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Simplistic model for the investigation of mechanical stability parameters of pyrochlore structured solids

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Abstract. Herein, we present a simplistic theoretical model for the calculation of bulk modulus, shear modulus and Young's modulus. These parameters indicates that investigated materials show stability or instability in nature. A stable material may be used in many applications like thermoelectric, photovoltaic, etc. In this paper, we have found all the materials have good stability. We have proposed a simple relation with plasmon oscillation theory. The calculated values are in better agreement with their experimental and reported values, and even for many pyrochlore compounds, these are revealed for the first time, and have great potential for technological applications of thermal barrier coatings (TBC) in aerospace, construction, nuclear reactors, and supercritical boiler industries.

Keywords: bulk modulus; shear modulus; Young's modulus; rare earth pyrochlores

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Introduction

During the last few years, increasing attention has been given to the theoretical study of physical, chemical and elastic properties of cubic phase $A_2^{+3}B_2^{+4}O_7$ pyrochlore oxide solids because of their important role in thermal barrier coatings (TBC) for gas turbine energies, superconductivity, fast ion conductors, catalyst design, dielectrics, nuclear waste encapsulation, high-temperature stability, boiler, thermoelectric and optoelectronic applications. These materials have thermal efficiencies, high melting temperatures, low thermal conductivities and low cost [1-6]. Pyrochlore materials are of great technical importance and have fundamental interest in aerospace, construction, and solid oxide fuel cells [7–10]. The REP (rare earth pyrochlores) has composition $A_2^{+3}B_2^{+4}O_7$, here A and B are metallic cations of the geometry trivalent, tetravalent, or divalent, pentavalent, respectively [11–14]. Pyrochlore complexes (stannate, titanate, zirconate, hafnate) are of face centered cubic (FCC) structure with a generic formula $A_2^{+3}B_2^{+4}O_7$. This system has unit cell with space group Fd-3m/227 and eight formula units (Z=8) with 88 ions; among them 16 A^{+3}cations, 16B^{+4}cations and 56 O^{-2}anions [15]. In this geometry, Ti^{+4} cations occupy the 16c (0, 0, 0) position, the A^{+3} cations are at the Wyckoff positions 16d (1/2, 12, 1/2), and O^{-2}anions reside at the 8b (3/8, 3/8, 3/8) and 48f (x, 1/8, 1/8) positions. In the conformation of pyrochlore $A_2^{+3}B_2^{+4}O_7$, A-site cations (atomic radius of ~100 pm) are coordinated with six 48f O^{-2} and two 8b O^{-2}; whereas B cations (atomic radius of 60.5 pm) are coordinated with six 48f O^{-2} anions. In the stereotype of pyrochlore structure

(x= 0.3125); The B and A atoms are coordinated by typical octahedra and skewed cubes, respectively. The B-site polyhedral deformed into a trigonal antiprism (when *x* rose to 0.375) and the rare earth A-site polyhedral changed to regular cubes. The stable structure pyrochlore is obtained when $1.46 \leq r_A/r_B \geq 1.78$ ($r_A$and r_B denote the radii of A^{+3} and B^{+4}cations, respectively) [15]; while the fluorite structure is stable when $r_A/r_B < 1.46$.

The rare earth stannate were synthesized using the solid state methods by Kennedy et al. [16]. They ascertained structural parameters and found $x48fO^{-2}$ decreases monotonically with increasing lattice parameters. In further course of time Liu et al. studied structural stability, theoretical elastic stiffness, and thermal conductivity of $La_2T_2O_7$(T = Ge, Ti, Sn, Zr, and Hf) [17]. They showed that comparatively weak bonds of La-O in $La_2T_2O_7$ contribute a predominant role in assessing the thermal, mechanical properties; and structural stability. Later, Chernyshev et al. [18] have used ab-initio calculations to study the elastic properties of rare earth titanate. Kushwaha [19] has studied the thermodynamic, vibrational and mechanical properties of $RE_2Ti_2O_7$ (RE = Sm, Gd, Dy, Ho, Er, Yb) pyrochlores using suggested eight parameter bond-bending force constant model. Feng et al. [20,21] have performed experimental and theoretical methods for calculating the thermal conductivity, chemical bonding, structural, and mechanical properties of $Ln_2Zn_2O_7$ (Ln = La, Pr, Nd, Sm, Eu, and Gd) by applying the LSDA+U methods and in $RE_2Sn_2O_7$ using DFT (density functional theory) and ultrasonic resonance methods. Again, Liu et al. [22,23] have executed the first principles approach to investigate structural and mechanical properties of rare earth stannate and titanate pyrochlores. Many other researchers [24–27] have evolved various theories to analyze the structural, mechanical, thermal, and chemical properties of ideal REP; such as bond angle, bond length, lattice parameters, elastic moduli, volume expansion coefficient, and linear thermal expansion coefficient (TEC). Due to hardships fetched by experimental processes and their high cost, as well as intricacies in obtaining accurate values of the above discussed parameters; researchers have moved to calculate these parameters by theoretical methods using a series of approximations, but such a method has always been complex [17,27]. In past years, many theoretical calculations based on empirical relationships have become the crucial part of the material research. Mostly, empirical formula has been found to be simple, easy to use and provide better results for physical parameters. Consequently, empirical formulae have accepted as the methods of choice for computational solid state researches.

In earlier researches, authors used the plasmon oscillation theory of solids to successfully develop empirical relationships for electronic, structural, and mechanical properties of zinc blende and rock salt structured solids and ternary chalcopyrite semiconductors [28–30]. These results validate the relevance plasmon oscillation theory, as it determines various characteristics of quantum aspects; until now this has remained closer to accuracy. Plasmon energy relies on the quantity of valance electrons, which varies as a metal form a compound. Empirical correlations sometimes don't produce incredibly exact findings for each unique substance; though, they may still be helpful, nevertheless, the plasmon energy dependent elastic properties of REP have been investigated. Thus, noticing the accuracy in previous researches provided by plasmon oscillations theory [31–33]; this study is focused to offer a different and more accurate explanation for the shear modulus (*G*), bulk modulus (*B*), and Young's moduli (*E*) of ternary compounds with cubic pyrochlore structure. As far as, it is acknowledged, besides a few earlier studies on this phenomenon, there have not been any studies on the impact of conduction *d*-electrons in REP (effect of conduction *d*-electrons) [6,34]. Whether, this occurrence is common among rare-earth pyrochlores is a crucial question. Hence, *d*-electrons effect persists in REP. In this respect, results of this investigation will have a favourable impact on further studies of physical and chemical properties; as well as promotes the applications REP in many diverse fields of material research.

The objectives of this study were to estimate the elastic properties of REP $A_2^{+3}B_2^{+4}O_7 (A = La \rightarrow Lu \text{ and } Y;\text{ and } B = Sn, Ti, Zr, Hf)$ applying the valance electron plasmon oscillation theory of solids.

Scientific backgrounds and results and discussion

The tendency of material to deform elastically when a deforming force is applied is described by elastic characteristics including bulk, shear, and Young's moduli; which are employed as measures of a material's mechanical strength. Kamran et al. suggested a semi-empirical formula of shear modulus based on ionicity fraction of bonding for diamond like and zinc-blende covalent crystals [35]. Li et al. [36] have proposed that the bond ionicity of compounds, and electronegativity of atoms A and B can be used to express the shear modulus (G) of zinc-blende structured solids as given below:

$$G = K_1(\chi_A\chi_B)^{K_2}(1 - f_i)^{K_3}, \quad (1)$$

where K_1, K_2, and K_3 are constants.

Cohen [37,38] has arrived at equations for bulk and shear moduli as the second order partial differential equation of total energy E with respect to some suitable deformation parameter at the equilibrium state:

$$G = \frac{1}{\Omega}\frac{\partial^2 E}{\partial \delta^2}\Big|_{\delta=\delta_\circ}, \quad (2)$$

$$B = \Omega\frac{\partial^2 E}{\partial \Omega^2}\Big|_{\Omega=\Omega_\circ}, \quad (3)$$

where δ and Ω are dimensionless parameters and volume, respectively. Thus, in order to create the equations for the bulk and shear moduli, it is evident that the energy derivatives must first be estimated in terms of the chemical bonding parameters.

Forst and Ashby [39] have suggested the empirical equations for Young's modulus (E) and shear modulus (G) in order to establish correlations among the elastic properties of polycrystalline solids and their melting temperature T_m.

$$E = 100\, K_B T_m/\Omega, \quad (4)$$

$$G = 44\, K_B T_m/\Omega, \quad (5)$$

where K_B is Botzmann's constant, T_m is melting temperature of compound and Ω is volume of unit cell.

They have improved their correlation (5) on shear modulus by analyzing the variation in numerical coefficient. These coefficients were determined based on the crystal structure and chemical bonding of the material class. This coefficient was constant for every category of material and varied from 20 to 95 for alkali metals to basic oxides with the crystal structure α-A_2O_3 (corundum). Applying this notion, concept of iso-mechanical group was developed by them. When combined with the suitable empirical normalization, this group of materials exhibits that mechanical and transport properties are quite comparable or identical.

Verma et al. [40,41] have proposed the following empirical relationships of lattice thermal conductivity K and bulk modulus B for ternary tetrahedral semiconductors as the function of the bond length and product of ionic charges.

$$K = T_m(Z_A Z_B Z_C)^{0.845} d^{-5}, \quad (6)$$

$$B = (Z_A Z_B Z_C)^S V d^{-5}, \quad (7)$$

where V and S are constants for chalcopyrite solids and depends upon crystal lattice, T_m-melting temperature, and Z_A, Z_B, Z_C are the ionic charges on the A, B and C elements.

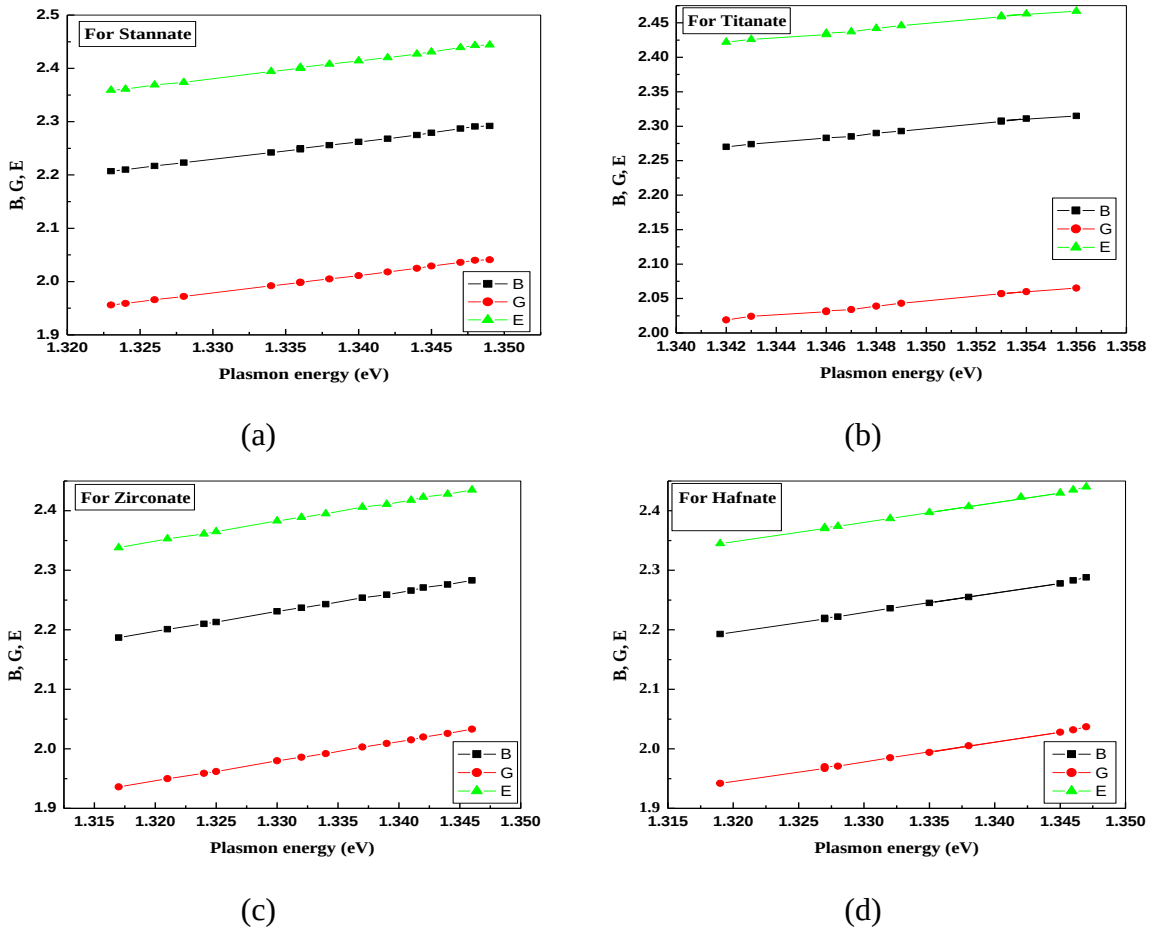

Fig. 1. Plot of elastic constants (B, G, E) versus plasmon energy on log-log scale for rare earth pyrochlores for stannate (a), titanate (b), zirconate (c), and hafnate (d)

Ionic charge is modified when a metal makes a compound because it depends on the amount of valance electrons and the plasmon energy therein. Here, the calculated results are reported in Fig. 1. The results show that bulk modulus (*B*), shear modulus (*G*), and Young's modulus (*E*) illustrate a linear relationships; lie on a straight line; and increasing trend when draw on a log-log scale against the plasmon energy of the compounds. Many authors have found that drastically lowered plasmon energy can be used to get better agreement with experimental values of electronic, mechanical, static and dynamic characteristics of binary solids, ternary chalcopyrite semiconductors, and rare earth mono-chalcogenides [40–42]. Now, we may extend relationships (1)-(5) as the function of plasmon energy with minor modifications for cubic structured rare earth pyrochlores, and consequently we get the better agreement between experimental and theoretical data.

$$\mathrm{B} = \zeta\left(\hbar\omega_{\mathrm{p}}\right)^{\mu}, \tag{8}$$

$$\mathrm{G} = \kappa\left(\hbar\omega_{\mathrm{p}}\right)^{\eta}, \tag{9}$$

$$\mathrm{E} = \varsigma\left(\hbar\omega_{\mathrm{p}}\right)^{\eta}, \tag{10}$$

where $\zeta, \kappa, \varsigma, \mu, and\ \eta$ are constants varies with the group of materials. The constants ζ, κ, ς have values 0.006254, 0.00335 and 0.004247 GPa/ eV, respectively. The exponents $\mu\ and\ \eta$ have values 3.35 and 3.344, respectively. The plasmon energy $\left(\hbar\omega_{\mathrm{p}}\right)$ of these compounds was estimated elsewhere [42].

Table 1. Calculated values of bulk, shear and Young's moduli of tin based rare earth pyrochlores with the available theoretical and experimental data

$A_2B_2O_7$	$\hbar\omega_p$ (eV)	Bulk modulus *B*, GPa			Shear modulus *G*, GPa			Young modulus *E*, GPa		
		Cal. Eq. (9)	Theo.	Expt.	Cal. Eq. (10)	Theo.	Expt.	Cal. Eq. (11)	Theo.	Expt.
$La_2Sn_2O_7$	21.05	161.06	155.75[a], 182.30[a] 190.00[q]	188.90[d]	90.37	95.00[q]		228.40	245.00[q]	
$Ce_2Sn_2O_7$	21.09	162.08	160.81[a]		90.95			229.86		
$Pr_2Sn_2O_7$	21.20	164.92	158.51[a]		92.55			233.89		
$Nd_2Sn_2O_7$	21.28	167.00	162.73[a], 187.4[a]	199.2[d]	93.72			236.86		
$Sm_2Sn_2O_7$	21.57	174.71	163.24[a], 187.50[a]	193.77[d]	98.07			247.84		
$Eu_2Sn_2O_7$	21.66	177.15	128.18[a]		99.45			251.32		
$Gd_2Sn_2O_7$	21.68	177.70	166.37[a], 176.60[a]	192.77[d]	99.75	89.00[r]		252.10	226.00[r]	
$Tb_2Sn_2O_7$	21.77	180.17	167.99[a]		101.15			255.62		
$Dy_2Sn_2O_7$	21.86	182.66	168.36[a]		102.56			259.17		
$Ho_2Sn_2O_7$	21.96	185.46	169.46[a]		104.14			263.16		
$Er_2Sn_2O_7$	22.07	188.58	170.36[a], 188.7[a]	193.50[d]	105.89			267.60		
$Tm_2Sn_2O_7$	22.13	190.29	170.69[a]		106.86			270.04		
$Yb_2Sn_2O_7$	22.24	193.46	127.69[a], 172.63[a]	192.23[d]	108.65			274.56		
$Lu_2Sn_2O_7$	22.30	195.21	176.07[a]		109.64			277.05		
$Y_2Sn_2O_7$	22.32	195.79			109.97			277.88		
$La_2Ti_2O_7$	21.980	186.03	176.72[b], 199[t]		104.45	99.00[t]		263.97	253.00[t]	
$Sm_2Ti_2O_7$	22.051	188.04	184.29[b], 206.00[h]		105.59	108.00[h]		266.83	277.00[h]	
$Eu_2Ti_2O_7$	22.161	191.73	140.60[b]		107.36			271.31		
$Gd_2Ti_2O_7$	22.180	191.73	186.91[b], 186.00[c], 206.00[e] 200.00[h]		107.67	107.00[h]		272.09	272.00[h]	
$Tb_2Ti_2O_7$	22.212	192.65	187.87[b], 207.00[e]	199±1[g] 204.00[f]	108.19			273.41		
$Dy_2Ti_2O_7$	22.293	195.00	188.91[b], 208.00[e], 194.00[h]	197.00[f]	109.52	105.00[h]		276.76	267.00[h]	
$Ho_2Ti_2O_7$	22.346	196.55	189.83[b], 209.00[e]	213±2[g] 200.00[f]	110.40	104[h]		278.97	264.00[h]	
$Er_2Ti_2O_7$	22.556	202.78	191.0[b], 209.00[e]		113.91	101.00[h]		287.84	256.00[h]	
$Tm_2Ti_2O_7$	22.615	204.55	190.69[b], 210.00[e]		114.91			290.37		
$Yb_2Ti_2O_7$	22.568	203.14	210.00[e], 178.00[h]		114.11	97.00[h]		288.36	246.00[h]	
$Lu_2Ti_2O_7$	22.683	206.61	191.89[b], 211.00[e]	181.00[f]	116.07			293.30		

[a]Ref. [23], [b]Ref. [22], [c]Ref. [45], [d]Ref. [20], [e]Ref. [18], [f]Ref. [45], [g]Ref. [46], [h]Ref. [19], [i]Ref. [21], [j]Ref. [47], [k]Ref. [48], [l]Ref. [49], [m]Ref. [50], [n]Ref. [25], [o]Ref. [24], [p]Ref. [51], [q]Ref. [17], [r]Ref. [52], [s]Ref. [53],[tr]Ref. [54].

The utility of relations (8)-(10) lies in the fact that they just need plasmon energy of the of rare earth pyrochlores as input values instead experimental data. A full explanation of the elastic properties of rare earth stannate, zirconate, titanate and hafnate has been given elsewhere [18–28]. Explicitly, an analogue evolves among the ternary pyrochlores, this may be used to calculate the elastic properties from their plasmon energy$\left(\hbar\omega_p\right)$. Equations (8)-(10) are the

expression of elastic properties for cubic structured rare earth pyrochlores. In this paper we employ equations (8)-(10) to study the elastic properties of pyrochlores depend upon plasmon energy of the material and presented in Tables 1 and 2. For comparison purposes theoretical and experimental values by earlier researchers are presented in this table. From this table it is evident that calculated values of elastic properties are in good conformity with experimental values as compared to others theoretical findings. From the table it is also clear that experimental and theoretical data is not available for most of the compounds; and the elastic constants values for these pyrochlores are calculated first time in this work. So, these values will be helpful in determining other characteristic values, which find technological applications especially in the TBC industry.

Table 2. Calculated values of bulk, shear and Young's moduli of zirconium based rare earth pyrochlores with the available theoretical and experimental data

$A_2B_2O_7$	$\hbar\omega_p$, eV	Bulk modulus *B*, GPa			Shear modulus *G*, GPa			Young's modulus *E*, GPa		
		Cal. Eq. (9)	Theo.	Expt.	Cal. Eq. (10)	Theo.	Expt.	Cal. Eq. (11)	Theo.	Expt.
$La_2Zr_2O_7$	20.758	153.73	176.00[i] 192.00[m] 200.00[n] 179.00[o] 191.00[p] 179.00[q]	175.00[j]	86.24	87[i] 107[m] 73[n] 83[o] 106[p] 93[q]	92[j]	217.97	208[i] 271[m] 195[n] 214[o] 268[p] 237[q]	186[j] 175[r] 239[*]
$Ce_2Zr_2O_7$	20.964	158.88			89.14			225.29		
$Pr_2Zr_2O_7$	21.088	162.03	155.00[i]	149.00[k]	90.92	103.00[i]	100.00[k]	229.78	224.00[i]	215.00[k]
$Nd_2Zr_2O_7$	21.135	163.24	164.00[r] 127.00[i]	131.00[l]	91.60	88.00[r] 60.00[i]	86.00[s]	231.50	224.00[r] 213.00[i]	219.00[s]
$Sm_2Zr_2O_7$	21.402	170.21	167.00[r] 197.00[i]	181.00[k]	95.53	89.00[r] 100.00[i]	96.00[k] 90.00[s]	241.44	226.00[r] 252.00[i]	231.00[s]
$Eu_2Zr_2O_7$	21.491	172.59	149.00[i]	140.00[k]	96.87	67.00[i]	72.00[k]	244.82	243.00[i]	229.00[k]
$Gd_2Zr_2O_7$	21.583	175.06	165.00[i]	156.00[s] 175.00[t] 158.00[l]	98.27	88.00[r] 63.00[i]	89.00[t] 80.00[s] 66.00[l]	248.34	224.00[r] 214.00[i]	238.00[t] 205.00[s]
$Tb_2Zr_2O_7$	21.743	179.42			100.73			254.56		
$Dy_2Zr_2O_7$	21.825	181.69			102.01			257.79		
$Ho_2Zr_2O_7$	21.922	184.39			103.53			261.64		
$Er_2Zr_2O_7$	21.998	186.53			104.74			264.69		
$Tm_2Zr_2O_7$	22.084	188.98			106.12			268.17		
$Yb_2Zr_2O_7$	22.187	191.93			107.79			272.38		
$La_2Hf_2O_7$	20.848	155.96	180.00[q]		87.50	88.00[q]		221.15	228.00[q]	
$Ce_2Hf_2O_7$	21.210	165.18			92.69			234.26		
$Pr_2Hf_2O_7$	21.246	166.11			93.22			235.60		
$Nd_2Hf_2O_7$	21.267	166.66			93.53			236.38		
$Sm_2Hf_2O_7$	21.469	172.00			96.54			243.98		
$Eu_2Hf_2O_7$	22.110	189.72			106.54			269.23		
$Gd_2Hf_2O_7$	21.610	175.79	170.00[r]		98.68	96.00[r]		249.38	242.00[r]	
$Tb_2Hf_2O_7$	21.765	180.03			101.07			255.42		
$Dy_2Hf_2O_7$	21.891	183.53			103.04			260.41		
$Ho_2Hf_2O_7$	21.998	186.53			104.74			264.69		
$Er_2Hf_2O_7$	22.094	189.26			106.28			268.58		
$Tm_2Hf_2O_7$	22.183	191.81			107.72			272.22		
$Yb_2Hf_2O_7$	22.254	193.87			108.88			275.14		

[a]Ref. [23], [b]Ref. [22], [c]Ref. [45], [d]Ref. [20], [e]Ref. [18], [f]Ref. [45], [g]Ref. [46], [h]Ref. [19], [i]Ref. [21], [j]Ref. [47], [k]Ref. [48], [l]Ref. [49], [m]Ref. [50], [n]Ref. [25], [o]Ref. [24], [p]Ref. [51], [q]Ref. [17], [r]Ref. [52], [s]Ref. [53], [t]Ref. [54].

Concluding remarks

From the discussion in scientific background, it is concluded that plasmon energy of valance electrons in the compound is an important parameter in determining elastic characteristics of rare earth pyrochlores and is a pioneering work. Henceforth, it is found that elastic properties of the materials investigated here present a linear relationship and lie on a straight line when potted on a log-log scale against the plasmon energy. The evaluated values revealed a predictable pattern and agreed with the information provided so far, demonstrating the validity of the proposed approach.

Briefly, a simple model is postulated for the calculation of bulk modulus, shear modulus and Young's modulus of cubic structured rare earth pyrochlores. Furthermore, predictions of this model on elastic properties are reasonably consistent with experimental and theoretical data obtained by using various methodologies. Confidently, this theory will present an important role where experimental data of these elastic properties is not available and to discover new compounds with targeted values of bulk modulus, shear modulus, Young's modulus and Poisson's ratio in a series of a large family of rare earth pyrochlores, which are of utmost technological applications, now-a-days.

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