations and is defined by Levine's bond charge model [29] as  $b = 0.089(N_c^\mu)^2$ . The Thomas Fermi screening parameter (TFSP) is given by-

$$K_s^\mu = (4K_F^\mu / \pi a_B)^{0.5} \quad (5)$$

Kumar *et al.* [40] reported the optical, electronic, and elastic properties of divalent and trivalent rare earth mono-chalcogenides in the form of plasma energy ( $\eta\omega_p$ ) as follows-

$$E_h = K(\hbar\omega_p)^{1.6533} \quad (6)$$

$$E_c = K_1 \exp(K_2 \hbar\omega_p) \quad (7)$$

$$E_g = K_3 + K_4(\hbar\omega_p) \quad (8)$$

Where  $K$ ,  $K_1$ ,  $K_2$ ,  $K_3$  and  $K_4$  are numerical constants for divalent and trivalent rare earth chalcogenide compounds and  $\hbar\omega_p$  is the plasma energy of such compounds. Gao *et al.* [41, 42] developed an empirical relationship between microhardness and some known characteristic parameters, such as effective number of valence electrons per  $\mu$ -bond, bond-volume, and bond ionicity. Thus, it is clear that the bond length and ionicity of the chemical bonds both depend on the actual number of valence electrons in a compound as well as their plasma energy. Explicitly, homopolar and heteropolar energy gaps for  $ABO_3$  perovskite oxides may also depend upon plasma energy of valance electrons. Now, to find the better accord between available theoretical and experimental data for  $ABO_3$  perovskite oxide solids in the cubic phase; the relations (2)-(3) are extended in term of plasma energy ( $\hbar\omega_p$  in eV) as-

$$E_h = K_1(\hbar\omega_p)^{K_2} \quad (9)$$

$$E_c = K_3(\hbar\omega_p)^{0.667} \exp[-K_4(\hbar\omega_p)^{-0.3334}] \quad (10)$$

where  $\eta\omega_p$  is the plasma oscillations energy of a quanta associated with valence electrons in metals or compounds [40].  $K_1$ ,  $K_2$ ,  $K_3$ , and  $K_4$  are numerical constants that have values 0.01651, 1.667, 60.9980, 10.10451 and 0.04041, 1.667,

26.9729, 6.82412 for A-O and B-O bonds respectively in ABO<sub>3</sub> perovskite materials. Now, substituting the values of E<sub>h</sub> and E<sub>c</sub> from equations (9) and (10) in equations (1) and (4); the values of ionicity (f<sub>i</sub>), covalence (f<sub>c</sub>), and average energy gap (E<sub>g</sub>) of the chemical bonds have computed and presented in Table 1.

### 2.1. Refractive Index

Based on plasma energy and average energy gap or Penn gap (E<sub>g</sub>) using Penn like model, the dielectric constant and subsequently refractive index ( $n = \sqrt{\epsilon_{\infty}}$ ) are investigated [73]

$$\epsilon_{\infty, X-Y} = 1 + \frac{\hbar \omega_p^2}{E_{g, X-Y}^2} S_0$$

$$\text{Where } S_0 = 1 - \left( \frac{E_g}{4E_f} \right) + \frac{1}{3} \left( \frac{E_g}{4E_f} \right)^2 \approx 0.95$$

$$(\epsilon_{\infty})_{Total} = (\epsilon_{\infty})_{A-O} + (\epsilon_{\infty})_{B-O} \quad (11)$$

### 2.2. Electronic Polarizability

The electronic polarizability were calculated using well-known Clausius-Mossotti model -

$$\alpha_{CM} = 0.395 \times 10^{-24} \frac{(\epsilon_{\infty} - 1)M}{(\epsilon_{\infty} + 1)d} \quad (12)$$

Where M is the molecular weight,  $\epsilon_{\infty}$  is the dielectric constant and  $d$  is the density of the perovskite material. The average bond polarizability of ABO<sub>3</sub> compounds in term of Penn gap or average energy gap (E<sub>g</sub>) was defined by Chemla [74] as -

$$\alpha_{A-O} = \frac{(2a_0)^3 E_0^2 D_{A-O}}{E_{g, A-O}^2} \quad \& \quad \alpha_{B-O} = \frac{(2a_0)^3 E_0^2 D_{B-O}}{E_{g, B-O}^2} \quad (13)$$

In the above relation,  $a_0 = \hbar^2/mc^2$ ,  $E_0 = me^4/2\hbar^2$  and  $D = 1.0$  for both type of the bonds. The total polarizability investigated by summing the individual polarizability of two bonds A-O and B-O in ABO<sub>3</sub> molecule.

$$\alpha_{Total} = \alpha_{A-O} + \alpha_{B-O} \quad (14)$$

The computed values of polarizability of these compounds from relations (12) & (14) are given in the Table 2. A fairly good agreement has been observed between the values of electronic polarizability obtained by Clausius-Mossotti and in this analysis.

### 2.3. Bulk Modulus

Employing the average value of ionicity of the bonds,  $f_i = (f_{i, A-O} + f_{i, B-O})/2$ , in well-known Neumann's scaling approach [47]; the bulk modulus of ABO<sub>3</sub> perovskite oxides can be determined. According to Neumann's approach, bulk modulus is inversely proportional to cell volume of a compound as-

$$B \propto V^{-n}$$

$$B = B_0 V^{-n} \quad (15)$$

where  $n$  is equal to 1.159;  $B_0$  is defined as  $B_0 = b_0(1 - b_1 f_c)$ ,  $b_0$  and  $b_1$  are adjustable parameters, which depend upon the crystal structure of a compound and have values  $2.5675 \times 10^4$  and 2.456, respectively; and  $f_c = (1 - f_i)$  is the covalence of the ABO<sub>3</sub> compound. In this calculation the structural parameter such as cell-volume was used from experimental data [24, 25].

## 3. Results and Discussion

Homopolar gap (E<sub>h</sub>), heteropolar gap (E<sub>c</sub>), average energy gap (E<sub>g</sub>), ionicity (f<sub>i</sub>), covalence (f<sub>c</sub>), dielectric constant ( $\epsilon_{\infty}$ ) and refractive index ( $n = \sqrt{\epsilon_{\infty}}$ ) of the chemical bonds in ABO<sub>3</sub> perovskite oxide materials have been calculated using the relations (1), (4), (9)-(11) in term of plasma energy ( $\hbar\omega_p$  in eV) and the estimated results are given in the Table 1. The values of ionicity, covalency and energy gaps of the chemical bonds A-O and B-O in ABO<sub>3</sub> (A → Ba, Sr, B → Hf, Zr, Ti) materials are compared with the values reported by previous theoretical findings [9]. Hence, these results of electronic properties showed a fairly good agreement with other such results. In order to further validate present investigations, the bulk modulus of such perovskites is to be calculated employing Neumann's relation (15) and is presented in Table 2. When a graph is plotted between B versus  $V^{-n}$  for these compounds, an increasing trend is observed as in Figure 1, which validates the current approach. It is obvious from Table 2 that calculated results for B are in fine tune with available experimental data [51, 66, 69] as compared to previous theoretical reports [5, 23, 48-50, 52-65, 67-70]. Consequently, reliability and accuracy of the presented formulae on electronic and mechanical properties is excellently verified.

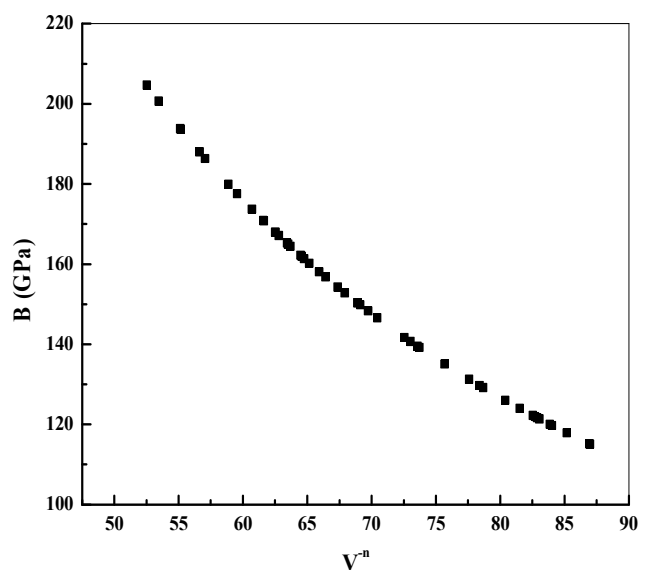


Figure 1. Plot of bulk modulus versus cell volume. This show an increasing trend and validates the present model.

**Table 1.** Energy gaps (in eV), ionicity, covalence, and dielectric constant for A-O & B-O bonds in ABO<sub>3</sub> perovskite oxides.

Structure	$\eta\omega_p$ (eV)	A-O Bonds					B-O Bonds					Dielectric constant ( $\epsilon_r$ )		
		$E_h$	$E_c$	$E_g$	$f_i$	$f_c$	$E_h$	$E_c$	$E_g$	$f_i$	$f_c$	$\epsilon_{r,A-O}$	$\epsilon_{r,B-O}$	$\epsilon_{r,Total}$
BaFeO <sub>3</sub>	22.772	3.021	13.893	14.218	0.954	0.046	7.398	19.540	20.894	0.874	0.126	3.437	2.128	5.565
BaMoO <sub>3</sub>	22.384	2.936	13.456	13.773	0.954	0.046	7.190	19.052	20.364	0.875	0.125	3.509	2.147	5.657
BaNbO <sub>3</sub>	22.055	2.865	13.091	13.400	0.954	0.046	7.015	18.641	19.917	0.875	0.125	3.573	2.164	5.738
BaSnO <sub>3</sub>	21.767	2.802	12.772	13.076	0.954	0.046	6.862	18.281	19.526	0.876	0.124	3.632	2.180	5.813
BaHfO <sub>3</sub>	21.337	2.711	12.303	12.598	0.953	0.047	6.638	17.748	18.949	0.877	0.123	3.725	2.204	5.929
Ref. [9]		2.524	11.892		0.956	0.044	5.961	15.921		0.877	0.123			
BaZrO <sub>3</sub>	21.170	2.675	12.122	12.413	0.953	0.047	6.551	17.541	18.725	0.877	0.123	3.763	2.214	5.977
Ref. [9]		2.677	12.602		0.956	0.044	6.323	16.907		0.877	0.123			
BaIrO <sub>3</sub>	21.894	2.830	12.912	13.219	0.954	0.046	6.929	18.440	19.699	0.876	0.124	3.606	2.173	5.779
BaPbO <sub>3</sub>	20.636	2.564	11.550	11.832	0.954	0.046	6.278	16.885	18.015	0.878	0.122	3.889	2.246	6.136
BaTbO <sub>3</sub>	20.492	2.534	11.398	11.676	0.953	0.047	6.205	16.709	17.824	0.878	0.122	3.926	2.255	6.181
BaPrO <sub>3</sub>	20.001	2.435	10.890	11.159	0.953	0.047	5.962	16.118	17.186	0.879	0.121	4.052	2.286	6.338
BaCeO <sub>3</sub>	19.714	2.376	10.587	10.851	0.952	0.048	5.818	15.764	16.803	0.880	0.120	4.135	2.307	6.443
BaAmO <sub>3</sub>	19.986	2.431	10.868	11.137	0.952	0.048	5.952	16.093	17.159	0.879	0.121	4.059	2.288	6.348
BaNpO <sub>3</sub>	19.829	2.399	10.706	10.971	0.952	0.048	5.874	15.903	16.953	0.879	0.121	4.103	2.299	6.403
BaUO <sub>3</sub>	19.781	2.389	10.657	10.921	0.952	0.048	5.851	15.845	16.891	0.880	0.120	4.116	2.302	6.419
BaPaO <sub>3</sub>	19.363	2.306	10.229	10.485	0.952	0.048	5.646	15.341	16.347	0.879	0.121	4.239	2.332	6.572
BaThO <sub>3</sub>	19.168	2.267	10.032	10.285	0.952	0.048	5.552	15.109	16.097	0.880	0.120	4.299	2.347	6.646
BaTiO <sub>3</sub>	22.618	2.988	13.720	14.042	0.954	0.046	7.316	19.347	20.684	0.875	0.125	3.464	2.136	6.50 <sup>54</sup>
Ref. [9]		3.035	14.244	14.563	0.956	0.044	7.170	19.191	20.486	0.877	0.123			
BaRuO <sub>3</sub>	22.301	2.918	13.364	13.679	0.954	0.046	7.145	18.948	20.251	0.874	0.126	3.525	2.152	5.677
BaPuO <sub>3</sub>	19.965	2.426	10.847	11.115	0.952	0.048	5.942	16.068	17.132	0.879	0.121	4.065	2.290	6.355
BaVO <sub>3</sub>	23.153	3.106	14.327	14.660	0.955	0.045	7.606	20.022	21.418	0.873	0.127	3.369	2.110	5.479
BaBkO <sub>3</sub>	19.494	2.332	10.362	10.621	0.952	0.048	5.710	15.499	16.517	0.880	0.120	4.200	2.323	6.523
SrMnO <sub>3</sub>	24.479	3.409	15.872	16.233	0.955	0.045	8.346	21.716	23.265	0.870	0.130	3.160	2.051	5.212
SrVO <sub>3</sub>	23.691	3.227	14.947	15.291	0.955	0.045	7.903	20.706	22.163	0.872	0.128	3.280	2.085	5.365
SrFeO <sub>3</sub>	24.061	3.312	15.378	15.731	0.955	0.045	8.110	21.179	22.678	0.871	0.129	3.222	2.069	5.291
SrTiO <sub>3</sub>	23.554	3.197	14.789	15.130	0.955	0.045	7.827	20.532	21.973	0.872	0.128	3.302	2.091	5.393
Ref. [9]		3.201	14.991		0.956	0.044	7.560	20.234		0.877	0.123			
SrTcO <sub>3</sub>	23.162	3.108	14.337	14.670	0.955	0.045	7.611	20.033	21.430	0.873	0.127	3.368	2.109	5.477
SrMoO <sub>3</sub>	22.935	3.058	14.078	14.407	0.955	0.045	7.487	19.746	21.118	0.873	0.127	3.407	2.120	5.528
SrNbO <sub>3</sub>	22.585	2.980	13.682	14.003	0.954	0.046	7.297	19.304	20.638	0.874	0.126	3.471	2.137	5.608

**Table 1.** Continued.

Structure	$\eta\omega_p$ (eV)	A-O Bonds					B-O Bonds					Dielectric constant ( $\epsilon_r$ )		
		$E_h$	$E_c$	$E_g$	$f_i$	$f_c$	$E_h$	$E_c$	$E_g$	$f_i$	$f_c$	$\epsilon_{r,A-O}$	$\epsilon_{r,B-O}$	$\epsilon_{r,Total}$
SrSnO <sub>3</sub>	22.434	2.947	13.512	13.830	0.954	0.046	7.216	19.115	20.432	0.874	0.126	3.499	2.214	5.648
SrHfO <sub>3</sub>	22.145	2.884	13.190	13.501	0.954	0.046	7.062	18.753	20.039	0.875	0.125	3.556	2.160	5.716
Ref. [9]		2.578	12.147		0.956	0.044	6.090	16.275		0.877	0.133			
SrTbO <sub>3</sub>	21.269	2.696	12.228	12.522	0.953	0.047	6.603	17.663	18.857	0.876	0.124	3.740	2.208	5.949
SrAmO <sub>3</sub>	20.893	2.617	11.824	12.110	0.953	0.047	6.409	17.200	18.355	0.877	0.123	3.827	2.230	6.058
SrPuO <sub>3</sub>	20.528	2.541	11.436	11.715	0.952	0.048	6.223	16.753	17.871	0.878	0.122	3.916	2.253	6.170
SrCeO <sub>3</sub>	19.494	2.330	10.345	10.604	0.951	0.049	5.542	14.989	15.980	0.879	0.121	4.379	2.488	6.867
SrCoO <sub>3</sub>	24.061	3.312	15.378	15.731	0.955	0.045	8.110	21.179	22.678	0.871	0.129	3.222	2.069	5.291
SrZrO <sub>3</sub>	21.862	2.823	12.877	13.183	0.955	0.045	6.912	18.400	19.656	0.876	0.124	3.612	2.175	5.787
Ref. [9]		2.765	13.007		0.956	0.044	6.530	17.469		0.877	0.123			
SrRuO <sub>3</sub>	23.330	3.146	14.530	14.867	0.954	0.046	7.703	20.246	21.663	0.873	0.127	3.339	2.101	5.441
SrThO <sub>3</sub>	19.560	2.345	10.430	10.690	0.952	0.048	5.742	15.579	16.603	0.878	0.122	4.480	2.318	6.498
SrGeO <sub>3</sub>	24.470	3.406	15.860	16.222	0.956	0.044	8.341	21.703	23.251	0.870	0.130	3.161	2.052	5.213
SrRhO <sub>3</sub>	22.987	3.069	14.138	14.467	0.954	0.046	7.516	19.812	21.190	0.874	0.126	3.398	2.117	5.516
CaVO <sub>3</sub>	24.861	3.497	16.325	16.696	0.956	0.044	8.564	22.207	23.802	0.870	0.130	3.106	2.036	5.142
CaHfO <sub>3</sub>	22.806	3.029	13.932	14.257	0.956	0.044	7.417	19.583	20.941	0.874	0.126	3.430	2.126	5.557
CaZrO <sub>3</sub>	22.635	2.991	13.739	14.061	0.955	0.045	7.325	19.368	20.707	0.874	0.126	3.461	2.135	5.596
CaRuO <sub>3</sub>	24.155	3.334	15.489	15.844	0.955	0.045	8.163	21.299	22.810	0.871	0.129	3.208	2.065	5.273
CaSnO <sub>3</sub>	23.153	3.106	14.327	14.660	0.955	0.045	7.606	20.022	21.418	0.873	0.127	3.369	2.110	5.479
CaCeO <sub>3</sub>	19.693	2.370	10.549	10.812	0.952	0.048	5.637	15.222	16.233	0.879	0.121	4.317	2.471	6.788
CaTiO <sub>3</sub>	24.155	3.334	15.489	15.844	0.955	0.045	8.163	21.299	22.810	0.871	0.129	3.208	2.065	5.273
CaGeO <sub>3</sub>	25.110	3.556	16.624	17.001	0.956	0.044	8.708	22.530	24.154	0.870	0.130	3.072	2.026	5.099
CaMoO <sub>3</sub>	23.627	3.213	14.873	15.216	0.955	0.045	7.868	20.624	22.074	0.873	0.127	3.290	2.088	5.378
SrZrO <sub>3</sub>	21.894	2.830	12.912	13.219	0.954	0.046	6.929	18.440	19.699	0.875	0.125	3.606	2.173	5.779
SrHfO <sub>3</sub>	21.656	2.779	12.650	12.952	0.953	0.047	6.804	18.143	19.377	0.876	0.124	3.655	2.186	5.842

Structure	$\eta\omega_p$ (eV)	A-O Bonds					B-O Bonds					Dielectric constant ( $\epsilon_r$ )		
		$E_h$	$E_c$	$E_g$	$f_i$	$f_c$	$E_h$	$E_c$	$E_g$	$f_i$	$f_c$	$\epsilon_{r,A-O}$	$\epsilon_{r,B-O}$	$\epsilon_{r,Total}$
MgRhO <sub>3</sub>	22.823	3.033	13.951	14.277	0.954	0.046	7.426	19.605	20.964	0.874	0.126	3.427	2.126	4.86 <sup>73</sup>
PbTiO <sub>3</sub>	25.070	3.547	16.576	16.951	0.955	0.045	8.685	22.478	24.098	0.874	0.126	3.078	2.028	5.106
PbZrO <sub>3</sub>	24.470	3.406	15.860	16.222	0.953	0.047	8.341	21.703	23.251	0.877	0.123	3.161	2.052	8.75 <sup>54</sup>
PbVO <sub>3</sub>	23.995	3.297	15.302	15.653	0.955	0.045	8.073	21.095	22.587	0.871	0.129	3.232	2.072	5.213
														5.304

Table 2. Refractive index, electronic polarizability and bulk modulus of ABO<sub>3</sub> perovskite oxides.

Structure	Refractive index ( $n=\sqrt{\epsilon_r}$ )			Electronic Polarizability		$f_{c,avg}$	Bulk-modulus B (in GPa)		
	Calc.	Expt.	Theo. <sup>54,72,73</sup>	$\alpha_{CM}$	$\alpha_{CHEMLA}$		Calc.	Expt.	Theo.
BaFeO <sub>3</sub>	2.359			10.539	9.428	0.0860	164.56		
BaMoO <sub>3</sub>	2.378			10.974	10.031	0.0855	158.25		
BaNbO <sub>3</sub>	2.395			11.361	10.583	0.0855	153.00		
BaSnO <sub>3</sub>	2.411		2.85, 2.52	11.719	11.100	0.0850	148.47		
BaHfO <sub>3</sub>	2.435			12.280	11.936	0.0850	141.86		173.0 <sup>61</sup>
BaZrO <sub>3</sub>	2.444		2.27, 2.20	12.510	12.285	0.0850	139.33		148.08 <sup>23</sup> , 140.6 <sup>61</sup>
BaIrO <sub>3</sub>	2.404			11.559	10.867	0.0850	150.46		
BaPbO <sub>3</sub>	2.477			13.284	13.490	0.0840	131.41		
BaTbO <sub>3</sub>	2.486			13.504	13.844	0.0845	129.31		
BaPrO <sub>3</sub>	2.517			14.284	15.123	0.0843	122.39		124.98 <sup>65</sup>
BaCeO <sub>3</sub>	2.538			14.790	15.972	0.0842	118.13		107.47 <sup>23</sup>
BaAmO <sub>3</sub>	2.519			14.321	15.181	0.0845	122.10		
BaNpO <sub>3</sub>	2.530			14.590	15.636	0.0845	119.90		
BaUO <sub>3</sub>	2.533			14.671	15.773	0.0840	119.24		137.18 <sup>65</sup>
BaPaO <sub>3</sub>	2.563			15.427	17.079	0.0845	113.51		
BaThO <sub>3</sub>	2.578			15.796	17.733	0.0840	110.90		124.34 <sup>63</sup> , 135.3 <sup>65</sup>
BaTiO <sub>3</sub>	2.366		2.39, 2.24, 2.54	10.707	9.660	0.0855	162.05	162 <sup>67</sup>	164 <sup>54</sup> , 186 <sup>56</sup> , 189 <sup>57</sup> , 178.1 <sup>61</sup> , 166 <sup>67</sup> , 159.76 <sup>23</sup>
BaRuO <sub>3</sub>	2.382			11.070	10.166	0.0860	156.92		
BaPuO <sub>3</sub>	2.520			14.356	15.240	0.0845	121.81		
BaVO <sub>3</sub>	2.340			10.259	8.882	0.0860	168.51		
BaBkO <sub>3</sub>	2.554			14.597	15.759	0.0840	115.38		120.52 <sup>53</sup>
SrMnO <sub>3</sub>	2.282			8.893	7.283	0.0875	193.92		
SrVO <sub>3</sub>	2.316			9.603	8.183	0.0865	180.05		
SrFeO <sub>3</sub>	2.300		3.97, 2.98	9.260	9.215	0.0870	186.49		
SrTiO <sub>3</sub>	2.322		2.35, 2.28, 2.55	9.734	8.924	0.0865	177.70	179 <sup>67</sup> , 184 <sup>51</sup>	200 <sup>52</sup> , 147.49 <sup>49</sup> , 168.1 <sup>54</sup> , 185 <sup>60</sup> , 164.78 <sup>23</sup> , 193 <sup>56</sup> , 183 <sup>61</sup> , 175 <sup>67</sup>
SrTcO <sub>3</sub>	2.340			10.127	9.589	0.0860	171.05		
SrMoO <sub>3</sub>	2.351			10.364	9.713	0.0860	167.26		163.37 <sup>49</sup>
SrNbO <sub>3</sub>	2.368			10.745	9.878	0.0860	161.50		

Table 2. Continued.

Structure	Refractive index ( $n=\sqrt{\epsilon_r}$ )			Electronic Polarizability		$f_{c,avg}$	Bulk-modulus (B in GPa)		
	Calc.	Expt.	Theo. <sup>54,72,73</sup>	$\alpha_{CM}$	$\alpha_{CHEMLA}$		Calc.	Expt.	Theo.
SrSnO <sub>3</sub>	2.375		2.4	10.919	9.951	0.0860	159.06		173-177 <sup>65</sup>
SrHfO <sub>3</sub>	2.390			11.337	10.429	0.0855	153.11		173.6 <sup>61</sup>
SrTbO <sub>3</sub>	2.439			12.374	12.078	0.0855	140.82		
SrAmO <sub>3</sub>	2.461			12.904	12.892	0.0850	135.18		
SrPuO <sub>3</sub>	2.484			13.449	13.754	0.0850	129.83		
SrCeO <sub>3</sub>	2.620			14.411	14.100	0.0850	115.14		104.95 <sup>23</sup>
SrCoO <sub>3</sub>	2.300		3.28, 3.70	9.260	7.742	0.0870	186.49		
SrZrO <sub>3</sub>	2.405		2.16, 2.02	11.598	10.925	0.0845	149.96	150 <sup>70</sup>	150.82 <sup>23</sup> , 127.76 <sup>49</sup> , 160 <sup>50</sup> , 163.7 <sup>61</sup> , 171 <sup>69</sup> , 163 <sup>68</sup>
SrRuO <sub>3</sub>	2.332			10.109	8.643	0.0865	170.84		
SrThO <sub>3</sub>	2.549			15.063	16.445	0.0850	116.19		
SrGeO <sub>3</sub>	2.283			8.651	7.292	0.0870	193.75		
SrRhO <sub>3</sub>	2.348			10.357	9.863	0.0860	172.77		132.01 <sup>49</sup>
CaVO <sub>3</sub>	2.267			8.623	7.293	0.0870	200.81		
CaHfO <sub>3</sub>	2.357			10.473	9.114	0.0850	165.13		191.56 <sup>71</sup>
CaZrO <sub>3</sub>	2.365		2.1, 1.96	10.345	9.894	0.0855	162.33		155.78 <sup>23</sup> , 154.8 <sup>66</sup>
CaRuO <sub>3</sub>	2.296			9.362	9.378	0.0870	188.15		
CaSnO <sub>3</sub>	2.340			10.216	9.634	0.0860	170.90		191.78 <sup>71</sup>

Structure	Refractive index ( $n=\sqrt{\epsilon_r}$ )			Electronic Polarizability		$f_{c,avg}$	Bulk-modulus (B in GPa)		
	Calc.	Expt.	Theo. <sup>54,72,73</sup>	$\alpha_{CM}$	$\alpha_{CHEMLA}$		Calc.	Expt.	Theo.
CaCeO <sub>3</sub>	2.605			14.083	13.590	0.0845	117.88		113.71 <sup>23</sup>
CaTiO <sub>3</sub>	2.296		2.47, 2.46	9.313	9.635	0.0870	184.94		185.2 <sup>64</sup> , 174.94 <sup>23</sup> , 179 <sup>67</sup> , 176.2 <sup>58</sup> , 176 <sup>58</sup> , 157 <sup>53</sup> , 196 <sup>56</sup>
CaGeO <sub>3</sub>	2.258			8.316	8.660	0.0870	205.40		
CaMoO <sub>3</sub>	2.319			9.643	8.882	0.0860	180.88		
SnZrO <sub>3</sub>	2.404		2.36	11.485	10.865	0.0855	150.46		
SnHfO <sub>3</sub>	2.417		2.21	11.478	10.693	0.0855	146.75		
MgRhO <sub>3</sub>	2.356			10.514	9.352	0.0860	165.41		
PbTiO <sub>3</sub>	2.259		2.22, 2.52, 2.53, 2.55	9.997	8.261	0.0855	167.38		172.8 <sup>46</sup> , 144 <sup>47</sup> , 197 <sup>50</sup>
PbZrO <sub>3</sub>	2.283		2.27, 2.14	11.799	10.867	0.0850	141.75		
PbVO <sub>3</sub>	2.303			9.485	8.205	0.0870	185.34		

## 4. Conclusions

In line with plasma oscillation theory of solids, empirical relations were put forward for homopolar gap ( $E_h$ ), heteropolar gap ( $E_c$ ), ionicity ( $f_i$ ), covalency ( $f_c$ ) of the chemical bonds A-O and B-O in cubic phase  $ABO_3$  perovskite and further applied to investigate their values for a series of perovskite oxides. The dielectric constant, refractive index and electronic polarizability of the materials have also been calculated and are presented in respective table. The pre-reported and current values of these properties are very closely correlated. By the way of comparison, it is evident that the plasmon energy of a compound is a crucial parameter for investigating its electronic and mechanical properties for cubic phase  $ABO_3$  perovskite oxides. The values of Phillips ionicity of these materials strongly support the determination of their bulk modulus, and the values were found to be in excellent agreement with previous experimental and theoretical reports. As a result of these findings, we draw the conclusion that the plasma oscillation theory of solids holds true even for cubic  $ABO_3$  perovskite solids. It is believed that the adopted methodology and data gathered in this study would be used as a guide for further initiatives on the development of examined materials and devices. This model can also easily be extended to other more complex compounds, of which work is in progress.

## CRedit Authorship Contribution Statement

Niharika Yadav: Writing original draft, review & editing, Review of Literatures. Preeti Varshney: Ideas, Final writing & editing, Data presentation, Rajesh Chandra Gupta: Analysis of figures, Critical revision, Supervision. Dheerendra Singh Yadav: Methodology, Conceptualization, Formal analysis, Data curation.

## Disclosure

The authors declare that they have no known financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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