

**RESEARCH ARTICLE**

## Shear-strain-induced switchable spin splitting and piezomagnetic properties in altermagnetic materials

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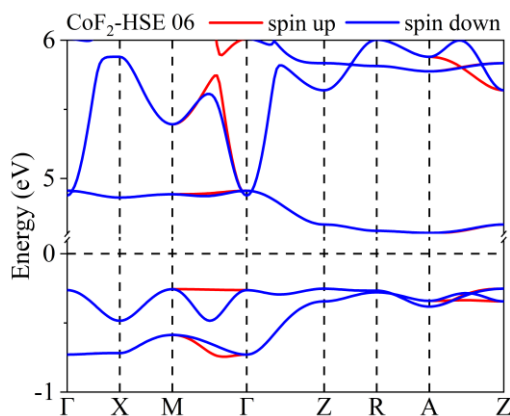
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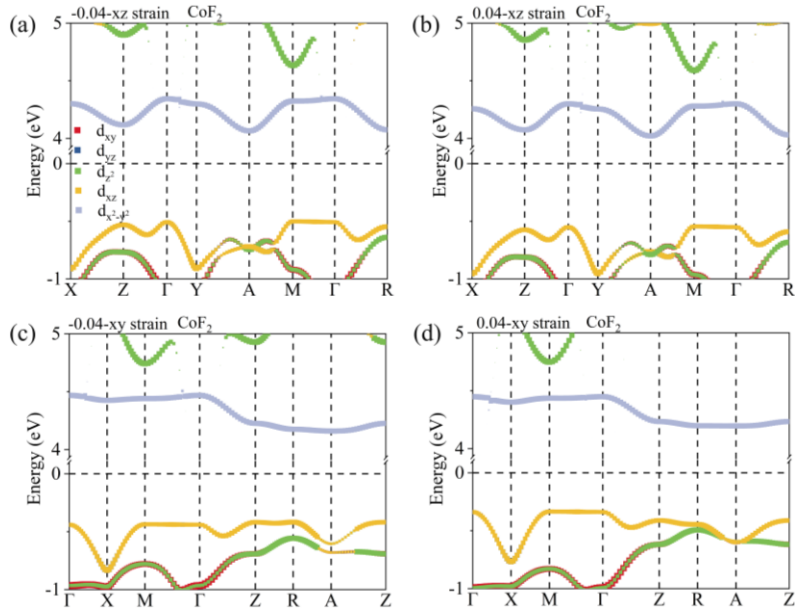
### Supporting Information

**Table 1** The symmetries of the space group before and after shear strain.

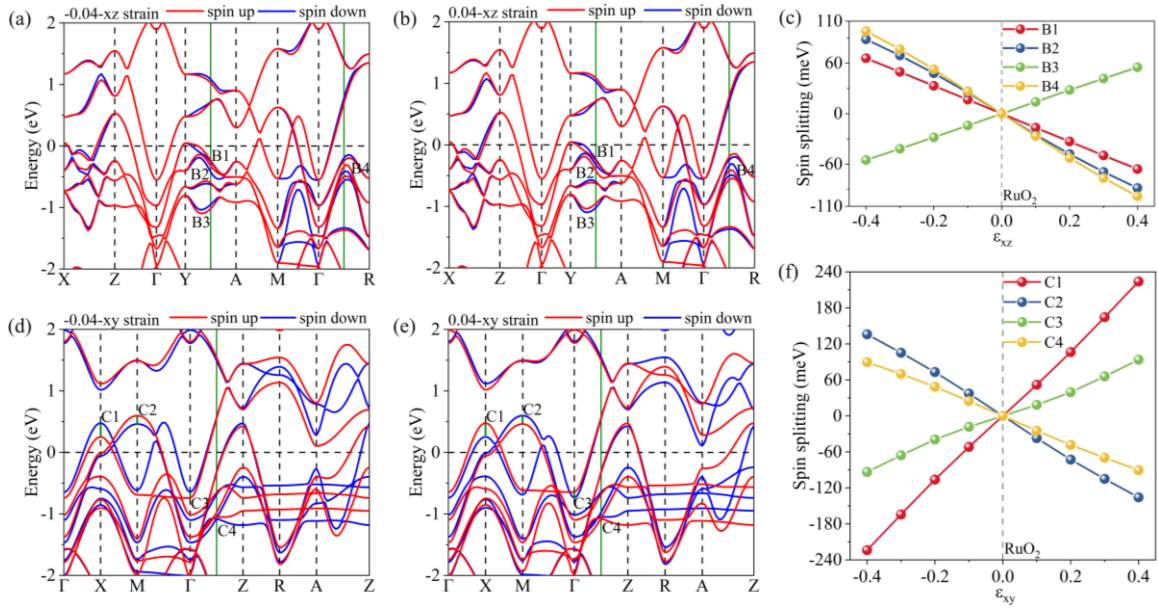
	CoF <sub>2</sub>		RuO <sub>2</sub>	
Strain	$\epsilon_{xz}$	$\epsilon_{xy}$	$\epsilon_{xz}$	$\epsilon_{xy}$
0	P4 <sub>2</sub> /mnm	P4 <sub>2</sub> /mnm	P4 <sub>2</sub> /mnm	P4 <sub>2</sub> /mnm
non-zero	P2 <sub>1</sub> /c	P2/m	P2 <sub>1</sub> /c	P2/m



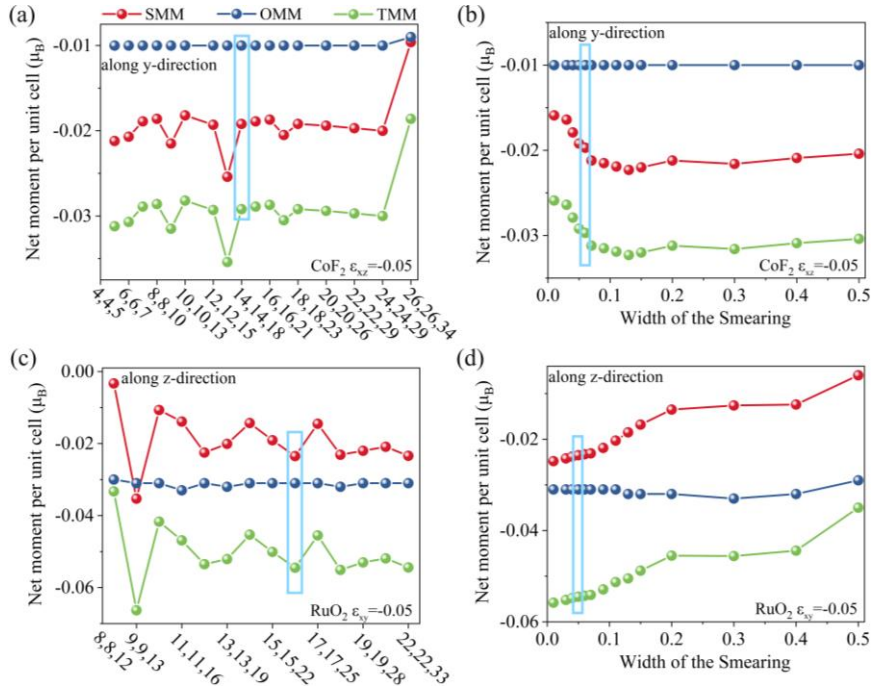
**Fig. S1** The band structure of altermagnetic CoF<sub>2</sub> calculated using the HSE06 hybrid functional.



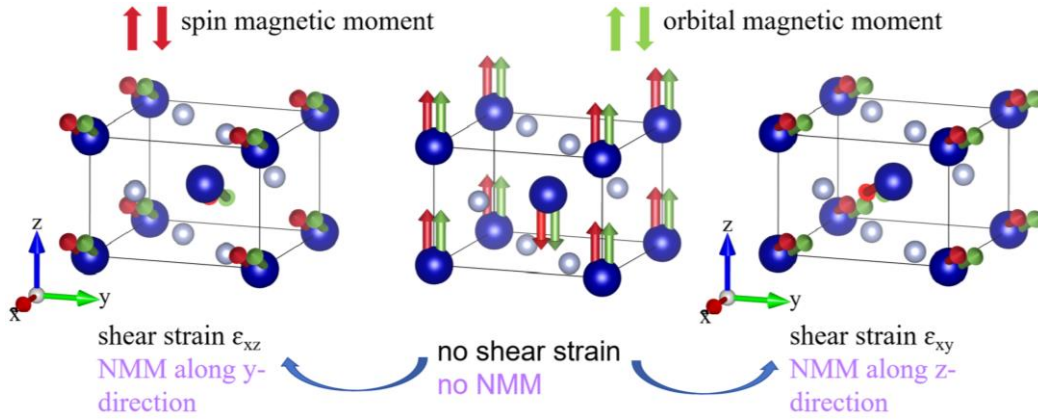
**Fig. S2** The 3d orbital-resolved band structure of antiferromagnetic  $\text{CoF}_2$  under shear strain  $\varepsilon_{xz}$  for (a) -0.04 and (b) 0.04, and under shear strain  $\varepsilon_{xy}$  for (c) -0.04 and (d) 0.04.



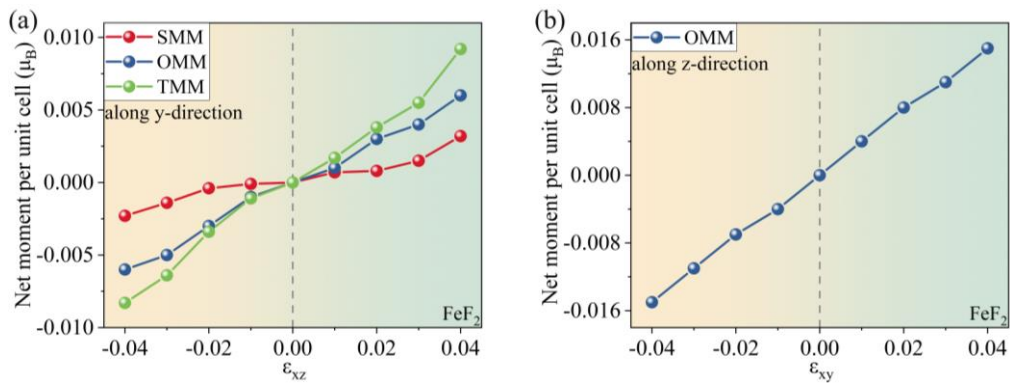
**Fig. S3** Band structures of  $\text{RuO}_2$  under shear strain  $\varepsilon_{xz}$  for (a) -0.04 and (b) 0.04, and under shear strain  $\varepsilon_{xy}$  for (d) -0.04 and (e) 0.04. The SOC effect is not considered in the calculations. Spin-up and spin-down components are marked in red and blue lines, respectively. The green line represents the individual SS energy difference. (c, f) SS corresponds to four selected points in (a,b) and (d,e).



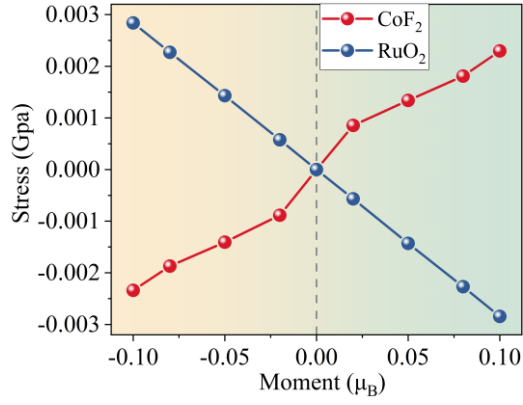
**Fig. S4** K-point and width of the smearing convergence tests of CoF<sub>2</sub> and RuO<sub>2</sub> by PBE+U [5.5 (1.5) eV] calculations.



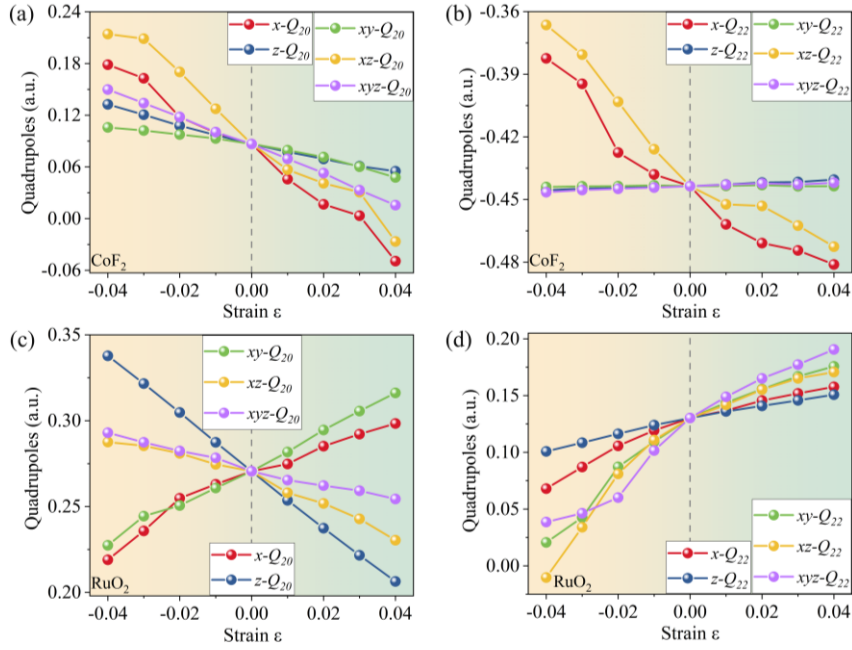
**Fig. S5** Spin and orbital magnetic moment distributions as functions of applied shear strain.



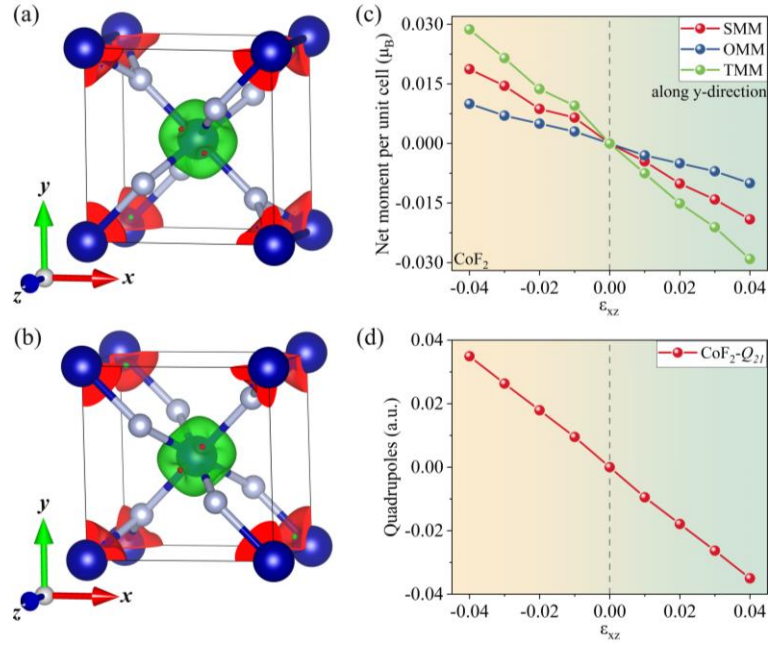
**Fig. S6** Piezomagnetic effects in altermagnet FeF<sub>2</sub>. The variation of (a) and (b) the net magnetic moment along the y and z direction as the shear strain  $\epsilon_{xz}$  and  $\epsilon_{xy}$  is varied.



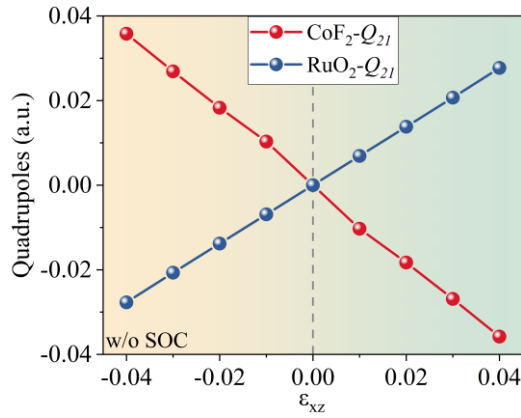
**Fig. S7** Variations in the  $xz$  direction stress of  $\text{CoF}_2$  and  $\text{RuO}_2$  with the magnetic moment of the  $y$  direction.



**Fig. S8** The charge quadrupole moments (a)  $Q_{20}$  and (b)  $Q_{22}$  of Co atoms in  $\text{CoF}_2$  as functions of the relative shear stress strength  $\varepsilon$ . The charge quadrupole moments (c)  $Q_{20}$  and (d)  $Q_{22}$  of Ru atoms in  $\text{RuO}_2$  as functions of the relative shear stress strength  $\varepsilon$ . Here,  $x$ ,  $z$  represents uniaxial strain,  $xy$ ,  $xz$  represents biaxial strain, and  $xyz$  represents triaxial strain.



**Fig. S9** The charge densities in the  $x$ - $y$  plane for the (a) crystal structure of CoF<sub>2</sub> and (b) modified structure. Piezomagnetic effects in CoF<sub>2</sub> with modified structure. (c) Variation of the net magnetic moment along the  $y$ -direction as the shear strain  $\epsilon_{xz}$ . Variations in the charge quadrupoles  $Q_{21}$  in the (d) shear strain  $\epsilon_{xz}$  on Co atoms, with the relative magnitude of shear strain  $\epsilon$ .



**Fig. S10** Variation of the charge quadrupole  $Q_{21}$  on Co and Ru atoms with relative strength of shear stress  $\epsilon_{xz}$  in CoF<sub>2</sub> and RuO<sub>2</sub> in the absence of spin-orbit coupling (SOC).