Effect of Pressure on Structural, Elastic and Electronic Properties of Perovskite PbTiO$_3$

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Abstract

We study the effect of pressure on Structural, elastic and electronic properties of Cubic and Tetragonal Perovskite using density function theory. The equilibrium parameters obtained are in good agreement with the available literature both experimental and theoretical. We found out that there is transition from tetragonal to cubic at a pressure of around 30GPa. Both crystals are stable in the pressure range of this study (0 – 50 GPa), and the stability increases with increasing pressure. The bulk modulus (**B**), Young modulus (**E**) and Shear modulus (**G**) all increase with increasing pressure. The band-gap increases and decrease around (*X-Gamma*) and (*M-Gamma*) for the case of Cubic and decrease for the case of Tetragonal Crystal around (*X-Gamma*), (*Z-Gamma*) and (*Z-X*) which converges at pressure of around 30GPa.

Introduction

Perovskite-type oxides displayed a number of extraordinary chemical, structural and physical properties [1], [2], they are considered to be among the most extensively studied and the most promising materials of twenty first century [3],[4], [6]. This attracted a quite number of researchers in both theoretical and experimental field to study these materials, experimental studies[1], [2], [7], [9]–[13], theoretical studies[4]–[6], [12], [14]–[18] just to mention few.

Perquisites have their way in many of solid state applications [18] with specific area of application includes memory, catalysis, waveguides [17] energy storage LED, photo-detectors[3], piezoelectricity, solar energy applications as well as transducers, multilayered capacitor[4], [7], [9], [19] among others

Generally, any material with a general formula of the form ABO_3 which is known to be calcium titanium oxide structure $CaTiO_3$ is considered to be Perovskite [20]. In this structure, the A-site is an ion which is at the corner of the lattice and usually it is alkaline or rare earth elements (e.g. Be, Ca, Sr, Pb etc.) B-site ions which is on the center of the lattice could be $3d$ to $5d$ transition metals (e.g. Ti, Al, Ni, Cu etc.).

Despite a lot of researches conducted on these materials both theoretically and experimentally, only few worked on the pressure effect on these materials [5], [8], [12] In this work, an effort is made to look into the effect of pressure on equilibrium, structural, elastic and electronic properties of $PbTiO_3$. This work will serve as a plus to the already available literature in the study of Perovskite.

The rest of the report is organized as; methodology where the general methodology will be discussed then followed by result and discussion in which the obtained results this include, the equilibrium and structural parameters, stability condition, elastic properties as well as electronic properties of the materials $PbTiO_3$ will be discussed, this will be followed by conclusion/summary finally.

Method

First-principle density functional theory (DFT) calculations were performed within the Generalized-Gradient-Approximation (GGA) as implemented in Quantum-Espresso package [40], [41] for the optimization and other calculations of the structures, Cubic crystal with space group Pm-3m (221) and Tetragonal Cubic crystal with space group P4mm (99) of $PbTiO_3$. A norm-conserving pseudo-potentials Pb.pw91-dn-rrkjus_psl.1.0.0.UPF, O.pw91-n-rrkjus_psl.1.0.0.UPF and Ti.pw91-spn-rrkjus_psl.1.0.0.UPF [43] were used for Pb, Ti and O respectively where the kinetic energy cut-off was set to $120Ry$ and automatic k-mesh grid of $8 \times 8 \times 8$ for Cubic and Tetragonal $PbTiO_3$ respectively. The kinetic energy cut-off as well as k-mesh were obtained after a convergence with total energy of the parameters with accuracy of $\sim 1mRy$ with respect to total energy and $0.5kbar$ respect to pressure.

The electron band structure calculations were performed through high symmetry points of the crystal along the path $\Gamma(0,0,0)$, $X(0.5,0,0)$, $M(0.5,0.5,0)$, $R(0.5,0,0.5)$ and $\Gamma(0,0,0)$ for Cubic crystal and $\Gamma(0,0,0)$, $X(0.5,0,0)$, $M(0.5,0.5,0)$, $Z(0,0,0.5)$, $R(0.5,0,0.5)$, $A(0.5,0.5,0.5)$ and $\Gamma(0,0,0)$ for the calculation of the density of the state (DOS) a denser grid of $32 \times 32 \times 32$ were used.

Result and Discussion

Convergence

The convergence of total energy with respect kinetic energy cut-off and k-mesh was shown in figure 1. The total energy and pressure accuracy are within the values of $1mRy$ and $0.5kbar$ for energy and pressure respectively.
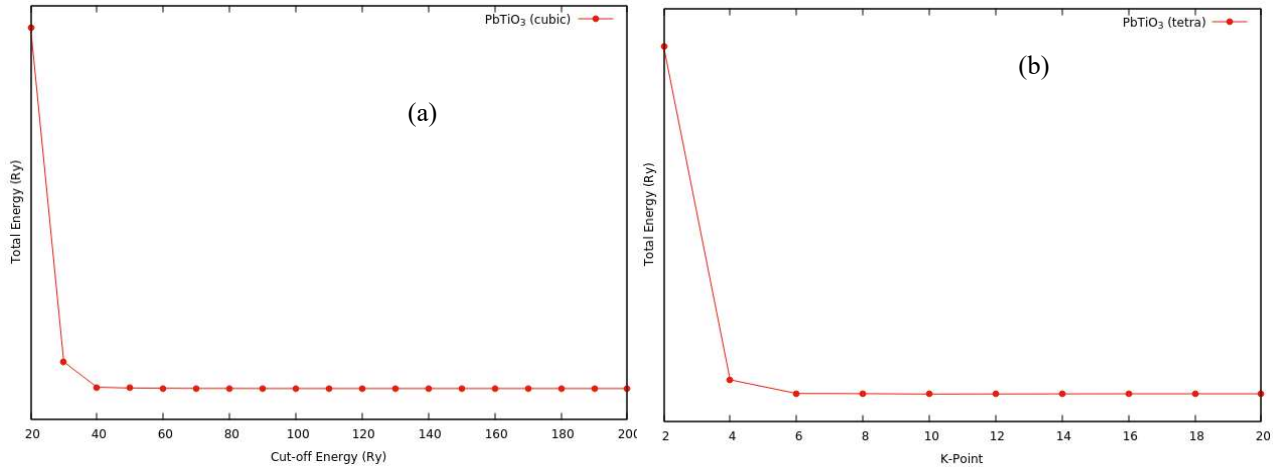
Figure 1: Convergence of (a) Kinetic energy cut-off and (b) K-point mesh with respect to total energy

It is good to mention that, the figures shown is the general convergence for both cubic and tetragonal cubic PTO, and this is because both the crystal show same behavior in the convergence parameters.

Equilibrium Parameters

The equilibrium parameters were obtained after a full relaxation of the two structures of $PbTiO_3$ Perovskite. The structural were relax till the forces on each atom is zero. The change in volume of the two crystals, cubic and tetragonal, were determine with respect to total energy of each system. Figure 2 shows the total energy as function of volume for $PbTiO_3$ both Cubic and Tetragonal crystal.
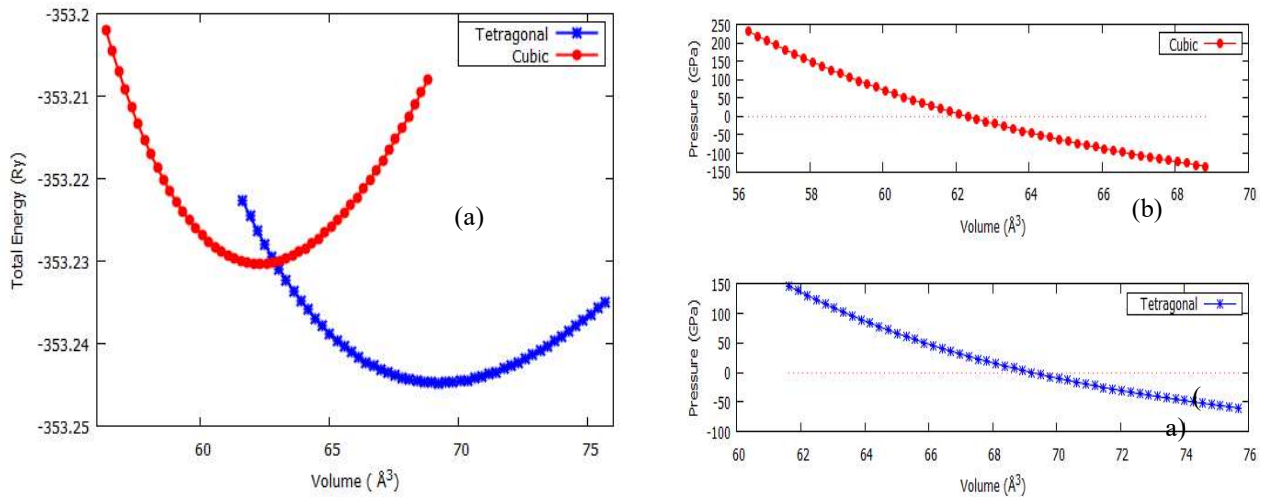

Figure 2: (a) Total energy as function of volume (b) Pressure as function of volume for Tetragonal and Cubic $PbTiO_3$
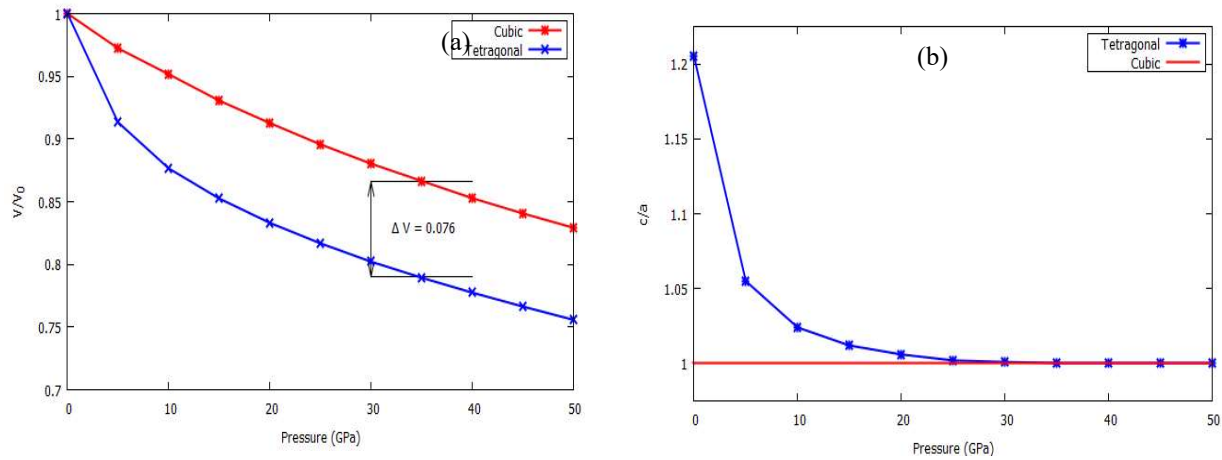
Figure 3:(a) Ratio V/V_0 for Cubic and Tetragonal PTO (b) Ratio c/a with Pressure for Cubic and Tetragonal $PbTiO_3$

The figure suggested that, Tetragonal PTO is more stable than the Cubic this is in agreement with work of [21] among others.

Structural Parameters

The volume change with respect to total energy of the two crystals were fitted into Murnaghan equation of the state[22], [23]where the lattice parameters, bulk modulus and its derivative as well as volume of the two crystal at equilibrium were determine, these parameters were presented in table 1.

$$E(V) = \frac{B_0 V}{B'_0(B'_0-1)}\left[B'_0\left(1-\frac{V_0}{V}\right)+\left(\frac{V_0}{V}\right)^{B'_0}-1\right]+Constant \quad (1)$$

Table 1: The equilibrium parameters for Cubic and Tetragonal $PbTiO_3$, lattice parameters a, b, c, the bulk modulus $\boldsymbol{B}_o$, the derivative of bulk modulus B' and equilibrium volume V_o

Parameters		PbTiO₃ (Cubic)	Reference	PbTiO₃ (Tetragonal)	Reference
Lattice	$a(\mathring{A})$	3.965	3.962[a], 3.960[b], 3.983[c], 3.887[e], 3.980[f] 3.883[g]	3.843	3.904[e] 3.79[j] 3.87[k] 3.81[n] 3.888[e] 3.805[o]
	$b(\mathring{A})$	3.965		3.843	3.904[e] 3.79[j] 3.87[k] 3.81[n] 3.888[e] 3.805[o]
	$c(\mathring{A})$	3.965		4.631	4.158[e] 3.85[j] 4.07[k] 4.686[n] 4.157[e] 4.361[o]
$\boldsymbol{B}_o$ (GPa)		174.30	200.56[a], 217.00[b] 229.00[h], 229.00[e] 235[j]		61[k] 35[b] 104[m] 60[i] 160[j] 50.22[o] 74[e]
B'		5.21		6.03	4.24[o]
$V_0(\mathring{A})^3$			62.193[a] 62.099[b]		67.89[p] 63.373[e]

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	62.32	63.187[c] 62.571[d] 58.728[e] 63.045[f] 58.547[g]	68.394	55.302[j] 60.956[k] 68.022[n] 62.839[e] 63.139[o]

[a] = Ref. [15] , [e] = Ref. [4] [b] = Ref. [25] [f] = Ref. [27] [j] = Ref. [18]
[c] = Ref. [27] [g] =Ref. [24]

Experimentally, the lattice parameter for the cubic crystal were found to be 3.970 [29] and 3.969 [29], the bulk modulus were determine experimentally to be 144.00 GPa [30]. The lattice parameters for tetragonal crystal were found experimentally to be 3.904$\mathring{A}$ for a and 4.152$\mathring{A}$ for c [31].

Elastic Properties

The calculated elastic constants at equilibrium for cubic and tetragonal PTO is presented in table 2, a comparison was made with theoretical and experimental values. These elastic constants were computed using a method developed recently [32].

Table 2: Equilibrium elastic constant for Cubic and Tetragonal PbTiO$_3$ Crystals

PbTiO$_3$	C$_{11}$ (GPa)	C$_{12}$(GPa)	C$_{13}$ (GPa)	C$_{33}$ (GPa)	C$_{44}$ (GPa)	C$_{66}$ (GPa)
Cubic	279.12	117.78	-	-	97.84	-
Ref Experiment	334.89[a], 342.60[b] 383.70[c], 383.6[h] 344.2[i]	133.99[a],155.20[b] 151.00[c] 151.0[h] 180.8[i]	- -	- -	103.11[a], 109.70[b] 120.30[c] 120.3[h] 103.5[i]	- -
	229[d]	-	-	-	-	-
Tetragonal	187.37	75.5	45.9	33.6	41.58	89.73
Ref	313.1[e] 280.5[g] 288.7[j] 230[k]	110.71[e] 118.5[g] 111.7[j] 96.2[k]	92.4[e] 118.5[g] 77.0[j] 65.2[k]	197[e] 279.7[g] 62.9[j] 41.9[k]	82.72[e] 98.6[g] 33.7[j] 46.6[k]	85.41[e] 98.6[g] 102.6[j] 98.8[k]
Experiment	235[f] 237[l]	101[f] 90[l]	99[f] 70[l]	105[f] 60[l]	65.1[f] 69[l]	104[f] 144[l]

[a] = Ref.[15] [d] = Ref.[30] [g] = Ref.[17] [j] = Ref.[4]
[b] = Ref.[25] [e] = Ref.[35] [h] = Ref.[4] [k] = Ref.[29]
[c] = Ref.[5] [f] = Ref.[33] [I] = Ref.[24] [l] = Ref.[34]

Stability

The stability of a crystal with pressure **P** can be checked using a generalized stability criteria [24]–[25]. For the case of our Tetragonal Perovskite (PbTiO$_3$), there are six independent elastic constants **C$_{ij}$**, thus, the generalized criteria is written as follows (equation 2):

$$C_{11}^P - C_{12}^P > 0 \qquad\qquad (2a)$$
$$C_{11}^P + C_{33}^P - 2C_{13}^P > 0 \qquad\qquad (2b)$$
$$C_{ii}^P > 0, \text{for } i = (1,3,4,6) \qquad\qquad (2c)$$
$$2C_{11}^P + C_{33}^P + 2C_{12}^P + 4C_{13}^P > 0 \qquad\qquad (2d)$$

Where $C_{\delta\delta}^{P} = C_{\delta\delta} - P$, for $(\delta = 1,3,4,6)$, $C_{1j}^{P} = C_{1j} + P$, for $(j = 2,3)$. for the cubic PbTiO$_3$, there are only three independent elastic constants $C_{11} = C_{22} = C_{33}$, $C_{12} = C_{13}$ and $C_{44} = C_{55} = C_{66}$, thus the criteria [38] at a given pressure (P) will reduced to (equation 3):

$$C_{11} + 2C_{12} - P > 0 \qquad (3a)$$
$$C_{44} - P > 0 \qquad (3b)$$
$$C_{11} - C_{12} - 2P > 0 \qquad (3c)$$

At equilibrium, the generalized stability criteria for Tetragonal and Cubic Crystal (PbTiO$_3$) will reduced to Born Stability criteria [39]. Figure 4 shows the stability criteria as function of pressure for the two crystals.
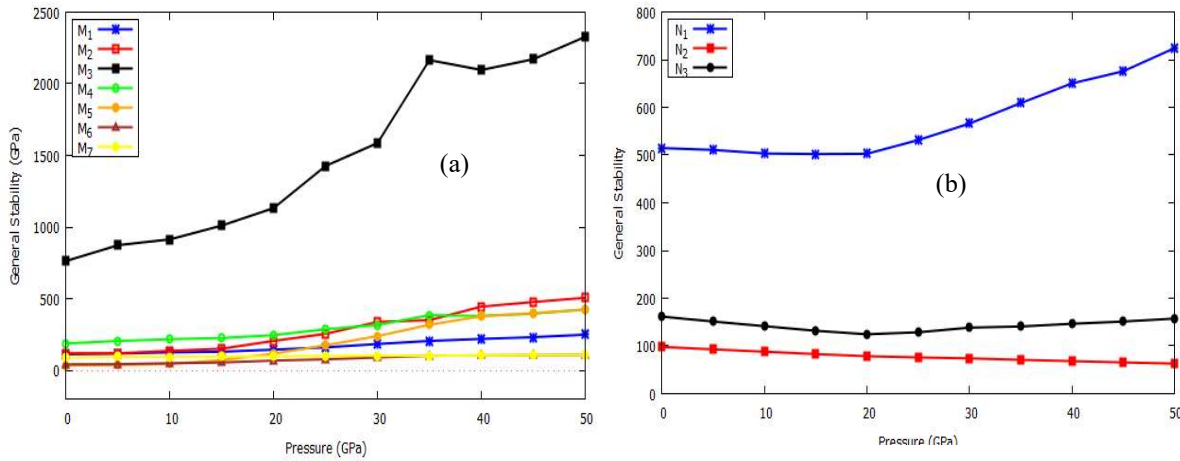

Figure 4: Generalized Stability criteria for (a) Tetragonal and (b) Cubic PbTiO$_3$

$$M_1 = C_{11}^{p} - C_{12}^{p} \qquad N_1 = (C_{11} + 2C_{12} + P)$$
$$M_2 = C_{11}^{p} + C_{33}^{p} - 2C_{13}^{P} \qquad N_2 = C_{44} - P$$
$$M_3 = 2C_{11}^{p} + C_{33}^{p} + 2C_{12}^{P} + 4C_{13} \qquad N_3 = (C_{11} - C_{12} - 2P)$$
$$M_4 \rightarrow M_7 = C_{ii}^{P} \; ; \; i = (1,3,4,6)$$

Mechanical Properties

The mechanic properties of a crystals can be evaluated through crystal moduli [15], Bulk modulus **B**, shear modulus **G** and Young modulus **E**. These moduli directly relates to resistance to deformations (Bulk modulus), shear deformations (Shear modulus) and elasticity (Young modulus). This properties of a material have been calculated through their elastic constants (equation 4). The moduli were computed using Viogt-Reuss-Hill approximations [33], the approximation is as follows in equation (4):

$$B = \frac{1}{2}(G_V + G_R) \qquad (4a)$$
$$G = \frac{1}{2}(B_V + B_R) \qquad (4b)$$
$$E = \frac{9BG}{3B + G} \qquad (4c)$$

Where $B_V = 1/9\,(2C_{11} + C_{33} + 2(C_{12} + C_{13} + C_{31}))$, $B_R = [2S_{11} + S_{33} + 2(S_{12} + S_{13} + S_{31})]^{-1}$ $G_V = 1/15\,[2C_111 + C_{33} - (C_{12} + C_{13} + C_{31}) + 3(2C_{44} + C_{66})]$ and $G_R = 15[4(2S_{11} + S_{33}) - (S_{12} + 2S_{13}) + 3(2S_{44} + S_{66})]^{-1}$.

With Tetragonal crystal having symmetries in the elastic constants C_{ij} and elastic compliance S_{ij} as $A_{11} = A_{22}, A_{44} = A_{55}, A_{12} = A_{23}, A_{12} = A_{21}$ and $A_{31} = A_{32}$, with A_{ij} being components of either elastic or compliance matrix. For the case of cubic crystal, there are only three independent elastic constants with $C_{11} = C_{22} = C_{33}, S_{11} = S_{22} = S_{33} C_{12} = C_{23} = C_{13}, S_{11} = S_{23} = S_{13} C_{44} = C_{55} = C_{66}$ and $S_{44} = S_{55} = S_{66}$.

Thus, the Viogt and Reuss Hill approximations for the Bulk and Shear modulus reduces to; $B_V = 1/3\,(C_{11} + 2C_{12})$, $B_R = [3S_{11} + 6S_{12}]^{-1}$, $G_V = 1/5\,(C_{11} - C_{12} + 3C_{44})$ and $G_R = 5[4S_{11} - S_{12} + 3S_{44}]^{-1}$. The elastic moduli and elastic constants are presented in figure 5.
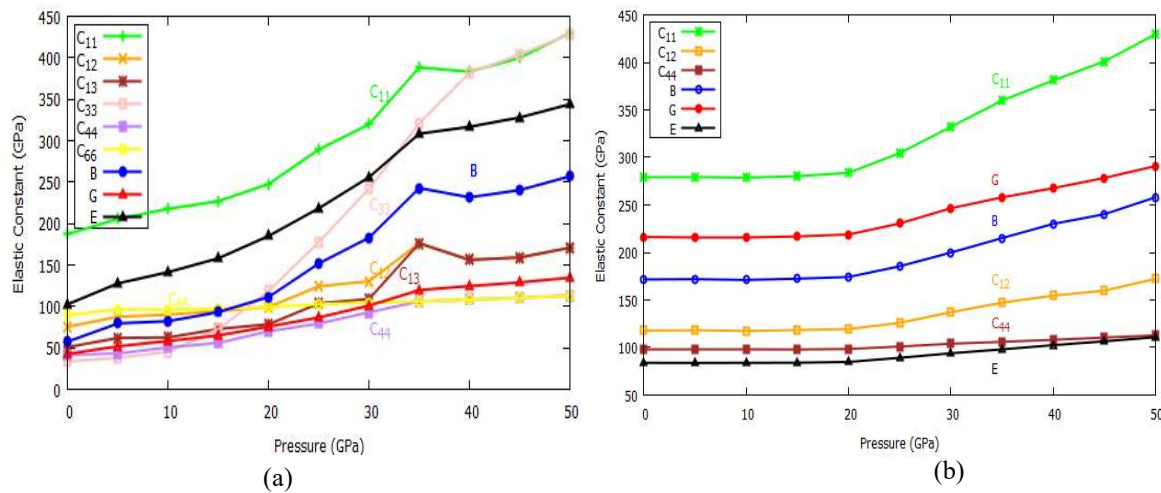

Figure 5: Elastic moduli as function of pressure for (a) Tetragonal and (b) Cubic PbTiO$_3$

The band structures were calculated following the path along high symmetry points, for cubic crystal $\Gamma - X - M - R - \Gamma$ and for Tetragonal through $\Gamma - X - M - Z - R - A - \Gamma$. Table 3 present the band-gaps at most important symmetry points. PTO can be seen to have an indirect band-gap this is in agreement with work of [6],[18] and in disagreement with work of [28] where he report them to be a direct band-gap materials. Table 3 present the band-gaps along some selected high symmetry points in Brillouin zone in compared with other works.
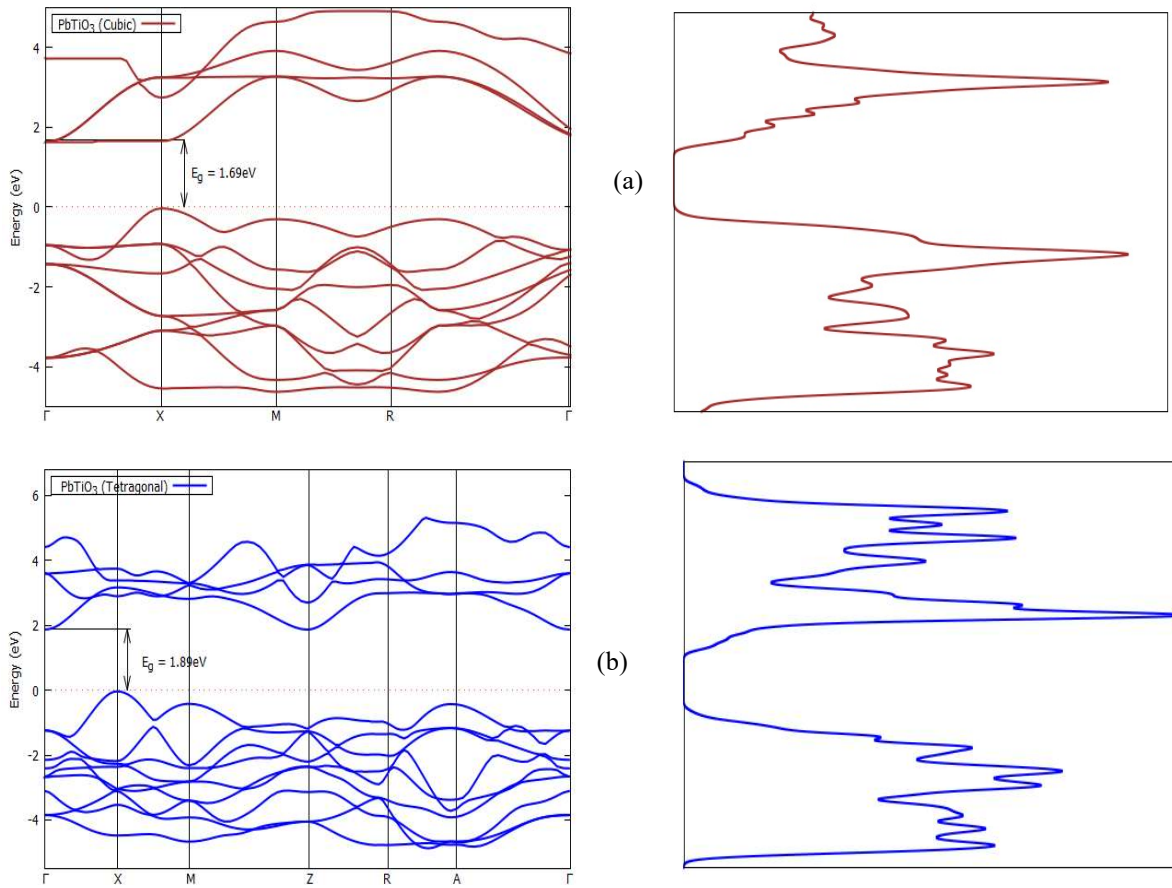
Figure 6: Band structure along high symmetry point in First Brillouin zone at 0 GPa pressure for (a) Cubic and (b) Tetragonal PbTiO$_3$

Table 3: Band-gaps at various symmetries for both Cubic and Tetragonal PbTiO$_3$ crystal at equilibrium

PbTiO$_3$	$X - \Gamma (eV)$	$M - \Gamma (eV)$	$Z - \Gamma (eV)$	$Z - X (eV)$
Cubic	1.65	1.93	-	-
Ref	3.045[d] 3.034[e]			
Tetragonal	1.86	-	3.03	4.06
Ref	1.70[a] 1.632[b] 1.47[c] 3.613[d] 2.21[f]			

[a] = Ref. [19]   [b] = Ref. [18]   [c] = Ref. [40]   [d] = Ref. [6]
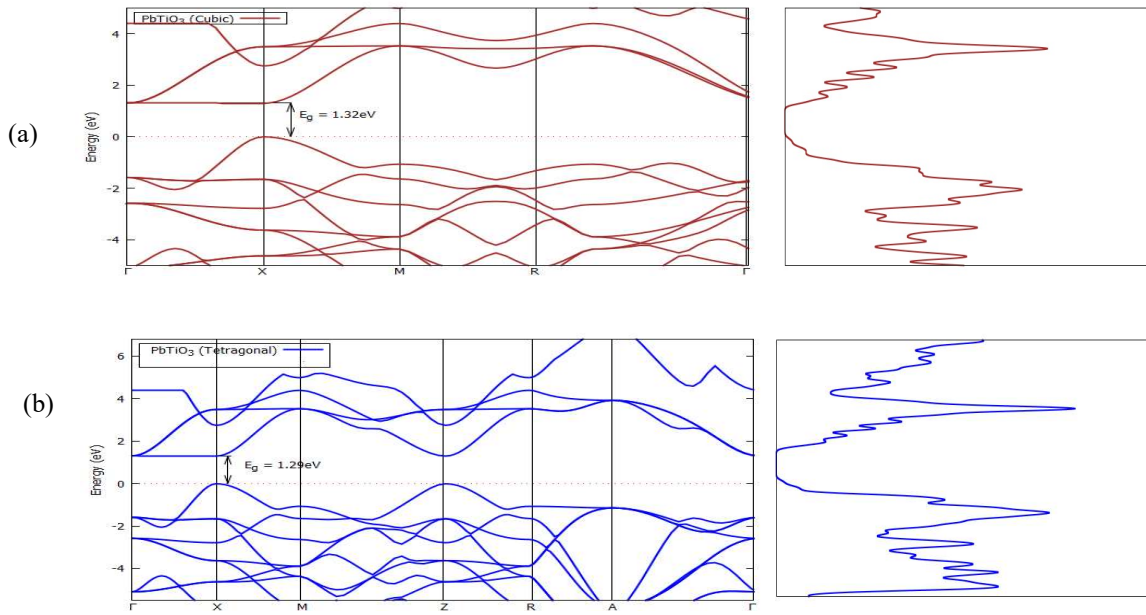[e] = Ref [6]   [f] = Ref. [17]

(a)

(b)

Figure 7: The band-gaps at some selected symmetry points at 50 GPa Pressure for (a) Cubic and (b) Tetragonal PbTiO₃
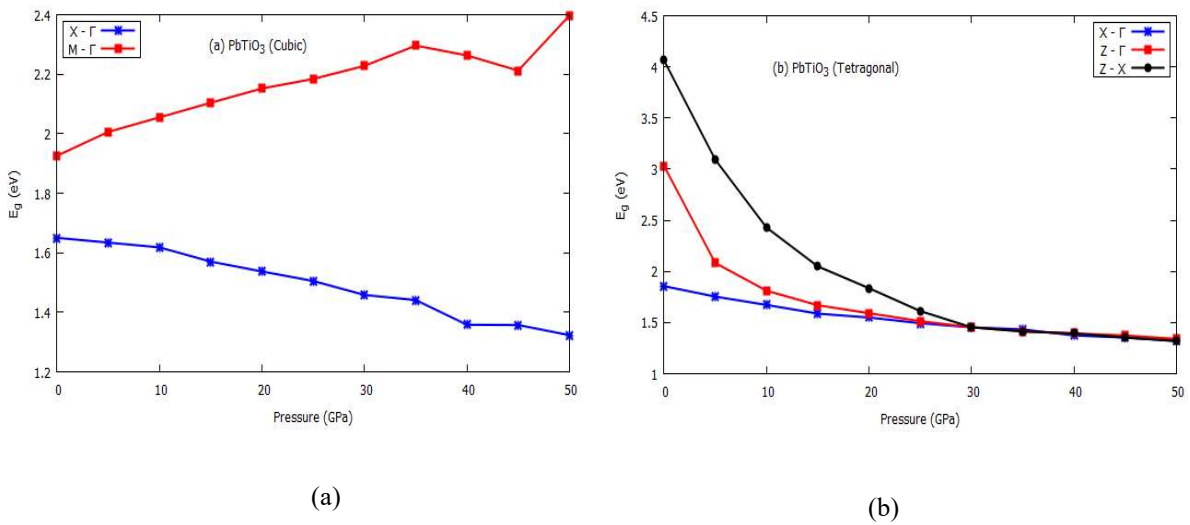
(a)

(b)

Figure 8: The band-gaps at some selected symmetry points (a) Cubic and (b) Tetragonal PbTiO₃

It can be seen from the figure, for the case of cubic PbTiO₃ the band-gap through the symmetry point $M - \Gamma$ increases with increasing pressure, for the point $X - \Gamma$ decreases in increasing pressure. For the case of of the tetragonal PbTiO₃ the gap decrease through all the three high-symmetry points under consideration $(X - \Gamma, \ Z - \Gamma, \text{and } Z - X)$ It is important to note that at a pressure of 30

GPa all these three higher symmetries converge, this corresponds to the transition pressure of the crystal (tetragonal) to cubic.

Conclusion

We present the effect of pressure on structural, elastic and electronic properties of Cubic and Tetragonal $PbTiO_3$ using density function theory as implemented in quantum-espresso package.

We obtained the equilibrium structural parameters which agreed with the available literature, both theoretical and experimental. The stability of the two crystal (Cubic and Tetra) where check. At equilibrium the stability check criteria known as Born Stability criteria was used to check their stability, they were found to all be stable at equilibrium. As the induced pressure increases, the stability was further check with the modified stability criteria, under this condition they were also found to all be stable.

The elastic moduli, Bulk modulus (B), Young modulus (E) and Shear modulus (G) were also determine at equilibrium and they compared well with the available literature. These moduli increase with increasing pressure.

Finally, the electronic bands were plotted for these two materials following a selected high symmetry point.

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