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Tuning ferroelectric photovoltaic performance in $R3c$ - CuNbO_3 through compressive strain engineering: a first-principles study

 Zu-Da He, Wen-Ce Li, Jin-Long Yang, Hua-Kai Xu, Xiang-Fu Xu, Guo-Xia Lai, You-Da Che, Wei-Ling Zhu, Xiao-Dong Yang* and Xing-Yuan Chen *

Most ferroelectric oxides exhibit relatively wide bandgaps, which pose limitations on their suitability for photovoltaics application. CuNbO_3 possesses potential ferroelectric properties with an $R3c$ polar structure that facilitate the separation of charge carriers under illumination, promoting the generation of photovoltaic effects. The optical and ferroelectric properties of $R3c$ - CuNbO_3 , as well as the effect of strain on the properties are investigated by first-principles calculation in this paper. The calculated results indicate that $R3c$ - CuNbO_3 possesses a moderate band gap to absorb visible light. The interaction of Cu–O and Nb–O bonds is considered to have a crucial role in the photovoltaic properties of CuNbO_3 , contributing to the efficient absorption of visible light. The bandgap of CuNbO_3 becomes smaller and the density of states near the conduction and valence bands becomes relatively uniform in distribution under compressive conditions, which improves the photoelectric conversion efficiency to 29.9% under conditions of bulk absorption saturation. The ferroelectric properties of CuNbO_3 are driven by the Nb–O bond interactions, which are not significantly weakened by the compressive strain. CuNbO_3 is expected to be an excellent ferroelectric photovoltaic material by modulation of compressive strain due to the stronger visible light absorption and excellent ferroelectric behavior.

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1. Introduction

Oxide-group materials have wide potential application in ferroelectric, photocatalysis and photovoltaic fields.^{1,2} Perovskite materials with $R3c$ structure show a unique application prospect in the field of ferroelectric photovoltaics due to the internal electric field.^{3,4} For example, BiFeO_3 and LiNbO_3 with $R3c$ structure have internal ferroelectric polarization electric fields, which can promote carrier separation without the p–n junction.^{5,6} Some ferroelectric oxides with a narrow band gap, such as $\text{Bi}_2\text{FeCrO}_6$, CuGaO_2 , ABiO_3 (A = Ca, Cd, Zn, and Mg) and $\text{Pb}(\text{Fe}_{1/2}\text{V}_{1/2})\text{O}_3$, exhibit strong visible light absorption, which is advantageous for achieving high photoconversion efficiency.^{7–10} However, the band gap of most $R3c$ -structured ferroelectric oxides is usually large and it is difficult for them to effectively absorb visible light.^{11,12} Niobium oxide (CuNbO_x) films have been shown to be excellent p-type semiconductors that can be stabilized as hole transport layers, significantly improving the efficiency of perovskite solar cells.¹³ In addition, CuNbO_3 with perovskite structure is also considered as a potential semiconductor material for photovoltaic and photoelectrochemical conversion.¹⁴ Narayanasamy successfully synthesized the $C/2m$

structure of CuNbO_3 by pulsed laser deposition technology, and applied it to dye-sensitized solar cells, achieving good photovoltaic performance.¹⁵ First-principles calculations show that CuNbO_3 with $C/2m$ structure can absorb visible light, and the optical properties are closely related to the Cu-d, Nb-d, and O-p energy level transitions.^{16,17} At the same time, Fukuda *et al.* synthesized CuNbO_3 with an $R3c$ structure, a polarized structural material with potential ferroelectric properties, although its light absorption properties have not been studied in detail.¹⁸ In addition to the choice of materials, strain is also a key factor in regulating the physical properties of materials. Strain can induce and regulate changes in the physical properties of materials, such as ferroelectric depolarization, piezoelectricity, magnetoresistance, electrical capacitance, and photovoltaic performance.^{19–22} By adjusting lattice parameters and electronic structure, strain can affect the band structure, ferroelectric polarization strength and optical properties to improve the photoelectric properties of the material.^{23,24} The wide band gap ferroelectric oxides, such as BiFeO_3 (ref. 25) and InFeO_3 ,^{26,27} have been shown to achieve significant bandgap adjustment while maintaining high ferroelectric polarization, which enhances the absorption of visible light and achieves excellent ferroelectric photovoltaic performance. In this paper, CuNbO_3 with an $R3c$ structure has been investigated by density functional theory for the ferroelectric photovoltaic performance. The calculated result indicated that CuNbO_3 with an $R3c$ structure is

Department of Physics, School of Science, Guangdong University of Petrochemical Technology, Maoming, Guangdong 525000, PR China. E-mail: chenxingyuan@gdupt.edu.cn; Fax: +86-668-2923567; Tel: +86-668-2923838



a new promising ferroelectric photovoltaic oxide. CuNbO_3 with an $R3c$ structure has a good ferroelectric polarization strength and can absorb visible light, which could improve the photovoltaic efficiency under the compressive strain conditions.

2. Computational method

All calculations in this paper are primarily conducted by using density functional theory implemented in the Vienna *Ab initio* Simulation Package (VASP) software, employing the pseudopotential plane wave method.^{28,29} Exchange–correlation interactions are treated by using the Perdew–Burke–Ernzerhof (PBE) functional combined with Hubbard U correction (PBE+ U).³⁰ The Hubbard U correction is particularly vital for the accurate calculation of the electronic structure with 3d transition metals.³¹ The plane-wave cutoff is set at 550 eV, and the K-point sampling density within the Brillouin region is maintained at 0.03 Å⁻¹. The crystal structure was relaxed until the force acting on the atoms reached a magnitude lower than 0.001 eV Å⁻¹. The Hubbard U value for the Cu element in $R3c$ - CuNbO_3 is set at 6 eV, with similar reports of Hubbard U correction available for other copper-based oxides.^{17,32,33} The calculated results indicate that the band gap of $R3c$ - CuNbO_3 , obtained through the PBE+ U approach, is approximately 1.7 eV. This value closely aligns with the band gap obtained using the HSE06 functional and is consistent with the experimental band gap of the $C/2m$ structure CuNbO_3 .¹⁴ Considering that the PBE+ U method offers an accurate calculation of the electronic structure for 3d elemental materials and is more cost-effective, we have chosen to employ the PBE+ U approach for subsequent calculations involving energy, electronic structure, band structure, ferroelectric and optical properties.

3. Calculation of the structure

The introduction of strain was achieved by simultaneous optimization of the *ab*-axis and *c*-axis lengths, as depicted in Fig. 1. The calculated results are summarized in Table 1. The calculated pristine CuNbO_3 lattice parameters are closed to the experimental values. MgSnO_3 and LiNbO_3 share structural similarities with CuNbO_3 . With the possibility of growing $R3c$ - MgSnO_3 films on LiNbO_3 substrates,^{6,34} the lattice constant of LiNbO_3 (5.15 Å) was chosen to optimize the lattice parameters of $R3c$ - CuNbO_3 , introducing lattice strain. This choice is based on the smaller lattice constant of LiNbO_3 compared to CuNbO_3 (5.28 Å), leading to compressive strain within the CuNbO_3 lattice. Using the lattice parameter *a* of LiNbO_3 as a reference, the lattice parameter *a* and *b* of $R3c$ - CuNbO_3 was adjusted to 5.15 Å through fitting, optimizing the lattice parameter *c*. The *c*-axis of $R3c$ - CuNbO_3 under compressive strain (C-CuNbO_3) is changing from 14.22 Å to 14.55 Å. To assess mechanical stability under compressive strain, the strain stress method³⁵ within VASP software was employed to calculate the elastic constants of CuNbO_3 with the $R3c$ space group. Six independent elastic constants exist within the $R3c$ space group structure, including C_{11} , C_{12} , C_{13} , C_{14} , C_{33} and C_{44} . Based on the crystal mechanics stability criteria proposed by Mouhat and Coudert *et al.*,³⁶

mechanical stability dictates that these independent elastic constants must adhere to specific inequalities.

$$C_{11} - C_{12} > 0, C_{11} + C_{12} > 0, C_{33} > 0, C_{44} > 0, (C_{11} + C_{12})C_{33} - 2C_{13}^2 > 0 \quad (1)$$

The calculated results, as presented in Table 2, confirm that both pristine CuNbO_3 and C-CuNbO_3 satisfy these inequalities, signifying their mechanical stability. The changes in the elastic constants of C-CuNbO_3 could be attributed to the compressive strain, which enhances the interatomic interactions, leading to bond shortening and an increase in the elastic constants. A similar situation exists for $R3c$ - InFeO_3 and $R3c$ - MgSnO_3 in our earlier research reports, where the compressive strain causes the bond length to become shorter resulting in a larger elastic constant.^{27,37} Cu–O bond lengths are transitioned from 2.03 Å to 1.99 Å, whereas Nb–O bond lengths are changed from 2.14 Å to 2.12 Å under compressive strain in $R3c$ - CuNbO_3 .

4. Calculation of optical properties

The optical and electronic properties of the material are closely correlated with its band structure. As illustrated in Fig. 2(a) and (c), the calculated band gaps for pristine CuNbO_3 and C-CuNbO_3 are 1.7 eV and 1.50 eV, respectively, both of which are indirect band gaps. Notably, the band gap of $R3c$ - CuNbO_3 closely aligns with the experimentally reported value for $C/2m$ -structured CuNbO_3 (2.0 eV).¹⁴ The band gap of $R3c$ - CuNbO_3 is smaller compared to the ferroelectric materials with $R3c$ structure such as BiFeO_3 (2.7 eV),³⁸ MgSnO_3 (4.0 eV),³⁹ and ZnSnO_3 (3.7 eV).³⁹ It shares the potential for strong visible light absorption with narrow bandgap ferroelectric oxides like $\text{Bi}_2\text{FeCrO}_6$ (1.8 eV),⁹ CuGaO_2 (1.46 eV),⁸ and ABiO_3 (A = Ca, Cd, Zn, and Mg) (2.0 eV).⁷ Under compressive conditions, the band gap of $R3c$ - CuNbO_3 decreases to 1.50 eV. The valence band maximum of both pristine CuNbO_3 and C-CuNbO_3 (Fig. 2(b) and (d)) is primarily composed of Cu-3d orbitals and O-2p orbitals, while the conduction band minimum is predominantly occupied by Nb-4d orbitals and O-2p orbitals. The bonding states of Cu–O and the anti-bonding states of Nb–O play a pivotal role in the optical properties of $R3c$ -structured CuNbO_3 . The influence of compressive strain results in a reduction of the interatomic distance in C-CuNbO_3 . The density of states (DOS) near the valence and conduction bands become relatively uniform distribution, resulting in a reduced bandgap and facilitating electron transitions. The band gap and dielectric function are intricately linked to the optical properties of the material. The optical properties can be obtained from the real (ϵ_1) and imaginary (ϵ_2) parts of the dielectric function within the Random Phase Approximation (RPA). The refractive index *n* and the extinction coefficient κ are determined from ϵ_1 and ϵ_2 with the photon energy *E* as follows.⁴⁰

$$n(E) = \frac{1}{\sqrt{2}} \sqrt{\epsilon_1(E) + \sqrt{\epsilon_1^2(E) + \epsilon_2^2(E)}} \quad (2)$$



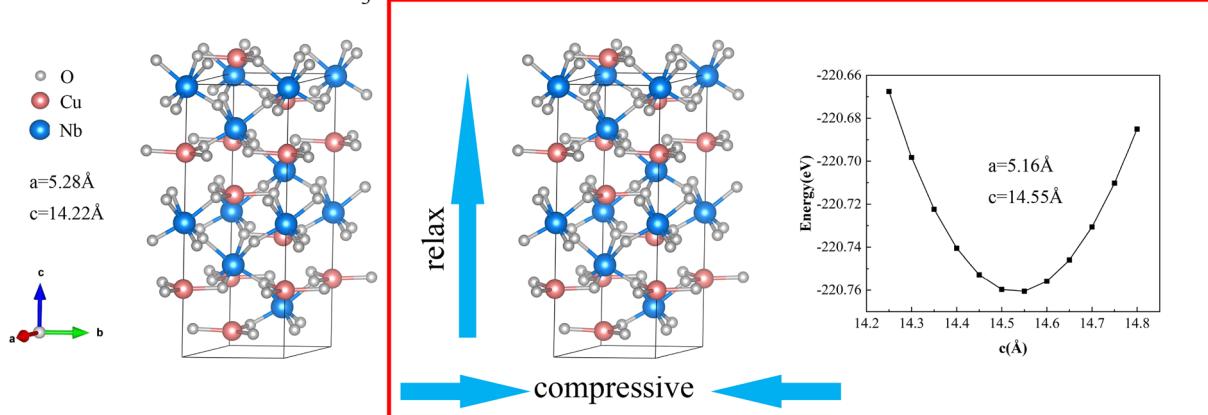
Pristine CuNbO₃Fig. 1 The calculated structure of pristine and compressive R3c-CuNbO₃.

Table 1 The calculated and experimental lattice parameters

	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)
CuNbO ₃ (exp) ¹⁴	5.24	5.24	14.00
CuNbO ₃ (cal)	5.28	5.28	14.22
C-CuNbO ₃ (cal)	5.15	5.15	14.55

Table 2 The calculated elastic constants and the unit given in GPa

	<i>C</i> ₁₁	<i>C</i> ₁₂	<i>C</i> ₁₃	<i>C</i> ₁₄	<i>C</i> ₃₃	<i>C</i> ₄₄
CuNbO ₃	204.167	138.897	88.539	6.668	193.172	31.948
C-CuNbO ₃	236.263	171.384	104.460	4.204	216.713	31.433

$$\kappa(E) = \frac{1}{\sqrt{2}} \sqrt{-\epsilon_1(E) + \sqrt{\epsilon_1^2(E) + \epsilon_2^2(E)}} \quad (3)$$

The reflectivity *R* and absorption *α* coefficient were calculated from *n* and κ .⁴⁰

$$R(E) = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} \quad (4)$$

$$\alpha(E) = \frac{4\pi\kappa}{hc/E} \quad (5)$$

Pristine R3c-CuNbO₃ exhibits a significant absorption coefficient within the visible light range, reaching 10^5 cm⁻¹ in the Fig. 3a. In contrast, under compressive strain conditions, C-CuNbO₃ displays a reduced band gap and stronger absorption in the visible light range compared to pristine CuNbO₃, which is highly advantageous for photovoltaic applications. The photovoltaic conversion efficiency was estimated to evaluate photovoltaic potential of CuNbO₃. The following approach was employed to calculate the photovoltaic conversion efficiency (PCE).⁴¹

$$PCE = \frac{\int_0^{\lambda_{max}} W(\lambda)[1 - R(\lambda)](1 - e^{-\alpha(\lambda)d})C(\lambda)d\lambda}{\int_0^{\infty} W(\lambda)d\lambda} \quad (6)$$

Here, λ represents the wavelength of light, λ_{max} is the maximum absorption wavelength related to the band gap *E_g* as follows.

$$\lambda_{max} = \frac{hc}{E_g} \quad (7)$$

$W(\lambda)$ represents the solar spectrum irradiance (AM1.5), where *d* represents the thickness of the material. The calculated absorption α and reflectivity *R* coefficient are shown in the Fig. 3a and b. *C*(λ) is the conversion factor, reflecting the ratio of photon energy converted to electron energy. It is related to the excitation energy of electron-hole pairs passing through the minimum band gap as follows.

$$C(\lambda) = \lambda \frac{E_g}{hc} \quad (8)$$

The calculated photovoltaic conversion efficiencies are illustrated in Fig. 3c. For pristine CuNbO₃ and C-CuNbO₃ with a thickness of 100 nm, the photovoltaic conversion efficiencies are 18.1% and 18.7%, respectively. The photovoltaic conversion efficiencies for pristine CuNbO₃ and C-CuNbO₃ with thickness of 500 nm are 25.6% and 27.5%, respectively. Both materials exhibit significantly high photovoltaic conversion efficiencies. The application of compressive strain further enhances the photovoltaic conversion efficiency of CuNbO₃ from 26.9% to 29.9% under conditions of bulk absorption saturation. The calculations of the optoelectronic properties suggest that R3c-CuNbO₃ is a promising photovoltaic material, with strain-induced enhancement of light absorption leading to increased photovoltaic conversion efficiency.

5. Calculation of ferroelectric properties

The ferroelectric polarization strength of both pristine CuNbO₃ and C-CuNbO₃ is determined by using the Berry phase method



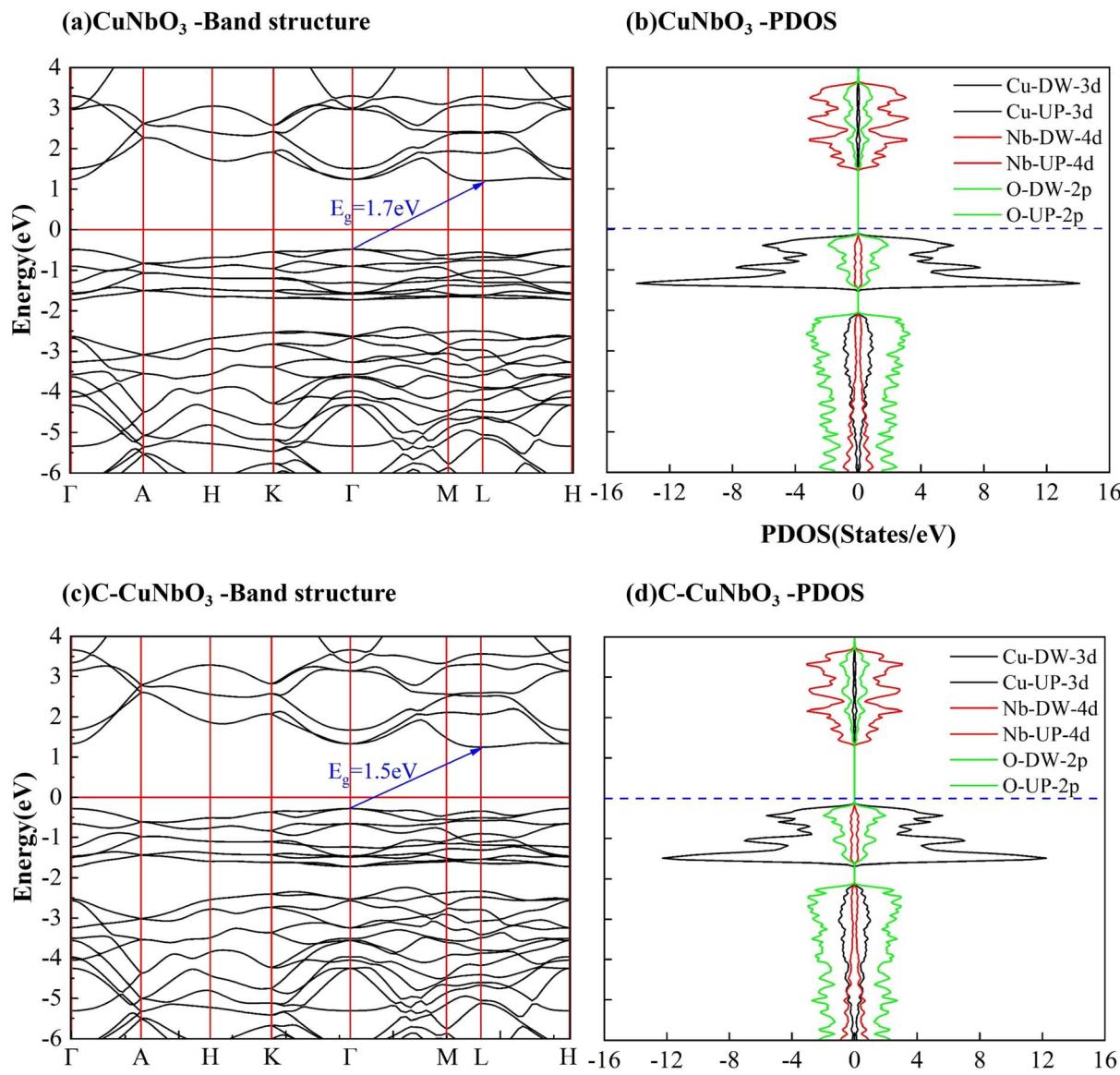


Fig. 2 The calculated energy band structure and partial density of states (PDOS) of (a and b) pristine and (c and d) compressive $R3c$ -CuNbO₃.

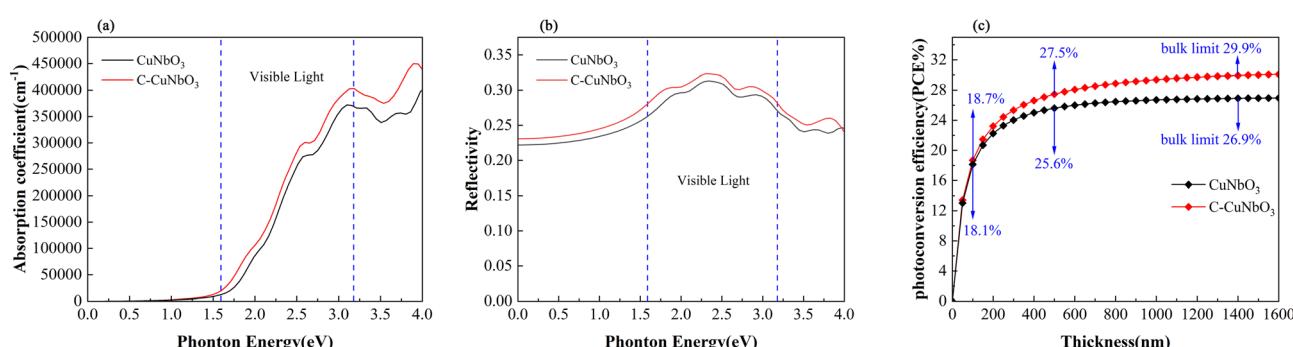


Fig. 3 The calculated (a) optical absorption coefficient, (b) reflection coefficient, and (c) photoelectric conversion efficiency. The range of visible light is indicated between the two dashed lines.



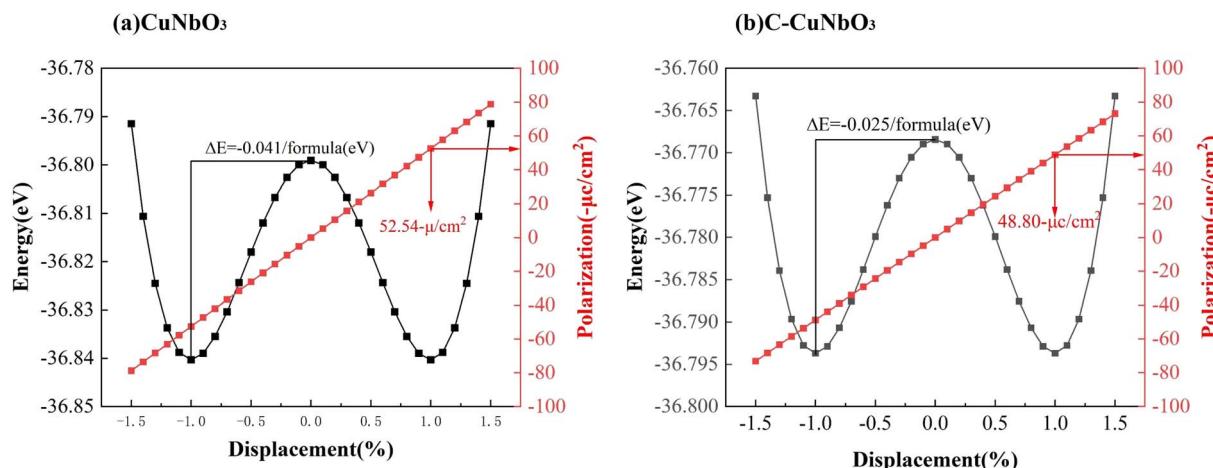


Fig. 4 The calculated ferroelectric polarization strength and energy changes as the atom interpolation shifts of (a) pristine and (b) compressive $R\bar{3}c$ -CuNbO₃.

Table 3 The calculated Born effective charges (e) and atomic offset (Å) away from centrosymmetric positions

		BEC _{xx}	BEC _{yy}	BEC _{zz}	Offset (Δz)
CuNbO ₃	O	-2.98	-2.98	-2.80	-0.09
	Cu	1.05	1.05	1.09	0.01
	Nb	7.92	7.92	7.30	0.12
C-CuNbO ₃	O	-2.99	-2.99	-3.02	-0.08
	Cu	0.93	0.93	1.03	-0.01
	Nb	8.03	8.03	8.04	0.10

within the framework of modern polarization theory.^{42,43} As shown in Fig. 4, the $R\bar{3}c$ space group is designated as the ferroelectric phase (state 1), while the centrosymmetric reference phase is labeled as $R\bar{3}c$ (state 0). The double-well potential energy curves and ferroelectric polarization strength are obtained by linearly interpolating between the centrosymmetric

phase (state 0) and the polar phase (state 1). These energy curves suggest that $R\bar{3}c$ -CuNbO₃ could exhibit promising ferroelectric properties similar to well-documented ferroelectric materials like BiFeO₃, ZnSnO₃ and MgSnO₃ in the literature.^{44–46} Under compressive strain conditions, the ferroelectric polarization value of $R\bar{3}c$ -CuNbO₃ decreases from 52.54 μ C cm⁻² to 48.80 μ C cm⁻². In Table 3, the Born effective charges (BEC) and atomic displacements away from centrosymmetric positions are calculated to investigate the ferroelectric properties of CuNbO₃. Born effective charges quantify the induced dipole moment of an atom in response to a slight displacement from its equilibrium position caused by the applied electric field. Greater Born effective charges generally correspond to more pronounced polarization effects, indicating increased susceptibility to atomic displacement in response to an applied electric field. The calculated results reveal that the BEC of Nb is larger than that of Cu (1e+), at approximately 8e+, and this significantly contributes to the ferroelectric polarization of $R\bar{3}c$ -CuNbO₃. The

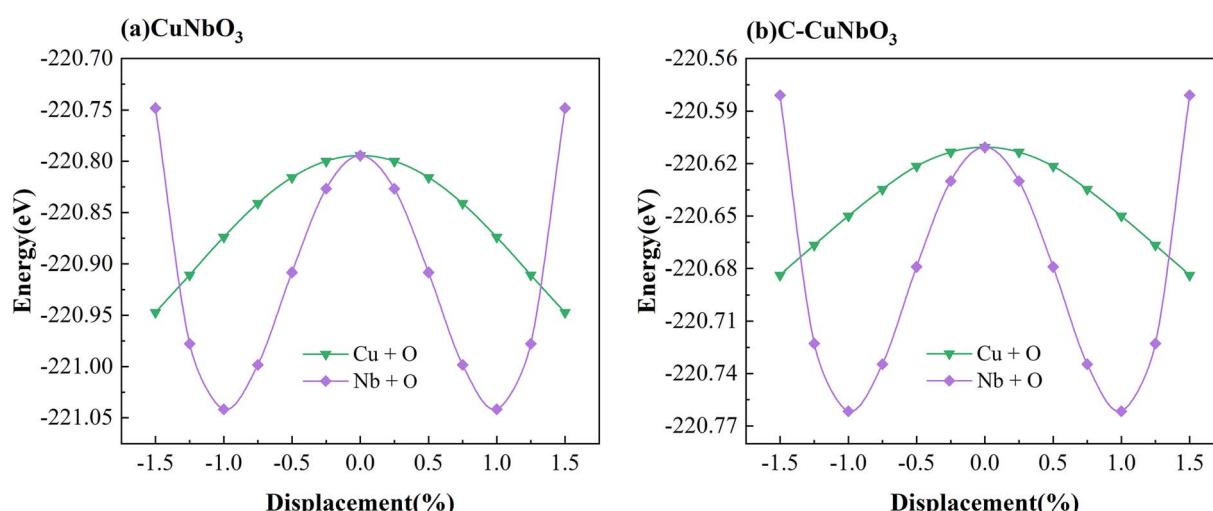


Fig. 5 The calculated energy changes as Cu–O and Nb–O movement of (a) pristine and (b) compressive $R\bar{3}c$ CuNbO₃.

calculated displacements show relatively substantial movements of Nb and O atoms in $R3c$ -CuNbO₃. Energy change diagrams for different atomic movements are also provided in Fig. 5, displaying a prominent double-well trend in atomic movement between Nb and O atoms, further affirming the pivotal role of Nb–O interaction in ferroelectric properties of $R3c$ -CuNbO₃. In Table 3, it is observed that the offset for O in pristine CuNbO₃ is approximately 0.09 Å, while the Nb offset is about 0.12 Å. For C-CuNbO₃, the O offset is roughly 0.08 Å, and the Nb offset is approximately 0.10 Å. Under compressive strain conditions, the ferroelectric polarization strength of CuNbO₃ experiences a slight reduction due to the diminished displacement offsets. However, it still exhibits excellent ferroelectric properties, evident from the distinct double-potential well curve and robust ferroelectric polarization strength. The introduction of compressive strain in CuNbO₃ enhances its light absorption, coupled with outstanding ferroelectric behavior, rendering it a highly promising ferroelectric photovoltaic oxide material.

6. Conclusion

The optical and ferroelectric properties of $R3c$ -CuNbO₃, as well as the impact of compressive strain, have been investigated by density functional theory. The calculated results showed that $R3c$ -CuNbO₃ has a more suitable band gap for absorbing visible light compared to ferroelectric materials with the $R3c$ structure, such as BiFeO₃, ZnSnO₃, and MgSnO₃. The interactions between Cu–O and Nb–O bonds play a crucial role in establishing the favorable bandgap in $R3c$ -CuNbO₃. The bandgap of $R3c$ -CuNbO₃ decreased under compressive strain, leading to increased uniform distribution DOS near the valence and conduction bands, improving photovoltaic conversion efficiency to 29.9% under conditions of bulk absorption saturation. The photoelectric conversion efficiency of CuNbO₃ can be enhanced by the compressive strain interaction, without weakening its ferroelectric properties driven by Nb–O bond interactions. CuNbO₃ under compressive strain exhibits enhanced visible light absorption and retains its exceptional ferroelectric characteristics, leading to a promising ferroelectric photovoltaic material.

Conflicts of interest

The authors declared that they have no conflicts of interest to this work. We declare that we do not have any commercial or associative interest that represents a conflict of interest in connection with the work submitted.

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