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Impact of stress on the optoelectronic properties of lead-free double perovskite Rb_2TeCl_6: A first-principles investigation

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Abstract. The effect of induced pressure on the physical properties of Rb_2TeCl_6 has been explored in the present work as a reversible material engineering approach. The investigation sheds lights on the potential of designing and optimizing materials with targeted properties for optoelectronic applications using pressure induced. The calculations were performed using density functional theory (DFT). The physical properties were investigated under pressure values between 0 and 40 GPa. The response of Rb_2TeCl_6 to applied stress was analyzed, revealing an ideal cubic structure with a lattice parameter of 10.3809 Å at 0 GPa which remain stable under pressure as revealing by the phonon dispersion calculations. The electronic band gap found to be decreasing from 2.622 eV at 0 GPa to 2.375 eV at 40 GPa, reflecting the high potential of induced pressure as an effective band-gap engineering tool. Optical properties were analysed in order to establish the optical response of the studied material under induced pressure.

1 Introduction

The importance of material optimization in many domains has been brought to light by the expanding development of optoelectronic devices. The promising qualities of halide perovskites (HPs) and their possible incorporation into environmentally friendly applications have been shown by ongoing research. Their amazing optoelectronic capabilities, easily tenable architectures, and simple production processes are the driving forces behind this interest [1], [2]. Because of their unique architectures made up of isolated metal-halide octahedral units or clusters, HPs are seen as promising materials for several applications, such as photovoltaics, thermoelectric, and energy storage. Rb-based compounds have garnered a lot of interest among the different halide perovskites because of their exceptional emission characteristics, non-toxicity, and adaptable synthesis techniques, which set them apart from other lead-free substitutes [3], [4]. This type of materials also exhibits significant electron-phonon interaction and a high exciton binding energy. Additionally, they exhibit exceptional stability under constraints like the presence of water, oxygen, heat, and UV light, underscoring their cheap cost of solution processing and eco-friendliness. Additionally, research on additional halide perovskite materials has revealed important optical and thermoelectric characteristics [5]–[7]. However, a variety of production methods, such as ceramics and flexible films, are now required due to the expanding range of uses for halide perovskites (HPs). The use of pressure as a useful tool

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for creating thick films and dense pellets is growing. In addition to changing the material's physical structure, pressure is a crucial thermodynamic variable that allows for the adjustment of its optoelectronic characteristics [8]. Previous works reported different effect responses to the applied pressure [9], [10]. In practical applications, studies of induced pressure heavily rely on technology and face greater challenges due to the complexity of crystal structures and chemical characteristics. However, advancements in computational tools, particularly first-principles methods, have demonstrated strong capabilities in exploring the physical properties of various materials. These methods also offer the ability to simulate material behaviour under different constraints [11]–[13]. Regarding the lack of scientific studies that focused on the effect of pressure on the physical properties of HPs and the potential that such understanding can hold, the present work has been initiated. The main goal of the present work is to investigate the impact of stress on the properties of halide perovskite Rb_2TeCl_6 providing new insights into the existing body of knowledge. To achieve this, we used density functional theory (DFT) calculations utilizing the WIEN2k code to explore the material's physical properties under varying pressure conditions.

2 Method of calculations

Hydrostatic pressure repairs to the application of an equal pressure on a material from all directions. To investigate its impact on the investigated sample we used the full-potential linearised augmented plane wave (FP-LAPW) approach as integrated into Wien2k [14]. The structural optimization is performed within the PBE-GGA approximation. The physical property was calculated using the Becke–Johnson potential. We set a a K-mesh point of 12 × 12 × 12 and an energy cut-off of 10^{-6} Ry.

3 Numerical results

3.1 Structural properties

Rb_2TeCl_6 has been investigated within $\boldsymbol{Fm\bar{3}m}$ (225) space group. The considered crystal structure is shown in Fig. 1-a. Table 1 shows its fractional coordinates. Optimization results show that the lattice constant of Rb_2PtCl_6 is found to be 10.3809 Å (Table 2). The energy as a fanction of volume curve was ploted in order to determine the most stable state of the crystal structure at 0 GPa, which corresponds to the minimum single-point energy. The calculation results are shown in Fig. 1-b. The physical properties of Rb_2PtCl_6 under hydrostatic pressure were then studied and calculated based on the optimization results. The theoretical presentation of the variation of the atomic constant a(Å) under pressure is given by the equation 01, Where P range from 0 to 40 GPa with steps of 10. The correspondent lattice parameter a(Å) of the Rb_2TeCl_6 compound at various pressures are presented in Table 3.

$$\boldsymbol{a(P) = a(0)\left[1 + \left(\frac{B^p}{B_m}\right)P\right]^{\left(\frac{-1}{3B^p}\right)}} \quad (01)$$

Table 1: Fractional coordinates

Atom	Positions		
	x	y	z
Rb	0.25	0.25	0.25
Te	0	0	0
Cl	0.25	0	0

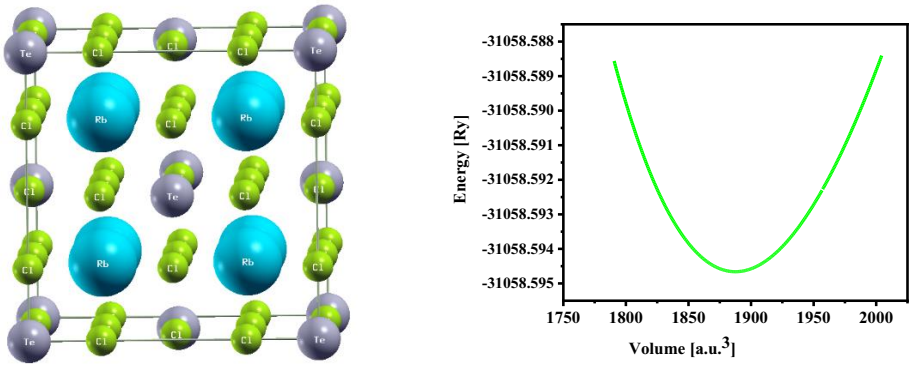

Fig. 1. (a) Unit cell structure and (b) the energy versus volume curve for Rb_2TeCl_6

Table 2: Observed and calculated values of a(Å), B_m (GPa), B_m (B^P), V_o (a.u.^{3}), and E_o (Ry) of Rb_2TeCl_6 double perovskite.

Parameters	Rb_2TeCl_6	
	Our work	Other works
a(Å)	10.3809	10.56 [7]
B_m (GPa)	30.6339	
B^P	8.5793	
V_o (a.u.^{3})	1887.2881	
E_o (Ry)	-31058.594659	

Table 3. The calculated lattice parameter a(Å) of the Rb_2TeCl_6 compound at various pressures.

P (GPa)	0	10	20	30	40
a(Å)	10.3809	9.8561	9.6469	9.5153	9.4193

The investigation of the phonon spectrum of the studied sample reveals consistent dynamical stability across the investigated pressure range. Figure 2 shows the phonon spectra at 0 and 30 GPa, where no imaginary frequencies are detected, confirming the stability of the material under the applied mechanical stress.

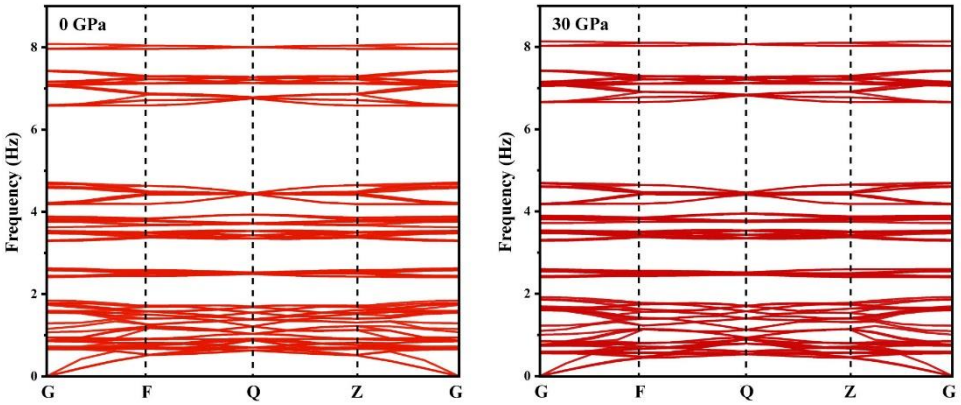

Fig. 2. The phonon dispersion curves of Rb_2TeCl_6 at 0 GPa and 30 GPa.

3.2 Electronic properties

To investigate the variation of the electronic properties of Rb_2TeCl_6 double perovskite under hydrostatic pressure, the associated band structure, TDOS, and PDOS have been calculated for different pressure values. The variation of the electronic gap value (Ef) of Rb_2TeCl_6 double perovskite oxide under hydrostatic pressure is presented in Fig.3. Ef is found to decrease with the increasing of the applied pressure, going from 2.622 eV at 0 GPa to 2.375 eV at 40 GPa (Table 4). Highlighting the potential application of pressure as an engineering tool to narrow the band gap value. The response of Rb_2TeCl_6 to applied pressure can be attributed to its layered structure, which becomes more tightly bound under compression, enhancing its suitability for photovoltaic applications [15], as illustrated in Fig. 3. These fluctuations can lead to further modifications in the lattice and electronic structures, along with their associated properties and functions. A deep analysis of the band structure plot (Fig. 3) shows that the conduction band minimum and valence band maximum of Rb_2TeCl_6 are not at the same high-symmetry point, indicating its indirect nature at all the applied pressure.

Table 4. The band gap energies of Rb_2TeCl_6 at different pressures.

P (GPa)	0	10	20	30	40
E_g (eV)	2.622	2.602	2.522	2.445	2.375

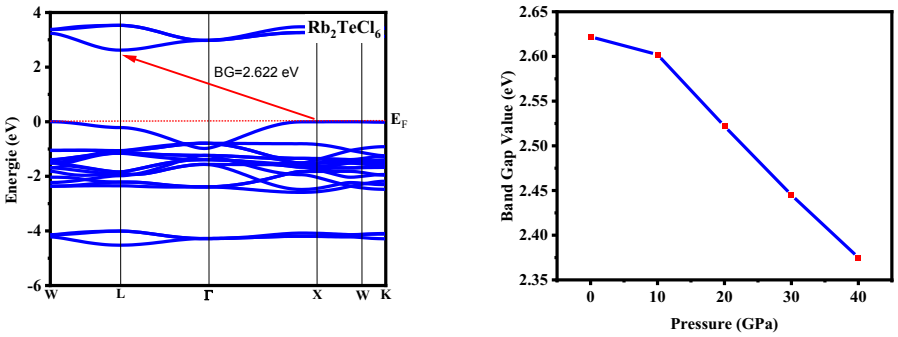

Fig. 3. Band gap structure of Rb_2TeCl_6 double perovskite and its variation at various pressure.

In order to elaborate the role of atoms in the electronic properties of the studied material the PDOS and TDOS have been computed as illustrated in Fig. 4. TDOS is decreasing under pressure. In the valence band the main contributor are p states of Cl with small contribution of s states of Te. In the conduction band the main contributors are p states of Te. Rb states do not contribute in the electronic behavior.

The electronic results under pressure demonstrate the ability of hydrostatic pressure to modulate the electronic properties and tailor materials with specific characteristics, offering the possibility of integrating these materials into targeted device applications.

3.3 Optical properties

For a better comprehension of the impact of induced pressure on the optical behavior of Rb_2TeCl_6, the refractive index (n(ω)), reflectivity (R(ω)), and optical absorption coefficient (α(ω)) are investigated (Fig. 5.).
The variation of n(ω) for Rb_2TeCl_6 s shown in Fig. 5-a. Rb_2TeCl_6 exhibits high n(ω) in the range of 0-5 eV and it decrees in higher energy values and under higher pressure. At 0 GPa the refraction index has a lower value of 0.5 at 6 eV. The static refractive indices is around 2 for all pressure values. Fig. 5-b shows the reflectance of Rb_2TeCl_6 double perovskite. At its ground state, Rb_2TeCl_6 shows several sharp peaks, especially a very strong one around 6 eV. Below 6 eV, the reflectivity fluctuates but remains relatively low. After 6 eV, there is a steep drop and then a rise again at higher energies. By applying pressure, the sharp peak around 6 eV (seen at 0 GPa) significantly smooths out and diminishes with increasing pressure. Overall, the curves become less sharp and smoother as pressure increases. Reflectivity generally increases slightly at higher energies (above 10 eV) when pressure is applied. The curves from 10 GPa to 40 GPa become closer together, suggesting pressure saturation effects at high pressures.

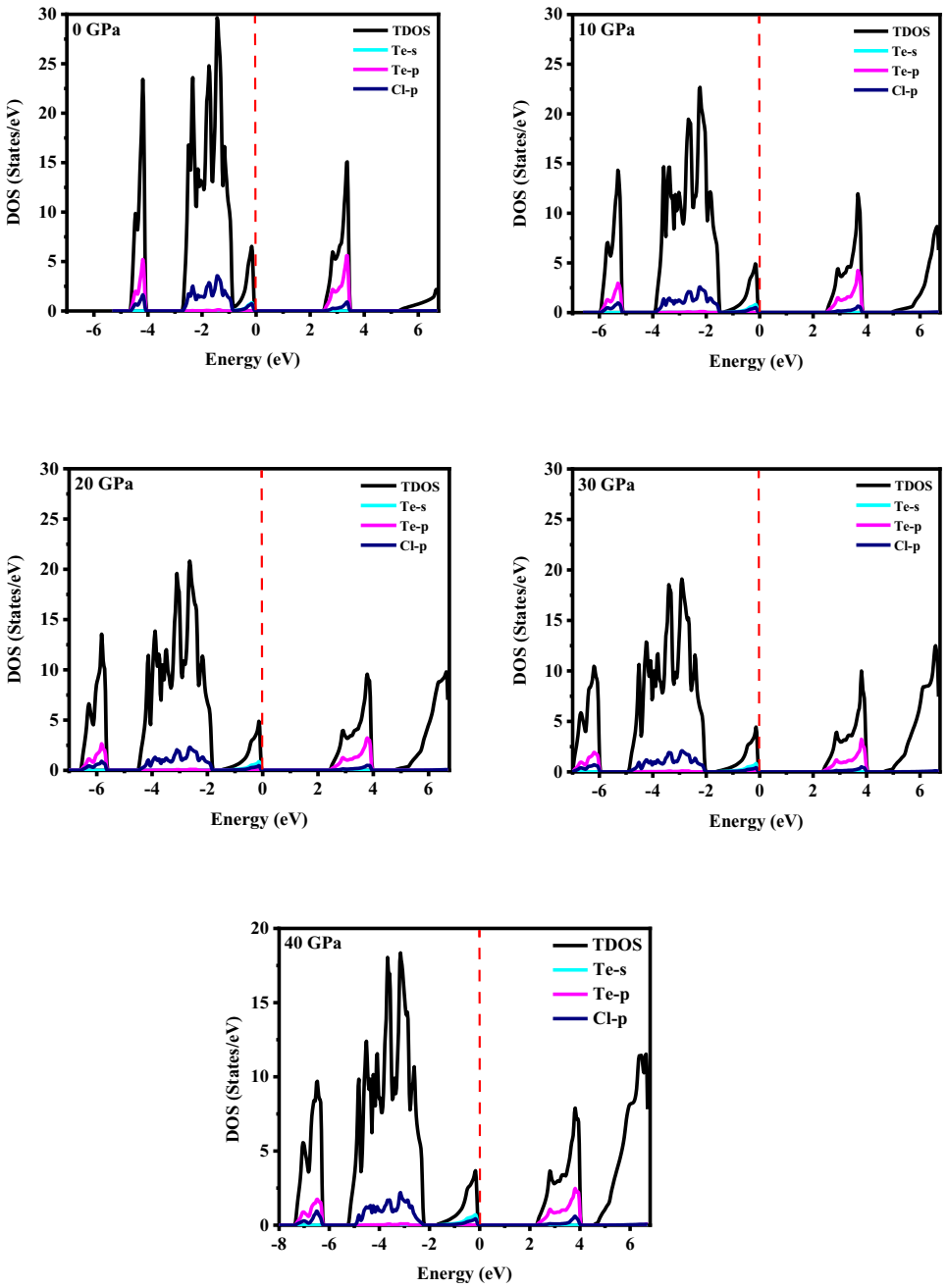

Fig. 4. Density of states plots of double perovskite Rb_2TeCl_6 under pressure

Fig. 5-c presents the optical absorption (α(ω)) of the studied material at the applied pressures. Around 3 eV, α(ω) increase slowly at 0 GPa. In the range of 5–9 eV, Sharp rises can be detected. When pressure rises from 10 to 40 GPa α(ω) moves toward lower energies. Furthermore, α(ω) increases throughout the energy range, especially after 8 eV. These

results confirm that the material is better suited for optoelectronic and photovoltaic applications thanks to its optical properties.

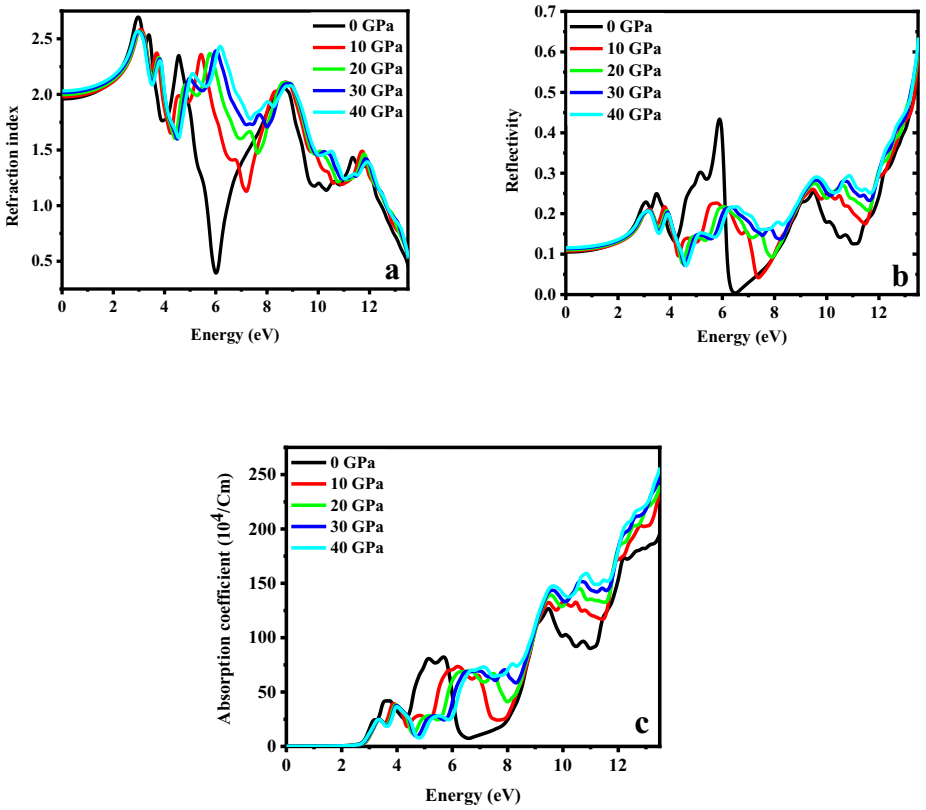

Fig. 5. (a) Refraction index, (b) Reflectivity, and (c) Absorption coefficient plots of Rb_2TeCl_6 under pressure

Conclusion

In this work, the DFT approach was used in order to comprehensively investigate the fluctuations of the structural, electrical, and optical characteristics of the cubic double perovskite Rb_2TeCl_6 under the application of hydrostatic pressure. The results show that Rb_2TeCl_6 crystallizes in the $Fm\bar{3}m$ (225) space group. The application of hydrostatic pressure does not affect the stability of the material, as confirmed by phonon calculations. However, the lattice constant decreases, reflecting a compression effect on the atomic structure. Rb_2TeCl_6 shows an indirect band gap character over the investigated pressure range. Additionally, the band gap decreases from 2.622 eV at 0 GPa to 2.375 eV at 40 GPa, indicating the potential of pressure for tuning the electronic parameters of Rb_2TeCl_6. The same response has been detected for the optical properties. These results confirm the sensitivity of the structural, electrical, and optical properties of Rb_2TeCl_6 to pressure, highlighting their potential for tailoring under such constraints.

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