American Journal of Physics and Applications
2023; 11(4): 80-88
http://www.sciencepublishinggroup.com/j/ajpa
doi: 10.11648/j.ajpa.20231104.11
ISSN: 2330-4286 (Print); ISSN: 2330-4308 (Online)

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

Niharika Yadav[1], Dhirendra Singh Yadav[1, *], Preeti Varshney[2], Rajesh Chandra Gupta[3]

[1]Department of Physics, Chaudhary Charan Singh P G College Heonra (Saifai), Etawah, India

[2]Department of Physics, Government Girls Inter College Iglas, Aligarh, India

[3]Department of Physics, B. S. A. College, Mathura, India

Email address:

dhirendra.867@rediffmail.com (Dhirendra Singh Yadav)

[*]Corresponding author

To cite this article:

Niharika Yadav, Dhirendra Singh Yadav, Preeti Varshney, Rajesh Chandra Gupta. Electronic and Mechanical Properties of Chemical Bonds (A-O & B-O) in Cubic Phase $A^{+2}B^{+4}O_3$ Perovskite Oxides. *American Journal of Physics and Applications*. Vol. 11, No. 4, 2023, pp. 80-88. doi: 10.11648/j.ajpa.20231104.11

Received: September 25, 2023; **Accepted**: October 16, 2023; **Published**: November 9, 2023

Abstract: In the present manuscript, electronic and mechanical properties of a series of ABO_3 (A→ alkaline earth metals, B→ 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 (ε_∞) 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 (α_{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 μ-type chemical bonds in complex materials as-

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

where E_h^{μ}, E_c^{μ} & E_g^{μ} are homopolar or covalent part, heteropolar or ionic part and average energy gap in binary μ-type bonds, which are defined as-

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

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

$$(E_h^{\mu})^2 = (E_g^{\mu})^2 - (E_c^{\mu})^2 \tag{4}$$

In the above relations, E_h^{μ} & E_c^{μ} are inversely related to the chemical bond length (d^{μ}); The valence states of various types of atoms differ by a factor called ΔZ, $d_0^{\mu} = d_{AB}^{\mu}/2$ (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-

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

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-

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

$$E_c = K_1 \exp(K_2 \hbar\omega_p) \tag{7}$$

$$E_g = K_3 + K_4(\hbar\omega_p) \tag{8}$$

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 μ-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-

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

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

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_3 perovskite materials. Now, substituting the values of E_h and Ec from equations (9) and (10) in equations (1) and (4); the values of ionicity (f_i), covalence (f_c), and average energy gap (E_g) 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 (Eg) using Penn like model, the dielectric constant and subsequently refractive index $(n = \sqrt{\varepsilon_\infty})$ are investigated [73]

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

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

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

2.2. Electronic Polarizability

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

$$\alpha_{CM} = 0.395\times10^{-24} \frac{(\varepsilon_\infty - 1)M}{(\varepsilon_\infty + 1)d} \quad (12)$$

Where M is the molecular weight, ε_∞ is the dielectric constant and *d* is the density of the perovskite material. The average bond polarizability of ABO_3 compounds in term of Penn gap or average energy gap (E_g) was defined by Chemla [74] as -

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

In the above relation, $a_0 = \hbar^2/me^2$, $E_0 = me^4/2\hbar^2$ 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_3 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_3 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 2.5675×10^4 and 2.456, respectively; and $f_c=(1-f_i)$ is the covalence of the ABO_3 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_h), heteropolar gap (E_c), average energy gap (E_g), ionicity (f_i), covalence (f_c), dielectric constant (ε_∞) and refractive index ($n=\sqrt{\varepsilon_\infty}$) of the chemical bonds in ABO_3 perovskite oxide materials have been calculated using the relations (1), (4), (9)-(11) in term of plasma energy ($\eta\omega_p$ 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_3 (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 Numann'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.

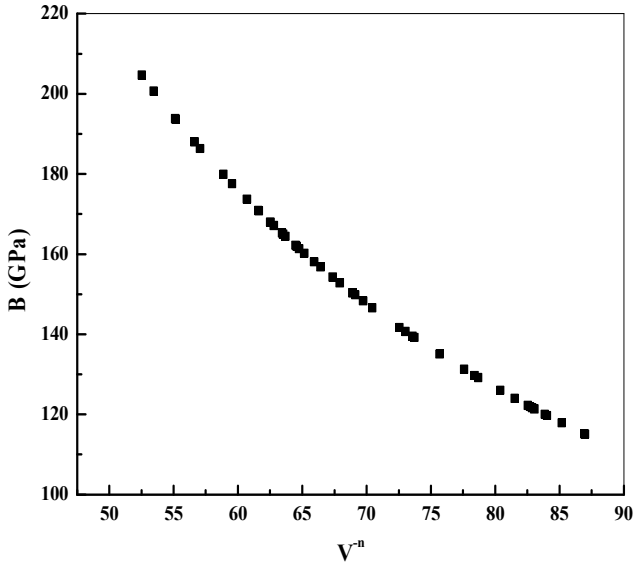

Figure 1. *Plot of bulk modulus versus cell volume. This show an increasing trend and validates the present model.*

Table 1. *Energy gaps (in eV), ionicity, covalence, and dielectric constant for A-O & B-O bonds in ABO_3 perovskite oxides.*

Structure	$\eta\omega_p$	A-O Bonds					B-O Bonds					Dielectric constant (ε_∞)		
	(eV)	E_h	E_c	E_g	f_i	f_c	E_h	E_c	E_g	f_i	f_c	$\varepsilon_{\infty,A\text{-}O}$	$\varepsilon_{\infty,B\text{-}O}$	$\varepsilon_{\infty,Total}$
$BaFeO_3$	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
$BaMoO_3$	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
$BaNbO_3$	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
$BaSnO_3$	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
$BaHfO_3$	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			
$BaZrO_3$	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			
$BaIrO_3$	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
$BaPbO_3$	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
$BaTbO_3$	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
$BaPrO_3$	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
$BaCeO_3$	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
$BaAmO_3$	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
$BaNpO_3$	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
$BaUO_3$	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
$BaPaO_3$	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
$BaThO_3$	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
$BaTiO_3$	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	5.600
Ref. [9]		3.035	14.244	14.563	0.956	0.044	7.170	19.191	20.486	0.877	0.123			6.50[54]
$BaRuO_3$	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
$BaPuO_3$	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
BaVO3	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
BaBkO3	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
$SrMnO_3$	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
$SrVO_3$	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
$SrFeO_3$	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
$SrTiO_3$	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			6.30[54]
$SrTcO_3$	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
$SrMoO_3$	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
$SrNbO_3$	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	$\eta\omega_p$	A-O Bonds					B-O Bonds					Dielectric constant (ε_∞)		
	(eV)	E_h	E_c	E_g	f_i	f_c	E_h	E_c	E_g	f_i	f_c	$\varepsilon_{\infty,A\text{-}O}$	$\varepsilon_{\infty,B\text{-}O}$	$\varepsilon_{\infty,Total}$
$SrSnO_3$	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
$SrHfO_3$	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			
$SrTbO_3$	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
$SrAmO_3$	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
$SrPuO_3$	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
$SrCeO_3$	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
$SrCoO_3$	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
$SrZrO_3$	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			
$SrRuO_3$	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
$SrThO_3$	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
$SrGeO_3$	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
$SrRhO_3$	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
$CaVO_3$	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
$CaHfO_3$	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
$CaZrO_3$	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
$CaRuO_3$	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
$CaSnO_3$	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
$CaCeO_3$	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
$CaTiO_3$	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
														6.25[54]
$CaGeO_3$	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
$CaMoO_3$	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
$SnZrO_3$	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
														5.59[73]
$SnHfO_3$	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 (ε_∞)		
		E_h	E_c	E_g	f_i	f_c	E_h	E_c	E_g	f_i	f_c	$\varepsilon_{\infty,A\text{-}O}$	$\varepsilon_{\infty,B\text{-}O}$	$\varepsilon_{\infty,Total}$
$MgRhO_3$	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[73] 5.553
$PbTiO_3$	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 8.75[54]
$PbZrO_3$	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	5.213
PbVO3	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	5.304

Table 2. *Refractive index, electronic polarizability and bulk modulus of ABO_3 perovskite oxides.*

Structure	Refractive index ($n=\sqrt{\varepsilon_\infty}$)			Electronic Polarizability		$f_{c\,avg}$	Bulk-modulus B (in GPa)		
	Calc.	Expt.	Theo.[54,72,73]	α_{CM}	α_{CHEMLA}		Calc.	Expt.	Theo.
$BaFeO_3$	2.359			10.539	9.428	0.0860	164.56		
$BaMoO_3$	2.378			10.974	10.031	0.0855	158.25		
$BaNbO_3$	2.395			11.361	10.583	0.0855	153.00		
$BaSnO_3$	2.411		2.85, 2.52	11.719	11.100	0.0850	148.47		
$BaHfO_3$	2.435			12.280	11.936	0.0850	141.86		173.0[61]
$BaZrO_3$	2.444		2.27, 2.20	12.510	12.285	0.0850	139.33		148.08[23], 140.6[61]
$BaIrO_3$	2.404			11.559	10.867	0.0850	150.46		
$BaPbO_3$	2.477			13.284	13.490	0.0840	131.41		
$BaTbO_3$	2.486			13.504	13.844	0.0845	129.31		
$BaPrO_3$	2.517			14.284	15.123	0.0843	122.39		124.98[65]
$BaCeO_3$	2.538			14.790	15.972	0.0842	118.13		107.47[23]
$BaAmO_3$	2.519			14.321	15.181	0.0845	122.10		
$BaNpO_3$	2.530			14.590	15.636	0.0845	119.90		
$BaUO_3$	2.533			14.671	15.773	0.0840	119.24		137.18[65]
$BaPaO_3$	2.563			15.427	17.079	0.0845	113.51		
$BaThO_3$	2.578			15.796	17.733	0.0840	110.90		124.34[63], 135.3[65]
$BaTiO_3$	2.366		2.39, 2.24, 2.54	10.707	9.660	0.0855	162.05	162[67]	164[54], 186[56], 189[57], 178.1[61], 166[67], 159.76 [23]
$BaRuO_3$	2.382			11.070	10.166	0.0860	156.92		
$BaPuO_3$	2.520			14.356	15.240	0.0845	121.81		
BaVO3	2.340			10.259	8.882	0.0860	168.51		
BaBkO3	2.554			14.597	15.759	0.0840	115.38		120.52[53]
$SrMnO_3$	2.282			8.893	7.283	0.0875	193.92		
$SrVO_3$	2.316			9.603	8.183	0.0865	180.05		
$SrFeO_3$	2.300		3.97, 2.98	9.260	9.215	0.0870	186.49		
$SrTiO_3$	2.322		2.35, 2.28, 2.55	9.734	8.924	0.0865	177.70	179[67] 184[51]	200[52], 147.49[49], 168.1[54], 185[60], 164.78[23], 193[56], 183[61], 175[67]
$SrTcO_3$	2.340			10.127	9.589	0.0860	171.05		
$SrMoO_3$	2.351			10.364	9.713	0.0860	167.26		163.37[49]
$SrNbO_3$	2.368			10.745	9.878	0.0860	161.50		

Table 2. *Continued.*

Structure	Refractive index ($n=\sqrt{\varepsilon_\infty}$)			Electronic Polarizability		$f_{c\,avg}$	Bulk-modulus (B in GPa)		
	Calc.	Expt.	Theo.[54,72,73]	α_{CM}	α_{CHEMLA}		Calc.	Expt.	Theo.
$SrSnO_3$	2.375		2.4	10.919	9.951	0.0860	159.06		173-177[65]
$SrHfO_3$	2.390			11.337	10.429	0.0855	153.11		173.6[61]
$SrTbO_3$	2.439			12.374	12.078	0.0855	140.82		
$SrAmO_3$	2.461			12.904	12.892	0.0850	135.18		
$SrPuO_3$	2.484			13.449	13.754	0.0850	129.83		
$SrCeO_3$	2.620			14.411	14.100	0.0850	115.14		104.95[23]
$SrCoO_3$	2.300		3.28, 3.70	9.260	7.742	0.0870	186.49		
$SrZrO_3$	2.405		2.16, 2.02	11.598	10.925	0.0845	149.96	150[70]	150.82[23],127.76[49], 160[50], 163.7[61], 171[69], 163[68]
$SrRuO_3$	2.332			10.109	8.643	0.0865	170.84		
$SrThO_3$	2.549			15.063	16.445	0.0850	116.19		
$SrGeO_3$	2.283			8.651	7.292	0.0870	193.75		
$SrRhO_3$	2.348			10.357	9.863	0.0860	172.77		132.01[49]
$CaVO_3$	2.267			8.623	7.293	0.0870	200.81		
$CaHfO_3$	2.357			10.473	9.114	0.0850	165.13		191.56[71]
$CaZrO_3$	2.365		2.1, 1.96	10.345	9.894	0.0855	162.33		155.78[23], 154.8[66]
$CaRuO_3$	2.296			9.362	9.378	0.0870	188.15		
$CaSnO_3$	2.340			10.216	9.634	0.0860	170.90		191.78[71]

Structure	Refractive index ($n=\sqrt{\varepsilon_\infty}$)			Electronic Polarizability		$f_{c\,avg}$	Bulk-modulus (B in GPa)		
	Calc.	Expt.	Theo.[54,72,73]	α_{CM}	α_{CHEMLA}		Calc.	Expt.	Theo.
$CaCeO_3$	2.605			14.083	13.590	0.0845	117.88		113.71[23]
$CaTiO_3$	2.296		2.47, 2.46	9.313	9.635	0.0870	184.94		185.2[64], 174.94[23], 179[67], 176.2[58], 176[58], 157[53], 196[56]
$CaGeO_3$	2.258			8.316	8.660	0.0870	205.40		
$CaMoO_3$	2.319			9.643	8.882	0.0860	180.88		
$SnZrO_3$	2.404		2.36	11.485	10.865	0.0855	150.46		
$SnHfO_3$	2.417		2.21	11.478	10.693	0.0855	146.75		
$MgRhO_3$	2.356			10.514	9.352	0.0860	165.41		
$PbTiO_3$	2.259		2.22, 2.52, 2.53, 2.55	9.997	8.261	0.0855	167.38		172.8[46], 144[47], 197[50]
$PbZrO_3$	2.283		2.27,2.14	11.799	10.867	0.0850	141.75		
$PbVO_3$	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. Dheerandra 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.

ORCID

Dheerendra Singh Yadav: https://orcid.org/0000-0001-8315-9743
Preeti Varshney: https://orcid.org/0000-0002-6014-7210
Rajesh Chandra Gupta: https://orcid.org/0000-0002-0560-7077

References

[1] M. Hasan, S. Nasrin, M. N. Islam, A. K. M. Akther Hossain, First-principles insights into the electronic, optical, mechanical, and thermodynamic properties of lead-free cubic ABO3 [A = Ba, Ca, Sr; B = Ce, Ti, Zr] perovskites AIP Advances (2022), 12, 085327. https://doi.org/10.1063/5.0104191.

[2] S. Cabuk, Magnetic, electronic and mechanical properties of $SeXO_3$ (X = Mn, Ni) with the LSDA +U framework, Journal of Alloys and Compounds (2021) 850, 156674. https://doi.org/10.1016/j.jallcom.2020.156674.

[3] P. M. Bulemo, and I. D. Kim, Recent advances in ABO_3 perovskites: their gas-sensing performance as resistive-type gas sensors, Journal of the Korean Ceramic Society 2020 57(1), 24-39. https://doi.org/10.1007/s43207-019-00003-1.

[4] N. Wagner, R. Seshadri, and J. M. Rondinelli, Property control from polyhedral connectivity in ABO_3 oxides, Phys. Rev. B (2019) 100, 064101. https://doi.org/10.1103/PhysRevB.100.064101.

[5] A. I. Lebedev, Ab initio calculations of phonon spectra in ATiO$_3$ perovskite crystals (A = Ca, Sr, Ba, Ra, Cd, Zn, Mg, Ge, Sn, Pb), Phys. Solid State (2009) 51, 362. https://doi.org/10.1134/S1063783409020279.

[6] H. P. Rooksby, Compounds of the Structural Type of Calcium Titanate, Nature, (1945) 155 484. https://doi.org/10.1038/155484a0.

[7] J. F. Scott, C. A. Pazde, Aurauj et al., J. Appl. Phys. 70 (1981) 382.

[8] S. Y. Lee, M. C. C Costodio, H. J. Lim et al., Growth and characterization of $Pb(Mg_{1/3}Nb_{2/3})O_3$ and $Pb(Mg_{1/3}Nb_{2/3})O_3$–$PbTiO_3$ thin films using solid source MOCVD techniques J. Cryst. Growth, (2001) 226, 247. https://doi.org/10.1016/S0022-0248(01)00796-5.

[9] Yuchen Liu, Bin Liu, Huimin Xiang, Yanchun Zhou, Hongqiang Nian, Hongfei Chen, Guang Yang, Yanfeng Gao, Theoretical investigation of anisotropic mechanical and thermal properties of ABO3 (A=Sr, Ba; B=Ti, Zr, Hf) perovskites, J. American Ceramic Society 10 (2018) 1. https://doi.org/10.1111/jace.15502

[10] Q. Mahmood, Bakhtiar Ul Haq, M. Yaseen, Shahid M. Ramay, Muhammad Gul Bahar Ashiq, Asif Mahmood, The first-principle study of mechanical, optical and thermoelectric properties of $SnZrO_3$ and $SnHfO_3$ for renewable energy applications, Solid State Communications 292 (2019) 17. https://doi.org/10.1016/j.ssc.2019.01.011.

[11] G. Gupta, T. Tautiyal, S. Auluck, Optical properties of the compounds $BaTiO_3$ and $SrTiO_3$, Phys. Rev. B. (2004), 69, 052101. https://doi.org/10.1103/PhysRevB.69.052101.

[12] M. P. Moret, M. A. C. Devillers et al., Optical properties of $PbTiO_3$, $Pb(Zr_xTi_{1-x})O_3$ and $PbZrO_3$, films deposited by metalorganic chemical vapor on $SrTiO_3$, J. Applied Physics 92 (2002) 468. https://doi.org/10.1063/1.1486048.

[13] D. Bauerle, W. Braum, V. Saile, Physica B 29 (1978) 179.

[14] S. Pikunov, E. Heifets R.I. Eglitis, G. Borstel, Bulk properties and electronic structure of SrTiO3, BaTiO3, PbTiO3 perovskites: an ab initio HF/DFT study, Compt. Mater. Sci. (2004) 29 165. doi: 10.1016/j.commatsci.2003.08.036.

[15] S. Saha, T. P. Shina, A. Mookerjee; Electronic structure, chemical bonding, and optical properties of paraelectric $BaTiO_3$, Phys. Rrev. B (2000) 62, 8828. https://doi.org/10.1103/PhysRevB.62.8828.

[16] M. Kamruzzaman, M. A. Helal, I. E. Ara et al., A comparative study based on the first principles calculations of ATiO3 (A = Ba, Ca, Pb and Sr) perovskite structure, Indian J Phys (2016) 90: 1105-1113. DOI 10.1007/s12648-016-0848-3.

[17] S. Y. Liu, M. Sun, S. Zhang, S. Liu, D. J. Li, Z. Niu, Y. Li, and S. Wang, First-principles study of thermodynamic miscibility, structures, and optical properties of $Cs_2Sn(X_{1-x}Yx)_6$ (X,Y = I, Br, Cl) lead-free perovskite solar cells, Appl. Phys. Lett. (2021) 118, 141903. https://doi.org/10.1063/5.0043809.

[18] Tariq Usman, G. Murtaza, Haijun Luo, Asif Mahmood, GGA and GGA+U Study of Rare Earth-Based Perovskites in Cubic Phase J. Superhard Nov. Magn. (2016) 10, 3953. DOI: 10.1007/s10948-016-3953-9.

[19] M. Rashid, Z. Abbas, M. Yasheen et al., J. Supercond. Nov. Magn. 4 (2017).

[20] Bin Amin, Farzana Majid, M. Bilal Saddique,. M. Rashid, Physical properties of half-metallic AMnO3 (A= Mg, Ca) oxides via ab initio calculations, Compt. Mat. Sci. (2018) 146, 248. DOI: 10.1016/j.commatsci.2018.01.033.

[21] Yuchen Liu, Wei Zhang, Banghui Wang, Luchao Sun, Fangzhi Li, Zhenhai Xue, Guohong Zhou, Bin Liu, Hongqiang Nian., Theoretical and experimental investigations on high temperature mechanical and thermal properties of $BaZrO_3$, Ceramic International (2018) 44 16475. https://doi.org/10.1016/j.ceramint.2018.06.064.

[22] Rasul Bakhsh Behram, M A Iqbal, Muhammad Rashid, M Atif Sattar, Asif Mahmood, Shahid M Ramay; Ab-initio investigation of AGeO3 (A=Ca, Sr) compounds via Tran–Blaha-modified Becke–Johnson exchange potential, Chin. Phys. B (2017) 26(11), 116103. DOI: 10.1088/1674-1056/26/11/116103.

[23] Narasak Pandech, Kanoknan Sarasamak and Sukit Limpijumnong, Elastic properties of perovskite $ATiO_3$ (A = Be, Mg, Ca, Sr, and Ba) and PbBO3 (B = Ti, Zr, and Hf): First principles calculations, J. Applied Physics (2015) 117, 174108. http://dx.doi.org/10.1063/1.4919837.

[24] Rehan Ullah, Malak Azmat Ali, Khadijah Mohammed Saleh Katubi, Norah Salem Alsaiari, Khamael M. Abualnaja, A.S. Verma, G. Murtaza, Modeling of bulk modulus of A2BX6 cubic crystals (A = K, Cs, Rb, TI, NH4; B = tetravalent cation; X = F, Cl, Br, I) using semi-empirical model, Inorganic Chemistry Communication (2022) 139, 109315. https://doi.org/10.1016/j.inoche.2022.109315.

[25] A. S. Verma, Vijay K Jindal, Lattice Constant of Cubic Perovskites, J. Alloys and Compounds 485 (2009) 514. DOI: 10.1016/j.jallcom.2009.06.001.

[26] M. Hasan and A. K. M. Akther Hossain, "Structural, electronic and optical properties of strontium and nickel co-doped BaTiO3: A DFT based study," Computational Condensed Matter (2021) 28, e00578. https://doi.org/10.1016/j.cocom.2021.e00578.

[27] J. C. Phillips, J. A. Van-Vechten, Dielectric Classification of Crystal Structures, Ionization Potentials, and Band Structures, Phys. Rev. Lett. (1969) 22, 705. https://doi.org/10.1103/PhysRevLett.22.705.

[28] J. A. Van-Vechten, Quantum Dielectric Theory of Electronegativity in Covalent Systems. I. Electronic Dielectric Constant, Phys. Rev. B 182 (1969) 891. https://doi.org/10.1103/PhysRev.182.891.

[29] B. F. Levine, Bond susceptibilities and ionicities in complex crystal structures, J. Chem. Phys. 59 (1973) 1463. https://doi.org/10.1063/1.1680204.

[30] D. S. Yadav, S. P. Singh, Electronic properties of aluminum, gallium and indium pnictides, Phys. Scr. (2010) 82(6), 065705. DOI: 10.1088/0031-8949/82/06/065705.

[31] M. Rabiei et al., Measurement Modulus of Elasticity Related to the Atomic Density of Planes in Unit Cell of Crystal Lattices, Materials 13 (2020) 4380. DOI: 10.3390/ma13194380.

[32] D. S. Yadav, A. S. Verma, Electronic, optical and mechanical properties of $A^{II}B^{VI}$ semiconductors, International Journal of Modern Physics B 26 (2012) 1250020. https://doi.org/10.1142/S0217979212500208.

[33] Shi-Yu Liu, Shuoxin Zhang, Shiyang Liu, De-Jun Li, Yaping Li, Sanwu Wang, Phase stability, mechanical properties and melting points of high-entropy quaternary metal carbides from first-principles, Journal European Ceramic Society. (2021) 41(13), 6267. https://doi.org/10.1016/j.jeurceramsoc.2021.05.022.

[34] A. S. Verma, Electronic and optical properties of rare-earth chalcogenides and pnictides, Afr. Phys. Rev. 3 (2009) 11.

[35] V. K. Srivastava, Ionicity in $A^{II}B$, Phys. Rev. B Condens Matter (1987) 36(9), 5044, DOI: 10.1103/physrevb.36.5044.

[36] V. P. Gupta, V. K. Srivastava, P. N. L. Gupta, Electronic properties of chalcopyrites, J. Phys. Chem. Solids 42 (1981) 1079. https://doi.org/10.1016/0022-3697(81)90133-5.

[37] O. P. Singh V. P. Gupta Phys. State Solidi B 137 (1986) 97.

[38] V. K. Srivastava, Homopolar and heteropolar energy gaps in zincblende crystals J. Phys. C, Solid State Physics (1986) 19, 5689. DOI 10.1088/0022-3719/19/28/019.

[39] R. C. Gupta, K. Singh, A. S. Verma, Empirical Relation for Electronic and Optical Properties of Binary Tetrahedral Semiconductors, East Eur. J. Phys. 1 (2021) 89. DOI: 10.26565/2312-4334-2021-1-11.

[40] V. Kumar, S. Chandra, J. K. Singh, Electronic, elastic and optical properties of divalent ($R^{+2}X$) and trivalent ($R^{+3}X$) rare earth monochalcogenides, Ind. J. Phys. (2017) 91 875-881, https://doi.org/10.1007/s12648-017-0983-5

[41] Faming Gao, Julong He, Erdong Wu, Shimin Liu, Dongli Yu, Dongchun Li, Siyuan Zhang, and Yongjun Tian, Hardness of Covalent Crystals, Phys. Rev. Lett. (2003) 91, 015502. https://doi.org/10.1103/PhysRevLett.91.015502.

[42] F. M. Gao, R Xu, K. Liu, Origin of hardness in nitride spinel materials, Phys. Rev. B (2005) 71, 052103. https://doi.org/10.1103/PhysRevB.71.052103.

[43] A. S. Verma, S R Bharadwaj, Electronic and optical properties of zinc blende and complex crystal structured solids, Phys. State Solidi B (2006) 243(15), 4025-4034. https://doi.org/10.1002/pssb.200844072

[44] D. S. Yadav, Electronic and mechanical properties of rare earth monochalcogenides, J. Alloys and Comp. 537 (2012) 250. https://doi.org/10.1016/j.jallcom.2012.05.016D. S. Yadav, D. V. Singh, Phys. Scr. 85 (2012) 015701.

[45] D. S. Yadav, D. V. Singh, Static and dynamical properties of II–VI and III–V group binary solids, Phys. Scr. (2012) 85, 015701. DOI 10.1088/0031-8949/85/01/015701.

[46] H. Neumann, Kristall imcl Tcchnik. (1980) 15, 849.

[47] S. Tariq, A. Ahmed, S. Saad, S. Tariq, Structural, electronic and elastic properties of the cubic CaTiO3 under pressure: A DFT study, AIP Advances (2015) 5, 077111. https://doi.org/10.1063/1.4926437.

[48] Md. L. Ali, Md. A Rahaman, Variation of the Physical Properties of Four Transition Metal Oxides SrTMO3 (TM = Rh, Ti, Mo, Zr) Under Pressure: An Ab Initio Study J. Adv. Phys. (2017) 6(2), 197. https://doi.org/10.1166/jap.2017.1329.

[49] R. Terki, H. Feraoun, G. Bertrand, H. Aourag, Full potential calculation of structural, elastic and electronic properties of BaZrO3 and SrZrO3, Phys. Status Solidi B (2005) 242(5), 1054-1062. DOI: 10.1002/pssb.200402142.

[50] L. Bornstein, T. Mitsui, S. Nomura, Crystal and Solid State Physics, vol. 16, Springer-Verlag, Berlin (1982).

[51] R. D. King-Smith, D. Vanderbilt, First-principles investigation of ferroelectricity in perovskite compounds, Phys. Rev. B (1994) 49, 5828. https://doi.org/10.1103/PhysRevB.49.5828.

[52] Khursheed Parrey, Nisha Devi, Rabah Khenata, Shakeel Ahmad, Shakeel Ahmad Khandy, Investigating structure, magneto-electronic, elastic and thermoelectric properties of alkaline earth actinide perovskite oxide (BaBkO3) from first principle calculations, Comp. Cond. Matter (2018) 16, 00340. DOI: 10.1016/j.cocom.2018.e00340.

[53] M. Kamruzzaman, M. A. Helal, I. E. Ara, A. K. M. Farid Ul Islam & M. M. Rahaman, A comparative study based on the first principles calculations of ATiO3 (A = Ba, Ca, Pb and Sr) perovskite structure, Ind. J. Phys. 90 (2016) 1105. https://doi.org/10.1007/s12648-016-0848-3.

[54] Shaheen Akhtar, Syed Muahmmad Alay-e-Abbas, Javaria Batool, Waqas Zulfiqar, Amel Laref, Ghulam Abbas, Nasir Amin, Investigation of structural, electronic and optical properties of (V+P) -doped $BaZrO_3$ for photocatalytic applications using density functional theory, J. Phys. Chem. Solids (2020) 147, 109662. https://doi.org/10.1016/j.jpcs.2020.109662.

[55] M. P. Moret, M. A. C. Devillers, K. Worhoff, P. K. Larsen, Optical properties of PbTiO3, PbZrxTi1-xO3, and PbZrO3 films deposited by metalorganic chemical vapor on SrTiO3, J. Appl. Phys. (2002) 92, 468. https://doi.org/10.1063/1.1486048.

[56] J. D. Axe, Apparent Ionic Charges and Vibrational Eigenmodes of BaTiO3 and Other Perovskites, Phys. Rev. 157 (1967) 429. https://doi.org/10.1103/PhysRev.157.429.

[57] J. Sun, X. F. Zhou, Y. X. Fan, J. Chen, H. T. Wang, First-principles study of electronic structure and optical properties of heterodiamond BC2, Phys. Rev. B (2006) 73, 045108. https://doi.org/10.1103/PhysRevB.73.045108.

[58] S. Tinte and M. G. Stachiotti, Applications of the generalized gradient approximation to ferroelectric perovskites, Phys. Rev. B (1998) 58, 11959. https://doi.org/10.1103/PhysRevB.58.11959.

[59] Bin Liu, Yuchen Liu, Changhua Zhu, Huimin Xiang, Hongfei Chen, Luchao Sun, Yanfeng Gao, Yanchun Zhou, Advances on strategies for searching for next generation thermal barrier coating materials, J. Mat. Sci. Technol. 35 (2019) 35(5) 833. https://doi.org/10.1016/j.jmst.2018.11.016.

[60] Mehwish K. Butt, Muhammad Yaseen, Ijaz A. Bhatti, Javed Iqbal, Misbah, Adil Murtaza, Munawar Iqbal, Murefah mana AL-Anazy, M. H. Alhossainy, A. Laref, A DFT study of structural, magnetic, elastic and optoelectronic properties of lanthanide based XAlO3 (X=Nd, Gd) compounds, J. Mater. Res. Technol. (2020) 9(6) 16488. https://doi.org/10.1016/j.jmrt.2020.11.055.

[61] G. Murtaza, Iftikhar Ahmad, B. Amin, A. Afaq, M. Maqbool, J. Maqssod, I. Khan, M. Zahid, Investigation of structural and optoelectronic properties of $BaThO_3$, Optical Materials (2011) 33 553. doi: 10.1016/j.optmat.2010.10.052.

[62] J. A. Souza, J. P. Rino, A molecular dynamics study of structural and dynamical correlations of CaTiO3Acta Materialia (2011) 59(4) 1409-1423. https://doi.org/10.1016/j.actamat.2010.11.003.

[63] B. Ghebouli, M. A. Ghebouli, T. Chihi, M. Fatmi, S. Boucetta, M. Reffas, First-principles study of structural, elastic, electronic and optical properties of SrMO3 (M=Ti and Sn), Solid State Comm. (2009) 149, 2249. https://doi.org/10.1016/j.ssc.2009.09.001.

[64] F. Hou, Ab initio calculations of elastic modulus and electronic structures of cubic $CaZrO_3$, Physica B (2008) 403(17) 2624-2628. https://doi.org/10.1016/j.physb.2008.01.025.

[65] A. P. Shakya., Electronic structure and elastic properties of ATiO3 (A= Ba, Sr, Ca) perovskites: A first principles study, Ind. J. Pure & Appl. Phys. (2015) 23(2) 102-109.

[66] Z. Feng, H. Hu, S. Cui, C. Bai, First-principles study of optical properties of $SrZrO_3$ in cubic phase, Solid State Comm. 148 (2008) 148(9), 472. DOI: 10.1016/j.ssc.2008.08.030.

[67] E. Mete, R. Shaltaf, S. Ellialtoglu, Electronic and structural properties of a 4d perovskite: Cubic phase of SrZrO3, Phys. Rev. B (2003) 68, 035119. https://doi.org/10.1103/PhysRevB.68.035119.

[68] D. de Ligny, P. Richet, High-temperature heat capacity and thermal expansion of $SrTiO_3$ and $SrZrO_3$ perovskites, Phys. Rev. B (1996) 53, 3013. https://doi.org/10.1103/PhysRevB.53.3013.

[69] Djellal Cherrad, D. Maouche, Mounir Reffas, Mounir Reffas. A Benamrani, Structural, elastic, electronic and optical properties of the cubic perovskites CaXO 3 (X = Hf and Sn), Solid State Comm. (2010) 150, 350. DOI: 10.1016/j.ssc.2009.11.048.

[70] A Lamichhane and N. M. Ravindra, Energy Gap-Refractive Index Relations in Perovskites, Materials (2020) 13(8), 1917. DOI: 10.3390/ma13081917.

[71] Q. Mahmood, Bakhtiar Ul Haq, M. Yaseen, Shahid M. Ramay, Muhammad Gul Bahar Ashiq, Asif Mahmood, The first-principle study of mechanical, optical and thermoelectric properties of SnZrO3 and SnHfO3 for renewable energy applicationsSolid State Comm. (2019) 292, 17-23. https://doi.org/10.1016/j.ssc.2019.01.011.

[72] D. R. Penn, Wave-Number-Dependent Dielectric Function of Semiconductors, Phys. Rev. (1962) 128, 2093. https://doi.org/10.1103/PhysRev.128.2093

[73] D. S. Chemla, Dielectric Theory of Tetrahedral Solids: Application to Ternary Compounds with Chalcopyrite Structure, Phys. Rev. Lett. (1971) 26, 1441. https://doi.org/10.1103/PhysRevLett.26.1441