

<https://doi.org/10.1038/s41535-025-00814-y>

Hybrid d/p-wave altermagnetism in $\text{Ca}_3\text{Ru}_2\text{O}_7$ and strain-controlled spin splitting

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The interplay of strong electronic correlations, sizable octahedral distortions, and pronounced spin-orbit coupling (SOC) makes perovskite oxides promising candidates for realizing altermagnetic phases. We study altermagnetic phases in $\text{Ca}_3\text{Ru}_2\text{O}_7$, a non-centrosymmetric layered perovskite whose ground state is a Kramers-degenerate antiferromagnet. We show that an alternative Néel-type spin arrangement hosts a P-2 *d*-wave altermagnetic state with orbital selectivity similar to Ca_2RuO_4 . Including SOC generates a symmetry-allowed *p*-wave component and yields a hybrid *d/p*-wave altermagnetic order. We further demonstrate that biaxial strain tunes both magnetic stability and band splitting: compressive strain beyond 2% favors the altermagnetic phase over the antiferromagnetic ground state, while tensile strain increases altermagnetic splittings by up to 9%. To quantify these trends, we define an altermagnetic figure of merit and trace its strain dependence to changes in electronic localization and octahedral geometry in this polar metal.

Altermagnets are a significant new magnetic material class, advancing fundamental research and spintronic applications^{1,2}. At the heart of altermagnetism (AM) lies crystal symmetry, which dictates the unique spin-splitting behavior. This inherent link makes strain a powerful tool for manipulating and controlling AM order in correlated materials, a frontier of active research^{3,4}. The potential of strain engineering has been recently demonstrated by the induced phase transition from an antiferromagnetic to an altermagnetic state in ReO_2 ⁴ and the discovery of an elasto-Hall conductivity in *d*-wave altermagnets⁵. The physics is further enriched by spin-orbit coupling (SOC), which, by breaking time-reversal symmetry, can induce phenomena such as weak ferromagnetism through spin canting or other mechanisms dependent on crystal symmetry^{6–12}. Collectively, these findings motivate the exploration of strain-induced AM order in new classes of correlated materials. In this context, Ruddlesden-Popper perovskites, renowned for hosting diverse quantum phases intrinsically coupled to lattice distortions, offer a compelling platform to investigate the interplay between strain, symmetry, and magnetism^{13–17}.

Ruddlesden-Popper compounds of the form $(\text{Ca}, \text{Sr})_{n+1}\text{Ru}_n\text{O}_{3n+1}$ exhibit strong electronic correlations and display phases that depend critically on symmetry and octahedral distortions. Rotations, Jahn-Teller distortions, and polar displacements break the operations that interchange opposite spin sublattices and enable the emergence of altermagnetic states¹⁸.

Over the past decade, researchers have observed Mott insulating behavior¹⁸, metamagnetism¹⁹, and unconventional superconductivity²⁰ in these systems. Revisiting their magnetic phases within the altermagnetic framework offers new insights into transitions among ferromagnetism, antiferromagnetism, and altermagnetism by linking symmetry, distortion, and magnetic order. Among the series, $\text{Ca}_3\text{Ru}_2\text{O}_7$ undergoes antiferromagnetic transitions as a function of temperature^{21–23} and exhibits pronounced tunability under magnetic field²⁴, pressure²⁵ and strain²⁶. These observations raise the question of whether $\text{Ca}_3\text{Ru}_2\text{O}_7$ (hereafter CRO) hosts an altermagnetic phase and what conditions might induce a transition from its native antiferromagnetic order.

We apply this framework to $\text{Ca}_3\text{Ru}_2\text{O}_7$, a non-centrosymmetric compound with strong spin-orbit coupling (SOC) that enables relativistic spin splitting and spin-momentum locking. SOC governs the magnetic anisotropy in this system and drives spin reorientation transitions, as previously reported²⁷. Investigating altermagnetism in $\text{Ca}_3\text{Ru}_2\text{O}_7$ offers a unique opportunity to reveal spin textures that emerge from the interplay of non-relativistic and relativistic effects. Most known altermagnets preserve inversion symmetry; finding altermagnetic order in a non-centrosymmetric metal would open new directions in the study of symmetry-protected spin transport phenomena^{28,29}.

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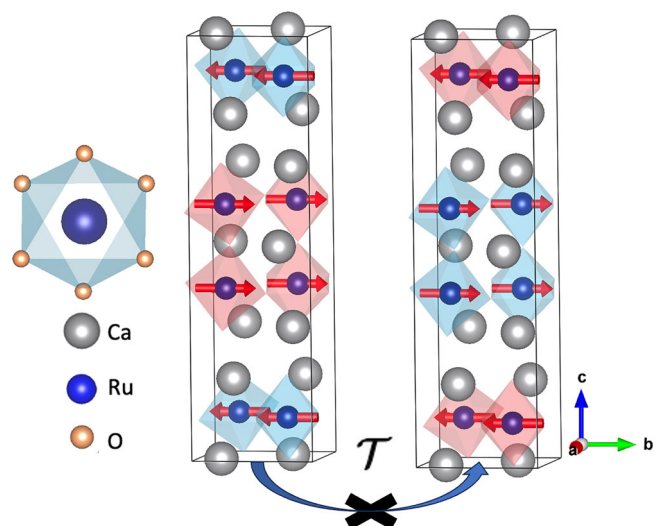


Fig. 1 | $\text{Ca}_3\text{Ru}_2\text{O}_7$ in its magnetic ground-state configuration exhibits spins aligned ferromagnetically (FM) within the plane and antiferromagnetically (AFM) between layers. This schematic illustrates that, under time-reversal operation, the spins cannot be connected by rotational symmetry alone because they can be connected through translational symmetry operations along the c -axis. These Kramers antiferromagnets are also named SST-3⁴⁸ in the literature. Consequently, $\text{Ca}_3\text{Ru}_2\text{O}_7$ exhibits Kramers antiferromagnetism in its ground state.

In this work, we identify magnetic configurations in $\text{Ca}_3\text{Ru}_2\text{O}_7$ that host altermagnetic order and analyze their symmetry and electronic structure under non-relativistic and relativistic spin splitting. In the absence of SOC, the system exhibits a d -wave altermagnetic state, while SOC introduces additional asymmetries and generates a hybrid d - and p -wave character. We demonstrate that biaxial strain tunes the altermagnetic response by enhancing or suppressing spin splitting depending on the strain direction and link this manipulation to changes in octahedral distortions and orbital localization. To quantify these effects, we define the altermagnetic quantity (AMQ) as a figure of merit that captures changes in band splitting and enables direct comparison across altermagnetic systems across different conditions.

Results

Exploring AM states

$\text{Ca}_3\text{Ru}_2\text{O}_7$ crystallizes in the non-centrosymmetric space group $Bb2_1m^{22}$, with associated point group $mm2$, which includes a twofold rotation axis along z and a vertical mirror plane. The full space group also contains a 2_1 screw axis along z , which plays a role in the nonsymmorphic symmetries relevant to the altermagnetic configuration.³⁰ The magnetic moment arises predominantly from the Ru $4d$ electrons, in which, at low temperatures, the Ru atoms order ferromagnetically within the bilayers while aligning antiferromagnetically between them, forming an A-type antiferromagnetic structure where the spins are oriented along the b -axis (see Fig. 1). Given this A-type antiferromagnetic order, the primitive cell of CRO contains spin-up sites, with a translational symmetry operation that maps spin-up into spin-down sites (along the z -axis). Consequently, the ground state is not altermagnetic (see Fig. 1)¹.

We analyzed CRO under different magnetic configurations to explore possible AM states and their stability. Specifically, we examined magnetic orderings commonly observed in AB_3 perovskites³¹, labeled as configurations A–D (see Fig. 2). Table 1 shows the energy differences relative to the ground-state configuration A, as well as some relevant structural, electronic, and magnetic properties for our study. Our results indicate that AM states appear in configurations B and C, where configuration B has an antiferromagnetic spin arrangement along the a , b , and c -axes, while configuration C shows this along the c -axis. Although these magnetic states have

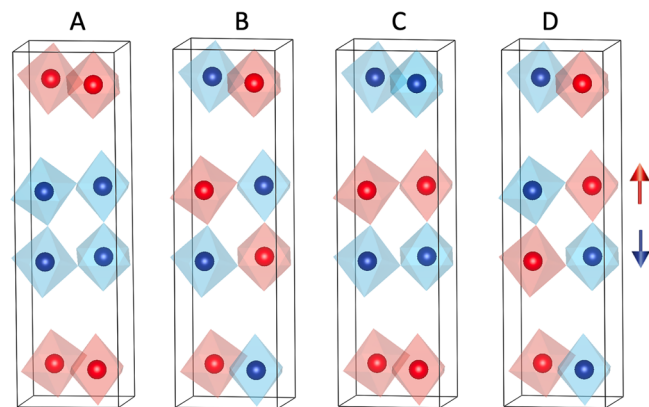


Fig. 2 | Magnetic configurations in $\text{Ca}_3\text{Ru}_2\text{O}_7$. The labels A–D correspond to the magnetic phases explored. Red and blue spheres denote atoms with majority spin-up and spin-down orientations, respectively. Ca and O atoms are omitted for clarity.

not been experimentally observed in CRO, similar phases have been reported in doped $\text{Ca}_3\text{Ru}_2\text{O}_7$ systems, such as Ti-doped $\text{Ca}_3(\text{Ru}_{1-x}\text{Ti}_x)_2\text{O}_7$ (configuration B)³², and in the sister compound $\text{Sr}_3\text{Ru}_2\text{O}_7$ (configuration D)³³.

Notably, variations in magnetic spin arrangements lead to significant structural and electronic changes (further structural details are given in Supplemental Material File (SM) Table S1). Specifically, FM and AFM in-plane arrangements result in metallic (A, C) and a narrow insular state (B, D), respectively. Next, we will focus on the AM phases of CRO, primarily in Configuration B.

In addition to the electronic differences, configuration B exhibits a lower magnetic moment than configuration A (details on Table S1). In configuration B, the magnetic moments form a Néel-type collinear ordering with alternating spin orientations. This promotes spin-compensated orbital overlap and wave function delocalization, which are characteristic of bonding-like states. As a result, configuration B is more sensitive to the Hubbard- U term due to the enhanced electronic proximity. As a result, a band gap opens at relatively low U values, specifically $U = 1.0$ eV. In contrast, configuration A remains metallic under the same conditions. The Supplemental Material (Section SII) provides further analysis. These contrasting results demonstrate CRO's highly correlated electronic nature, driven by the tight interplay between magnetic and structural degrees of freedom^{34–37}. Finally, we confirm that these characteristics are predominantly electronic, arising from the magnetic spin configuration, and are independent of volume changes or structural distortions.

We now examine the electronic structure of both configurations. Figure 3 shows the total and orbital-resolved density of states. While configuration A is metallic, configuration B exhibits a narrow gap at the Fermi level. In an ideal octahedral environment, the Ru d_{xy} , d_{xz} , and d_{yz} orbitals are degenerate. Orthorhombic distortions lift this degeneracy slightly, but it is the Néel-type magnetic order in the ab -plane (conf. B) that drives orbital differentiation by enhancing π -type hybridization between Ru- d_{xy} and O- p_x/p_y orbitals. This leads to a strong bonding–antibonding splitting, pushing the d_{xy} bonding states to lower energy and making them nearly filled. The resulting spectral redistribution lowers the d_{xy} chemical potential relative to the less-affected, half-filled d_{xz} and d_{yz} orbitals. The gap thus reflects an orbital-selective mechanism driven by the interplay between magnetism and crystal-field effects, as proposed for Ca_2RuO_4 ³⁸.

Figure 4 shows the non-relativistic band structure for the A and B magnetic configurations. The A configuration (ground state) exhibits metallic behavior, consistent with previously reported results that neglect SOC effects^{27,34}. In contrast, configuration B displays a narrow gap and a k -dependent non-relativistic spin splitting, a hallmark of altermagnetic states (see Fig. 4b). The shaded regions on the band structure indicate regions in

k -space where the altermagnetic spin splitting is maximal. Figure 5 shows the detailed Brillouin zone (BZ) corresponding to these paths.

The presence of the non-relativistic spin-splitting is independent of the value of k_y . The observed spin splitting exhibits what is known as a d -wave symmetry in momentum space. This terminology refers to how the splitting changes sign across the Brillouin zone, in analogy to the lobes of a d -orbital. Specifically, the splitting changes sign upon inversion of the k_x or k_z coordinate, but remains unchanged when inverting k_y . This independence from the k_y component allows for a more precise classification as a d_{xz} -wave character. According to the formal symmetry classification of altermagnets¹, this behavior corresponds to a P-2 d_{xz} -wave state. These paths, which extend beyond the xy plane, have not been explored in previous studies, where ARPES experiments primarily focused on the xy plane^{27,39}. The following section discusses the preference for a specific direction in the AM character.

Table 1 | The first column represents the label for each magnetic configuration

	ΔE	E-state	M-phase	m (μ_B)
A	0	Metallic	AFM	1.44
B	34.90	N-Insulator	AM	1.35
C	36.46	Metallic	AM	1.38/1.45
D	39.22	N-Insulator	AFM	1.35

ΔE is the energy difference relative to configuration A ($E_{\text{conf.}} - E_A$) (meV/Ru) without spin-orbit coupling; E-phase and M-phase indicate the electronic state and the AFM/AM ordering, respectively; and m denotes the magnetic moment per Ru atom. Conf. A–C are metallic and Conf. B–D displays a Narrow (N) insulator state.

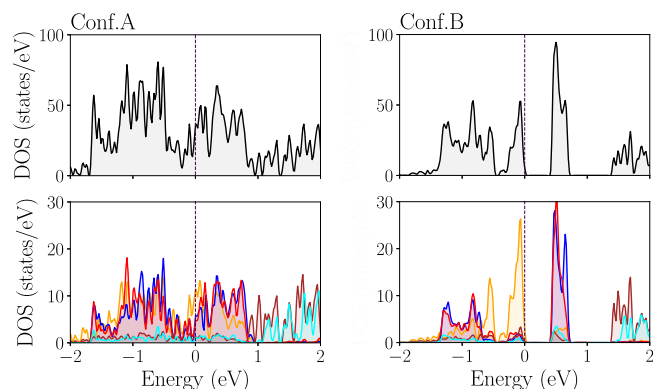
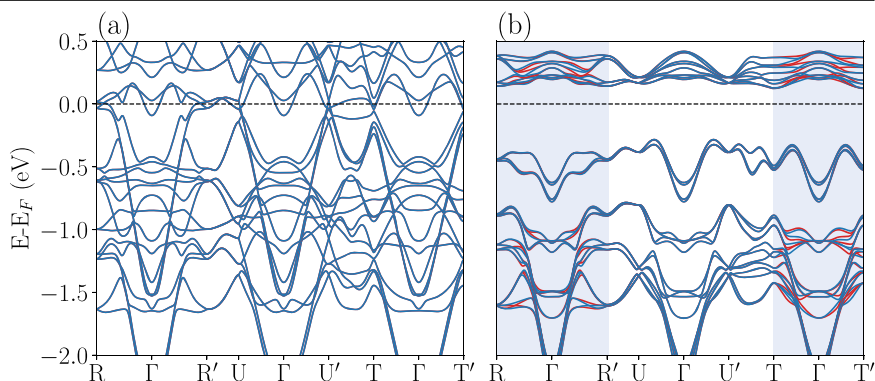


Fig. 3 | Density of states for $\text{Ca}_3\text{Ru}_2\text{O}_7$ in magnetic configurations A and B. The upper and lower panels display the total and Ru-4d projected density of states, respectively, for configurations A and B, shown in the left and right panels.

Fig. 4 | Spin-resolved band structure.

a, b Electronic band structure for configurations A and B, respectively. The blue region highlights the altermagnetic bands. The AM region along the R – Γ – R' and T – Γ – T' directions. In contrast, the AFM region is defined along the yz direction, represented by the U – Γ – U' path. Red and blue lines correspond to spin-up and spin-down, respectively. The Brillouin zone is given in Fig. 5.



The bands located between $[-2.0, -1.0]$ eV exhibit significant non-relativistic spin splitting, corresponding to the d_{xz} – d_{yz} orbitals. In contrast, the bands between $[-0.7, -0.5]$ eV, dominated by the d_{xy} orbital character, show negligible spin splitting (see, Fig. S3). Therefore, configuration B exhibits orbital-selective altermagnetism with the altermagnetism present in the d_{xz} – d_{yz} bands but not in the d_{xy} bands, this is similar to that observed in Ca_2RuO_4 ³⁸. When the k_x or k_z coordinate is inverted in reciprocal space, the non-relativistic spin splitting changes sign, while inversion of k_y leaves it unchanged. Notably, this altermagnetic order matches that found in Ca_2RuO_4 , despite its crystallization in a different space group³⁸. The orbital-selective magnetism depends on the magnetic space group and orbital character. In conf. B, the nearly filled d_{xy} orbitals do not contribute to magnetism, leading to orbital-selective AM. Consequently, conf. C displays different magnetic states in which all the t_{2g} orbitals contribute to the AM character; therefore, it does not exhibit orbital selective AM, see more details in Fig. S3.

The lack of inversion symmetry in $\text{Ca}_3\text{Ru}_2\text{O}_7$ enables sizable SOC effects, which play a central role in its magnetic properties²⁷. In configuration B, as in configuration A, the spins align primarily along the y -axis, with a slight canting toward z -axis ($(0, 1.3, 0.1) \mu_B$). SOC enriches the spin textures and activates symmetry-breaking mechanisms that lift band degeneracies, thereby enabling access to AM states that remain hidden in the collinear case.

Our spin-projected band structure analysis reveals how SOC qualitatively transforms the nature of altermagnetism in this system. The non-relativistic ground state exhibits a clear d -wave character, dominated by d_{xz} -like states along the high-symmetry paths shown in Fig. 4. Upon including SOC, a complex landscape emerges. The original d -wave features remain most evident in the $\langle S_y \rangle$ projection (Fig. 6a, b), consistent with the magnetic anisotropy along the b -axis. In stark contrast, the $\langle S_z \rangle$ projection unveils a completely new altermagnetic signature between -0.5

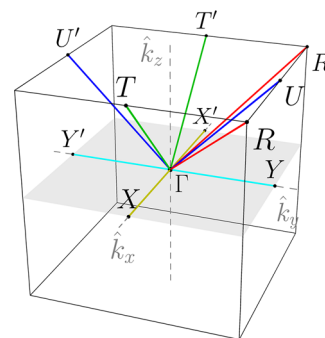


Fig. 5 | Brillouin zone of the orthorhombic structure. High-symmetry points related by symmetry are labeled as $R/R' = (\pm 0.5, 0.5, 0.5)$, $T/T' = (\pm 0.5, 0, 0.5)$, $U/U' = (0, \pm 0.5, 0.5)$, $Y/Y' = (0, \pm 0.5, 0)$, and $X/X' = (\pm 0.5, 0, 0)$, in units of the reciprocal lattice vectors.

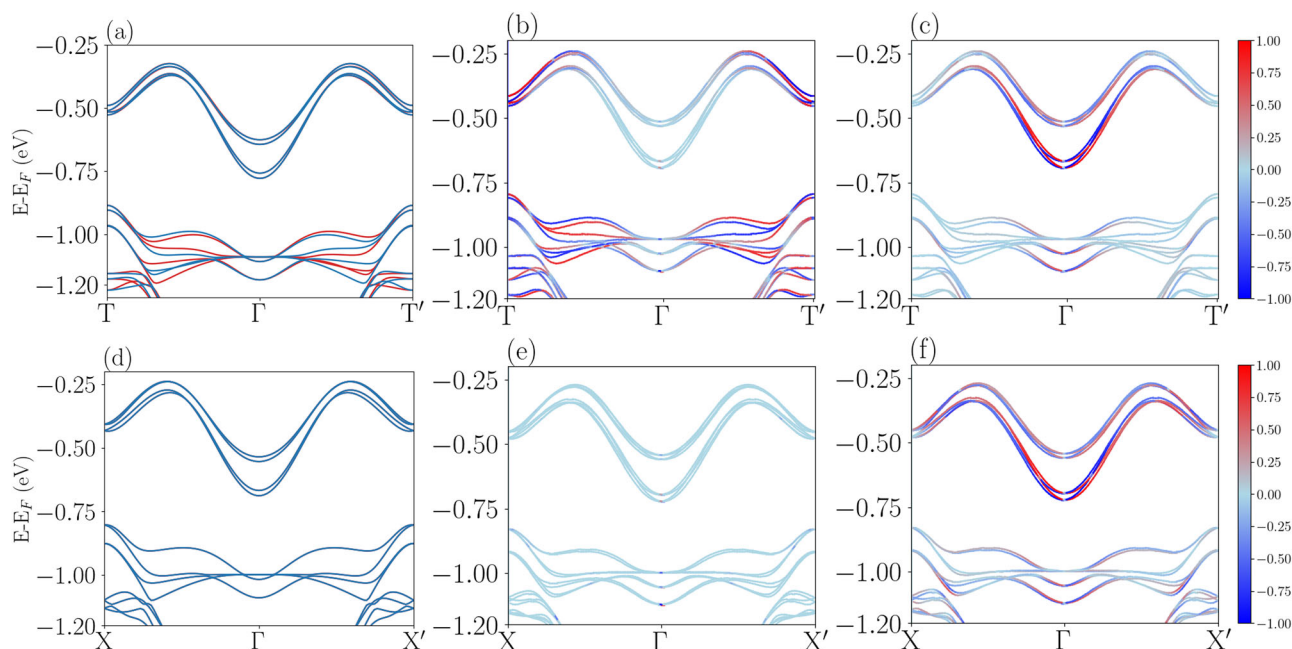


Fig. 6 | Comparison of band structures for $\text{Ca}_3\text{Ru}_2\text{O}_7$ without (NSOC) and with (SOC) spin-orbit coupling. Top row: Band structure along the $T - \Gamma - T'$ path. Bottom row: Band structure along the $X - \Gamma - X'$ path. For both paths, panels show

the NSOC case (a, d) and SOC projections along S_y (b, e) and S_z (c, f). The color scale indicates the spin expectation value (red: positive, blue: negative). The full energy range is shown in Fig. S4.

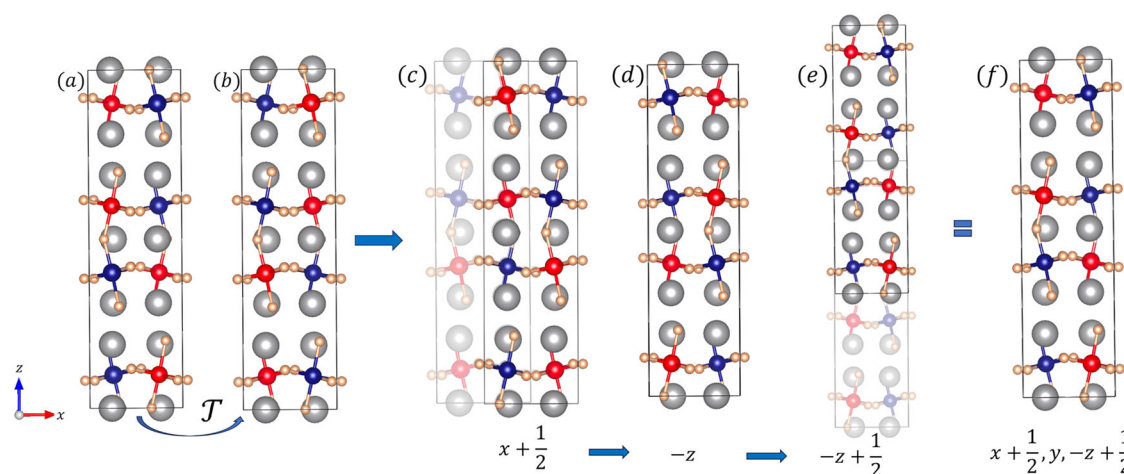


Fig. 7 | Symmetry operations responsible for the altermagnetic character of $\text{Ca}_3\text{Ru}_2\text{O}_7$ in the B magnetic configuration. \mathcal{T} denotes the time-reversal operator, which interchanges spin-up and spin-down states, represented by red and blue spheres, respectively. a Configuration B. b Spin exchange between spin-up and spin-

down via $\{\mathcal{T}\}$. c Half-unit-cell translation along the x axis ($x \rightarrow x + 0.5$). d Screw symmetry operation with $z \rightarrow -z$. e Half-unit-cell translation along the z axis. f Summary of combined nonsymmorphic operations yielding k-dependent splitting states.

and -0.75 eV, emerging from bands that were purely antiferromagnetic in the collinear case (Fig. 6a, c). The influence of SOC is particularly evident along the $X - \Gamma - X'$ direction. Here, SOC lifts the band degeneracy in the $\langle S_z \rangle$ channel, creating a spin splitting where the non-relativistic bands were degenerate (Fig. 6e, f) (similar results are found for $\langle S_x \rangle$ along k_z). This purely relativistic splitting exhibits a characteristic antisymmetric behavior for momentum inversion ($\mathbf{k} \rightarrow -\mathbf{k}$), which is the defining hallmark of a p -wave altermagnetic component.

Therefore, these findings demonstrate the emergence of a novel hybrid d/p -wave altermagnetic order. The AM+SOC phase in CRO is best described as a state where the non-relativistic d -wave component coexists with a purely SOC-driven p -wave character. This hybridization arises from the interplay between the magnetic structure and the crystal's nonsymmorphic symmetries.

While these results highlight a recently emerging regime of altermagnetism in the presence of SOC^{10,28}, a formal classification of this hybrid order, for instance, through advanced group-theoretical analysis, remains a substantial theoretical challenge. We describe the emergent AM + SOC features through their direct, symmetry-resolved signatures in the spin-projected electronic structure. Future studies will address a more systematic classification of AM + SOC spin textures.

Symmetry analysis

To understand the role of symmetry in AM-CRO, consider applying a time-reversal operator (TR), which in practical terms consists of an exchange between spin-up and spin-down (see Fig. 7a, b). Due to the distinct symmetry properties of many altermagnets, the original magnetic configuration cannot be recovered using only rotational symmetry operations. Following a

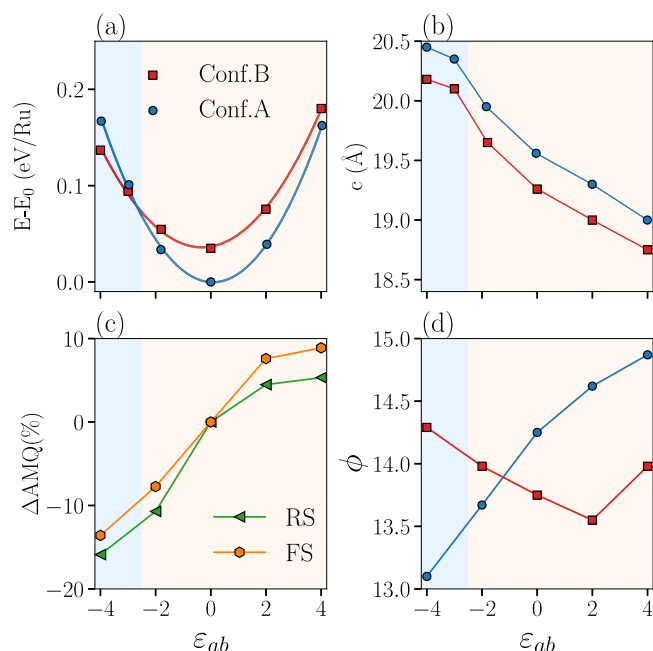


Fig. 8 | Effect of biaxial strain on structural and altermagnetic responses. **a** Total energy variation as a function of biaxial strain (ϵ_{ab}) for configurations A and B without spin-orbit coupling. **b** Evolution of the c -lattice parameter as a function of strain. **c** Variation of the altermagnetic merit quantity (AMQ), relative to the unstrained system, as defined in Eq. (3). Hexagons and triangles represent calculations performed under relaxed-structure (RS) and fixed-structure (FS) conditions, respectively, for configuration B. **d** Evolution of the RuO octahedral distortion angle (ϕ) for configurations A and B. Blue (red) shaded regions indicate strain ranges where the AM (AFM) phases are energetically favored.

time-reversal operation, a half-unit cell translation along the x -axis, shifting $x \rightarrow x + 0.5$ (Fig. 7c), is combined with a screw symmetry operation by inverting $z \rightarrow -z$ and adding a half-unit cell translation along the z -axis (Fig. 7d, e). In summary, the operation $(x + \frac{1}{2}, y, -z + \frac{1}{2})$ becomes necessary (Fig. 7f). These combined nonsymmorphic operations result in the k -dependent splitting states¹. Due to the symmetry operations that connect the spins, which are determined by rotations and translations along the x and z directions while leaving the y direction unchanged, the AM character is found along these axes, as shown in Fig. 4. In the case of the C configuration, the symmetry operation $(x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2})$ becomes necessary to achieve AM order. This symmetry operation is specific to the orthorhombic space group Bb2₁m. Since the crystallographic axes are not symmetry-equivalent, this operation does not remain valid under the replacement $x \rightarrow y$.

Tuning AFM to AM phases

To analyze the stability of configurations A and B, we calculated their total energies under various biaxial strain conditions (Fig. 8a). Configuration B shows the lowest energy within a compressive strain below -2% . Figure 8b shows the c -lattice parameter for each strain. These results suggest a potential magnetic transition from AFM to AM states in CRO.

Next, we investigate the effects of compressive ($-\epsilon$) and tensile ($+\epsilon$) strain on the AM features of CRO. Figure 9 shows the band structure of configuration B under strains of $\epsilon = -2\%$, 0 , and 2% (biaxial). It can be observed that compressive strain suppresses the AM features among the energy range $[-2; -1]$ eV (compare Figs. 9a with Fig. b). Moreover, the tensile strain enhances the splitting and shifts it to higher energies.

To quantify the effect of strain on the altermagnetic features of CRO, we calculate the average difference between spin-up and spin-down eigenvalues $\langle \Delta E(\mathbf{k}) \rangle$ for each occupied band along the entire \mathbf{k} -path. Additionally, we define the altermagnetic quantity (AMQ) as the altermagnetic

figure of merit, which integrates $\Delta E(\mathbf{k})$ over the Brillouin zone. The AMQ is a numerical measure of the overall altermagnetic character of a system, providing a quantitative basis for comparing different strain conditions.

In our implementation, we read the spin-resolved eigenvalues from the EIGENVAL file generated by VASP, then compute the \mathbf{k} -dependent average splitting $\langle \Delta E(\mathbf{k}) \rangle$ as the cumulative sum over occupied states along a particular set of \mathbf{k} points (over a \mathbf{k} -path or \mathbf{k} -grid), given by:

$$\langle \Delta E(\mathbf{k}) \rangle = \sum_{j=1}^{N_{occ}} \left| \frac{1}{N_k} \sum_{i=1}^{N_k} [E_{down}(\mathbf{k}_{i,j}) - E_{up}(\mathbf{k}_{i,j})] \right|, \quad (1)$$

where N_k is the numbers of bands at \mathbf{k} -point within specified energy range and N_{occ} is the occupied bands.

Note that the integration to obtain the AMQ can be performed either over the entire Brillouin zone or along a specific \mathbf{k} -path. We verified that both methods yield similar solutions; the only difference is a constant multiplicative factor, which cancels out when computing percentage changes.

We sum up all the occupied states rather than comparing only a few selected bands. This approach proves more reliable because the most strongly split bands can vary across different systems and even within the same material under strain, depending on details such as band character and crystal symmetry. Consequently, integrating over the entire set of occupied bands offers a more robust assessment of the altermagnetic spin-splitting.

The AMQ quantifies the spin-splitting across momentum space by integrating $\langle \Delta E(\mathbf{k}) \rangle$:

$$AMQ = \int_{BZ} \langle \Delta E(\mathbf{k}) \rangle d\mathbf{k}, \quad (2)$$

in our code, Simpson's rule is used for numerical integration. When \mathbf{k} points are expressed in inverse angstroms (\AA^{-1}), the resulting AMQ is in units of $\text{eV} \times \text{\AA}$. Although the AMQ is not a formal symmetry-derived order parameter like magnetic multipoles⁴⁰, it provides a symmetry-consistent and practical metric to quantify momentum-resolved spin splitting in systems with zero net magnetization. While this approach is robust, it may fail near band crossings or overlapping bands. A more rigorous treatment, such as disentanglement via Wannier-based orbital tracking, could refine the analysis but lies beyond the scope of this study. Nonetheless, the observed vanishing of spin splitting at high-symmetry points and the overall internal consistency strongly support the identification of altermagnetic behavior.

Since our primary goal is to evaluate strain effects on the altermagnetic state, we compare the AMQ under strain to the unstrained scenario. We define the percent variation ΔAMQ as:

$$\Delta AMQ = \frac{AMQ(\epsilon) - AMQ(\epsilon = 0)}{AMQ(\epsilon = 0)} \times 100. \quad (3)$$

This relative measure properly captures how strain modifies the degree of altermagnetic spin-splitting throughout the Brillouin zone.

Figure S6 shows the evolution of the spin splitting $\langle \Delta E(k) \rangle$ across the full \mathbf{k} -path and occupied bands under different strain conditions (see Brillouin zone in Fig. 4). The magnitude of band-dependent altermagnetic splitting varies with strain, increasing notably under tensile strain. The AQM response varies by approximately $+8\%$ under tensile strain (2%) and -11% under compressive strain (-2%), as shown in Fig. 8c. All computational details and equations are provided in the SM file (Fig. S7).

To further dissect the symmetry of the spin splitting in three dimensions (details provided in the SM, section SVI), we perform a multipolar analysis of the energy texture $\Delta E^{\theta}(\mathbf{k})$. In the non-relativistic limit, the response is purely even in k , confirming the expected pure d-wave altermagnetic state dictated by symmetry. Including SOC activates odd-parity components and transforms the system into a hybrid state with concurrent

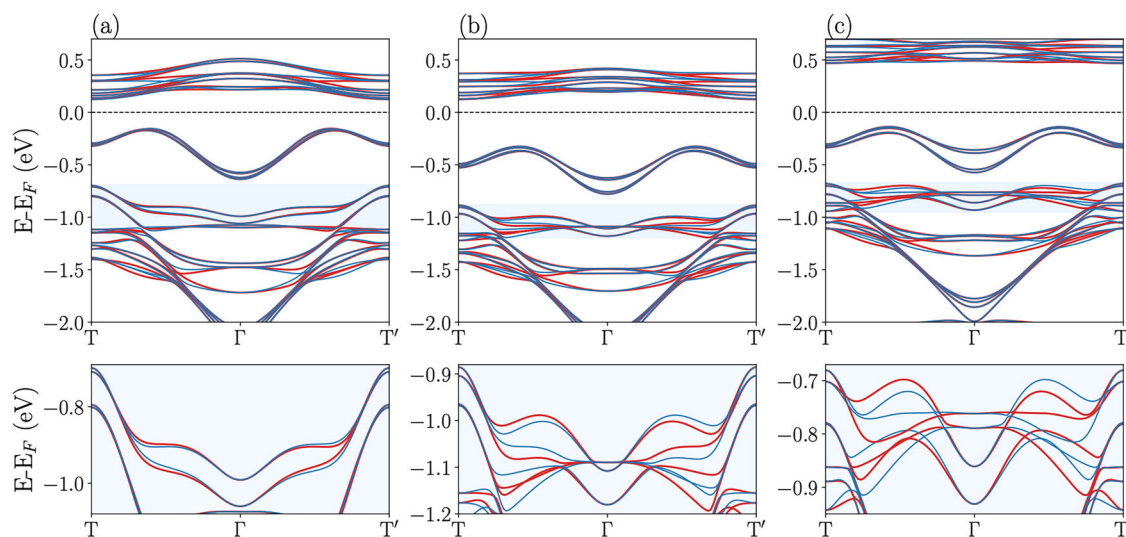


Fig. 9 | Strain dependence of altermagnetic band splitting. Top row: non-relativistic band structures of configuration B under three strain conditions: **a** -2% compressive, **b** 0% (unstrained), and **c** +2% tensile, plotted along the selected path.

Bottom row: zoomed-in view of the region showing the strongest altermagnetic features, which varies with strain. Red and blue lines correspond to spin-up and spin-down, respectively.

p -, d -, and f -wave character. Using spinor band pairs near the Fermi level, we find overall p -wave dominance, with fractional L^1 -norm weights $f_p \approx 0.47$, $f_d \approx 0.29$, and $f_f \approx 0.24$. The hybridization is strongly anisotropic across spin channels: the x and z components are p -dominated (f_p 0.59, $f_p \approx 0.60$), whereas the y component is d -dominated ($f_d \approx 0.59$).

Discussion

The non-relativistic spin-splitting in CRO arises from the interplay between hopping parameters and the opposite on-site spin polarizations in the two magnetic sublattices. Strain introduces competing effects that influence these parameters: compression along one axis promotes electronic delocalization, weakening magnetism and reducing the AM band splitting, whereas tensile strain favors localization, enhancing magnetic exchange and increasing the AM band splitting.

From the energy-strain relationship shown in Fig. 8a, we observe that configuration B (the AM phase) becomes energetically more favorable than configuration A (the AFM phase) under biaxial compressive strain ($\varepsilon_{ab} < -2\%$). Compressive strain decreases the in-plane Ru–O bond lengths, forcing an expansion along the c -axis. This expansion modifies the balance of structural distortions and stabilizes configuration B over configuration A. At the electronic level, the in-plane compression broadens the bands, weakening the magnetic exchange interactions and consequently reducing the AM band splitting. Conversely, under tensile strain, the lattice is stretched in the ab -plane while slightly contracting along c , effectively narrowing the bandwidth and reinforcing the altermagnetic character (Fig. S5). This effect is reflected in the rising AMQ values in Fig. 8c RS line (relaxed structures), demonstrating how strain can selectively enhance or suppress altermagnetic character.

To further assess the role of structural distortions, we performed an additional set of calculations where the atomic positions remained fixed at their zero-strain configuration. At the same time, only the lattice parameters were modified (fixed structure (FS) calculations). The results, depicted by the FS line in Fig. 8c, reveal a similar overall trend: AMQ increases under tensile strain and decreases under compressive strain. However, for $\varepsilon_{ab} > 2\%$, the deviation between the relaxed and non-relaxed calculations becomes more pronounced, suggesting that octahedral distortions (ϕ) play a secondary but non-negligible role in the strain response of the AM phase. Specifically, as seen in Fig. 8d, ϕ increases under compressive strain for configuration B, further enhancing localization effects that help sustain the AM band splitting. A direct comparison between the relaxed structures and

the non-relaxed structures allows us to disentangle the effects of strain-induced delocalization/localization from those arising purely from octahedral distortions. In particular, the density of states in Fig. S5 confirms that compressive strain broadens states, reducing AM features. In contrast, tensile strain narrows the bandwidth, reinforcing the AM character. Moreover, the band structures shown in Fig. S7 illustrate how freezing the atomic positions primarily alters the gap structure rather than the AM spin splitting itself, reinforcing the observation that the observed strain-dependent AM behavior is primarily dictated by electronic exchange interactions, with octahedral distortions acting as a secondary fine-tuning mechanism.

Furthermore, Fig. 8d reveals how the RuO octahedral distortion angle ϕ responds to biaxial strain in each magnetic configuration. In configuration A, ϕ increases smoothly from -4% to $+4\%$ strain. Configuration B shows a more intricate pattern: under compressive strain ($\varepsilon_{ab} < 0$), ϕ increases as the lattice compresses in the plane. This response reflects stronger electronic localization in the antiferromagnetic arrangement (see Fig. 3b), which preserves magnetic exchange by enhancing octahedral distortion. Under tensile strain, in-plane expansion tends to relax distortions while the slight contraction along the c axis reinforces them. The net change in ϕ depends on the balance between these two opposing effects.

The evolution of ϕ in configuration B correlates directly with the energy profile in Fig. 8a. Above 2% compressive strain, configuration B becomes lower in energy than configuration A and ϕ increases sharply. This coincidence demonstrates that enhanced octahedral distortion drives the AFM-to-AM transition. Although such strain levels are challenging to achieve in bulk crystals, epitaxial oxide films can routinely accommodate comparable lattice mismatches, providing a practical platform to realize and probe distortion-driven magnetic and electronic phase transitions in layered perovskites^{41–44}.

This work investigates the emergence of altermagnetic states in the correlated oxide $\text{Ca}_3\text{Ru}_2\text{O}_7$. While its ground state is not altermagnetic, symmetry-allowed AM order arises in alternative spin configurations. In the non-relativistic case, Configuration B, characterized by a Néel-type spin pattern, hosts a P-2 d_{xz} -wave altermagnetic state.

Including spin-orbit coupling with the Néel vector along b induces additional symmetry breaking, allowing a p -wave component in the spin texture. This hybridization between d - and p -wave features may result from the absence of inversion symmetry and the presence of nonsymmorphic operations. A complete understanding of the p -wave origin will require

further analysis based on spin space group symmetries under non-collinear magnetism.

Although configuration B has not been reported in pristine $\text{Ca}_3\text{Ru}_2\text{O}_7$, it appears in doped compounds such as $\text{Ca}_3(\text{Ti}_x\text{Ru}_{1-x})_2\text{O}_7$, suggesting that suitable conditions can stabilize the AM state. Our results further demonstrate that biaxial strain acts as an effective tuning parameter for the alternative magnetic band splitting: tensile strain (or equivalently, compression along the c -axis) enhances the splitting by approximately 9% at 2% strain, whereas compressive strain reduces it by about 11%. We also predict a strain-induced transition from the AFM ground state to the AM state beyond 2% compressive strain. While prior studies have used uniaxial strain to manipulate magnetic anisotropy²⁶, the effects of biaxial strain remain largely unexplored.

Inducing altermagnetism in $\text{Ca}_3\text{Ru}_2\text{O}_7$ would create a rare non-centrosymmetric altermagnetic material and provide a platform to explore the interplay between odd- and even-wave spin-momentum locking. Identifying such phases would broaden the spectrum of quantum phenomena known in the $\text{Ca}_{n+1}\text{Ru}_n\text{O}_{3n+1}$ family, which already exhibits strain-tunable transitions, including Mott suppression in Ca_2RuO_4 (~4% strain)¹⁸, the emergence of a Kondo effect, and a metal-to-semiconductor transition in CaRuO_3 (~3.6% strain)⁴¹. Our results highlight biaxial strain as a promising route to control altermagnetic phases in $\text{Ca}_{n+1}\text{Ru}_n\text{O}_{3n+1}$ -related materials, aligning with recent proposals to manipulate antiferromagnetic-altermagnetic phase transitions via strain^{4,45}. These findings motivate further exploration of symmetry-driven spin textures in systems with strong spin-orbit coupling.

Note: Recent studies have shown that SOC can induce interesting phenomena such as polarization switching in $\text{Ca}_3\text{Mn}_2\text{O}_7$, driven by magnetic anisotropy²⁸. Given its structural similarity to $\text{Ca}_3\text{Ru}_2\text{O}_7$, our results suggest that $\text{Ca}_3\text{Mn}_2\text{O}_7$ may also host mixed-symmetry altermagnetic order under SOC. Further exploration of this system could offer new pathways for tuning altermagnetic behavior via SOC.

Methods

We perform a theoretical analysis using the density functional theory with and without spin-orbit coupling. We use the plane-wave pseudopotential method implemented in the Vienna ab-initio simulation package (VASP)⁴⁶ within the generalized gradient approximations (GGA), and it gives structural properties closer to the experimental values. The electronic valence considered are: Ru: $5s^14d^7$ and O: $2s^22p^4$, and Ca: $3s^3p^4s$. We use a plane-wave energy cutoff of 650 eV and set a Regular Monkhorst–Pack grid of $7 \times 7 \times 5$ to perform the atomic relaxation and $11 \times 11 \times 7$ to perform the self-consistent calculation. We use a fine k-grid of $14 \times 14 \times 7$ within the tetrahedron method for the density of states. We perform the structural optimization of the unit cell until a force convergence threshold of at least 10^{-3} eV/Å per atom.

To account for electronic correlations in the Ru d -orbitals, we use the Dudarev approach⁴⁷ with an effective Hubbard parameter $U = 1.0$ eV, previously shown to yield accurate structural and electronic properties for CrO_2 ³⁴. We use a Cartesian coordinate system with crystallographic axes aligned as $\mathbf{a} \parallel \hat{x}$, $\mathbf{b} \parallel \hat{y}$, and $\mathbf{c} \parallel \hat{z}$.

Data availability

All data supporting the findings of this study are included in the article and its Supplementary Information.

Code availability

Density functional theory calculations were performed using the Vienna ab initio Simulation Package (VASP), accessed under an institutional license through the high-performance computer at the NHR Center of TU Dresden and on the high-performance computers Noctua 2 at the NHR Center PC2. Custom Python scripts developed for post-processing and analysis are available from the corresponding author upon reasonable request.

Received: 6 April 2025; Accepted: 12 August 2025;

Published online: 26 September 2025

References

- Šmejkal, L., Sinova, J. & Jungwirth, T. Beyond conventional ferromagnetism and antiferromagnetism: a phase with nonrelativistic spin and crystal rotation symmetry. *Phys. Rev. X* **12**, 031042 (2022).
- Bai, L., Feng, W., Liu, S., Šmejkal, L., Mokrousov, Y. & Yao, Y. Altermagnetism: Exploring new frontiers in magnetism and spintronics. *Adv. Funct. Mater.* **34**, 2409327 (2024).
- Sato, T., Haddad, S., Fulga, I. C., Assaad, F. F. & van den Brink, J. Altermagnetic anomalous hall effect emerging from electronic correlations. *Phys. Rev. Lett.* **133**, 086503 (2024).
- Chakraborty, A., González Hernández, R., Šmejkal, L. & Sinova, J. Strain-induced phase transition from antiferromagnet to altermagnet. *Phys. Rev. B* **109**, 144421 (2024).
- Takahashi, K., Steward, C. R., Ogata, M., Fernandes, R. M. & Schmalian, J. Elasto-Hall conductivity and the anomalous Hall effect in altermagnets. *Phys. Rev. B* **111**, 184408 (2025).
- Dzyaloshinsky, I. A thermodynamic theory of “weak” ferromagnetism of antiferromagnetics. *J. Phys. Chem. Solids* **4**, 241–255 (1958).
- Autieri, C., Sattigeri, R. M., Cuono, G. & Fakhredine, A. Staggered Dzyaloshinskii–Moriya interaction inducing weak ferromagnetism in centrosymmetric altermagnets and weak ferrimagnetism in noncentrosymmetric altermagnets. *Phys. Rev. B* **111**, 054442 (2025).
- Roig, M., Yu, Y., Ekman, R. C., Kreisel, A., Andersen, B. M. & Agterberg, D. F. Quasimagnetism-constrained spin ferromagnetism in altermagnets. *Phys. Rev. Lett.* **135**, 016703 (2025).
- Cheong, S. W. & Huang, F. T. Altermagnetism classification. *npj Quantum Mater* **10**, 38 (2025).
- Cheong, S.-W. & Huang, F.-T. Altermagnetism with non-collinear spins. *npj Quantum Mater.* **9**, 13 (2024).
- Kluczyk, K. P. et al. Coexistence of anomalous Hall effect and weak magnetization in a nominally collinear antiferromagnet MnTe. *Phys. Rev. B* **110**, 155201 (2024).
- Jo, D., Go, D., Mokrousov, Y., Oppeneer, P. M., Cheong, S. W. & Lee, H. W. Weak ferromagnetism in altermagnets from alternating g-tensor anisotropy. *Phys. Rev. Lett.* **134**, 196703 (2025).
- Bernardini, F., Fiebig, M. & Cano, A. Ruddlesden–Popper and perovskite phases as a material platform for altermagnetism. *J. Appl. Phys.* **137**, 103903 (2025).
- Autieri, C., Cuono, G., Chakraborty, D., Gentile, P. & Black-Schaffer, A. M. Conditions for orbital-selective altermagnetism in Sr_2RuO_4 : Tight-binding model, similarities with cuprates, and implications for superconductivity. *Phys. Rev. B* **112**, 014412 (2025).
- Naka, M., Motome, Y. & Seo, H. Altermagnetic perovskites. *npj Spintronics* **3**, 1 (2025).
- Bernardini, F., Fiebig, M. & Cano, A. Ruddlesden–popper and perovskite phases as a material platform for altermagnetism. *J. Appl. Phys.* **137**, 103903 (2025).
- Li, Y., Leeb, V., Wohlfeld, K., Valenti, R. & Knolle, J. d-wave magnetism in cuprates from oxygen moments. *arXiv preprint arXiv:2412.11922* (2024).
- Ricco, S. et al. In situ strain tuning of the metal-insulator-transition of Ca_2RuO_4 in angle-resolved photoemission experiments. *Nat. Commun.* **9**, 4535 (2018).
- Tiwari, P. et al. Suppression of field-induced spin density wave order in $\text{Sr}_3\text{Ru}_2\text{O}_7$ with pressure. *Phys. Rev. B* **108**, 115154 (2023).
- Maeno, Y., Yonezawa, S. & Ramires, A. Still mystery after all these years—unconventional superconductivity of Sr_2RuO_4 . *J. Phys. Soc. Jpn* **93**, 062001 (2024).
- Yoshida, Y. et al. Crystal and magnetic structure of $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Phys. Rev. B* **72**, 054412 (2005).
- Kikugawa, N. et al. $\text{Ca}_3\text{Ru}_2\text{O}_7$: electronic instability and extremely strong quasiparticle renormalisation. *J. Magn. Magn. Mater.* **310**, 1027–1029 (2007).
- von Arx, K. et al. Resonant inelastic x-ray scattering study of $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Phys. Rev. B* **102**, 235104 (2020).

24. Ohmichi, E., Yoshida, Y., Ikeda, S., Shirakawa, N. & Osada, T. Colossal magnetoresistance accompanying a structural transition in a highly two-dimensional metallic state of $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Phys. Rev. B* **70**, 104414 (2004).
25. Karpus, J. et al. Spectroscopic study of the field- and pressure-induced phases of the bilayered ruthenate $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Phys. Rev. B* **73**, 134407 (2006).
26. Dashwood, C. et al. Strain control of a bandwidth-driven spin reorientation in $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Nat. Commun.* **14**, 6197 (2023).
27. Marković, I. et al. Electronically driven spin-reorientation transition of the correlated polar metal $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Proc. Natl Acad. Sci. USA* **117**, 15524–15529 (2020).
28. Šmejkal, L. Altermagnetic multiferroics and altermagnetoelectric effect. Preprint at *arXiv* <https://doi.org/10.48550/arXiv.2411.19928> (2024).
29. Grzybowski, M. J. et al. Wurtzite vs. rock-salt MnSe epitaxy: electronic and altermagnetic properties. *Nanoscale* **16**, 6259–6267 (2024).
30. Schiff, H., McClarty, P., Rau, J. G. & Romhányi, J. Collinear altermagnets and their Landau theories. Preprint at *arXiv* <https://doi.org/10.48550/arXiv.2412.18025> (2024).
31. Gallego, S. V., Tasci, E. S., Flor, G., Perez-Mato, J. M. & Aroyo, M. I. Magnetic symmetry in the Bilbao crystallographic server: a computer program to provide systematic absences of magnetic neutron diffraction. *J. Appl. Crystallogr.* **45**, 1236–1247 (2012).
32. Ke, X. et al. Emergent electronic and magnetic state in $\text{Ca}_3\text{Ru}_2\text{O}_7$ induced by Ti doping. *Phys. Rev. B* **84**, 201102 (2011).
33. Rivero, P. et al. Predicting hidden bulk phases from surface phases in bilayered $\text{Sr}_3\text{Ru}_2\text{O}_7$. *Sci. Rep.* **7**, 10265 (2017).
34. León, A., González, J. & Rosner, H. $\text{Ca}_3\text{Ru}_2\text{O}_7$: Interplay among degrees of freedom and the role of the exchange correlation. *Phys. Rev. Mater.* **8**, 024411 (2024).
35. González, J., León, A., González-Fuentes, C. & Gallardo, R. Altermagnetism in two-dimensional Ca_2RuO_4 perovskite. *Nanoscale* **17**, 4796–4807 (2025).
36. Puggioni, D., Horio, M., Chang, J. & Rondinelli, J. M. Cooperative interactions govern the fermiology of the polar metal $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Phys. Rev. Res.* **2**, 023141 (2020).
37. Liu, G.-Q. Mott transition and magnetic anisotropy in $\text{Ca}_3\text{Ru}_2\text{O}_7$. *Phys. Rev. B* **84**, 235137 (2011).
38. Cuono, G., Sattigeri, R. M., Skolimowski, J. & Autieri, C. Orbital-selective altermagnetism and correlation-enhanced spin-splitting in strongly-correlated transition metal oxides. *J. Magn. Magn. Mater.* **586**, 171163 (2023).
39. Horio, M. et al. Electronic reconstruction forming a C 2-symmetric Dirac semimetal in $\text{Ca}_3\text{Ru}_2\text{O}_7$. *npj Quantum Mater.* **6**, 29 (2021).
40. Bhowal, S. & Spaldin, N. A. Ferroically ordered magnetic octupoles in d-wave altermagnets. *Phys. Rev. X* **14**, 011019 (2024).
41. Wang, Z. et al. Transport and magnetic properties of Hund's metal CaRuO_3 under strain modulation. *Phys. Rev. B* **110**, L041403 (2024).
42. Burganov, B. et al. Strain control of fermiology and many-body interactions in two-dimensional ruthenates. *Phys. Rev. Lett.* **116**, 197003 (2016).
43. Dong, M. et al. Polar metallicity controlled by epitaxial strain engineering. *Adv. Sci.* **11**, 2408329 (2024).
44. Tsubaki, K. et al. Significant effects of epitaxial strain on the nonlinear transport properties in Ca_2RuO_4 thin films with the current-driven transition. *Jpn. J. Appl. Phys.* **63**, 01SP03 (2023).
45. Xun, W., Liu, X., Zhang, Y., Wu, Y.-Z. & Li, P. Stacking-, strain-engineering induced altermagnetism, multipezo effect, and topological state in two-dimensional materials. *Appl. Phys. Lett.* **126**, 161903 (2025).
46. Kresse, G. & Furthmüller, J. Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set. *Comput. Mater. Sci.* **6**, 15–50 (1996).
47. Dudarev, S. L., Botton, G. A., Savrasov, S. Y., Humphreys, C. & Sutton, A. P. Electron-energy-loss spectra and the structural stability of nickel oxide: an LSDA+U study. *Phys. Rev. B* **57**, 1505 (1998).
48. Yuan, L.-D., Zhang, X., Acosta, C. M. & Zunger, A. Uncovering spin-orbit coupling-independent hidden spin polarization of energy bands in antiferromagnets. *Nat. Commun.* **14**, 5301 (2023).

Acknowledgements

A.L. thanks the Technische Universität Dresden Professor Fellowship Program. C. A. acknowledges the useful discussion with G. Cuono and A. Fakhredine about altermagnetism in Ca_2RuO_4 . C. A. is supported by the Foundation for Polish Science project “Mag- Top” no. FENG.02.01-IP.05-0028/23 co-financed by the European Union from the funds of Priority 2 of the European Funds for a Smart Economy Program 2021–2027 (FENG). J.W.G. acknowledges financial support from Chilean ANID-FONDECY grants N. 1220700 and 1221301. T.B. would like to thank the German Science Foundation (DFG) for supporting this work via the German–Israeli Project Cooperation with the Grant No. HE 3543/42-1. The authors gratefully acknowledge the computing time made available to them on the high-performance computer at the NHR Center of TU Dresden and on the high-performance computers Noctua 2 at the NHR Center PC2.

Author contributions

A.L. and J.G. performed the calculations and contributed to the organization of the article. A.L. and C.A. held foundational discussions about the study. A.L., J.G., and C.A. carried out the symmetry analysis. A.L. and T.B. performed the electronic structure analysis. A.L., J.G., and C.A. wrote the initial draft. All authors contributed to the discussion of the results and collaborated in editing and shaping the final version of the paper.

Funding

Open Access funding enabled and organized by Projekt DEAL.

Competing interests

The authors declare no competing interests.

Additional information

Supplementary information The online version contains supplementary material available at <https://doi.org/10.1038/s41535-025-00814-y>.

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