

Electronic Supplementary Information

Elastic Properties and Piezoelectric Energy Harvesting of a Lead-Free Hybrid Perovskite, (DABCO)RbBr₃

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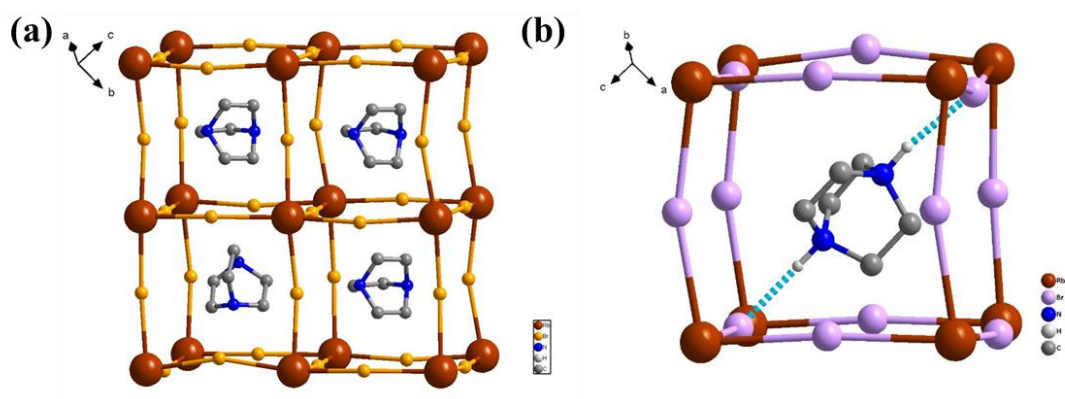


Figure S1. 3D packing structure and hydrogen bonding of (DABCO)RbBr₃ (a and b).

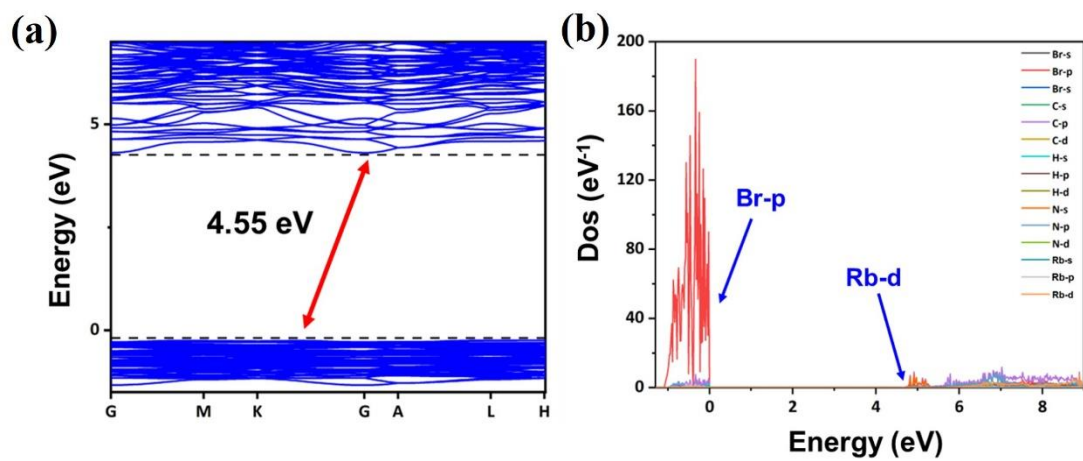


Figure S2. Band gap and density of states of (DABCO)RbBr₃ (a and b).

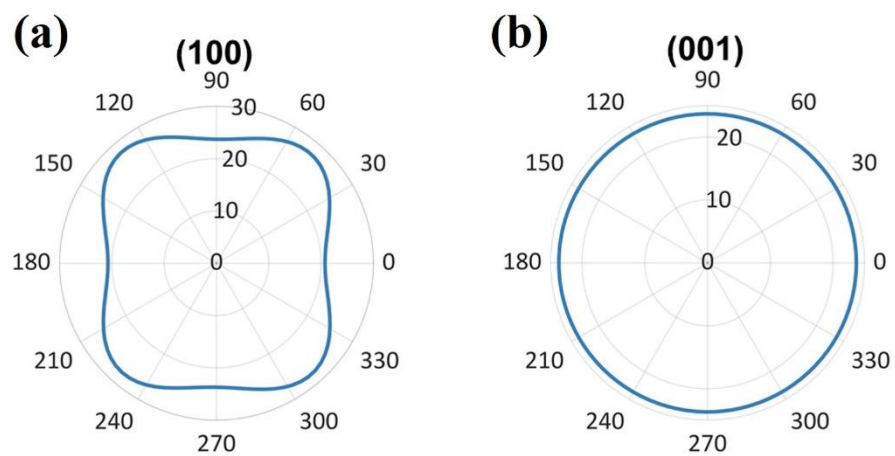


Figure S3. 2D representations of Young's moduli.

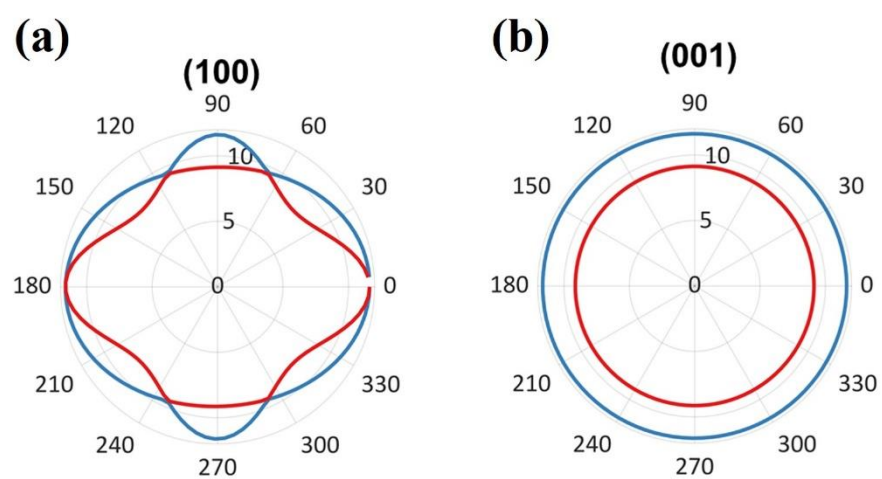


Figure S4. 2D representations of shear moduli.

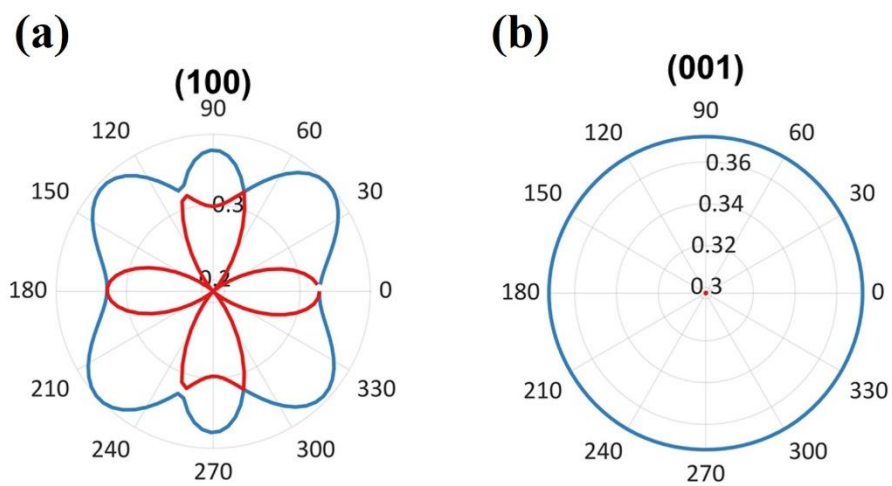


Figure S5. 2D representations of Poisson's ratios.

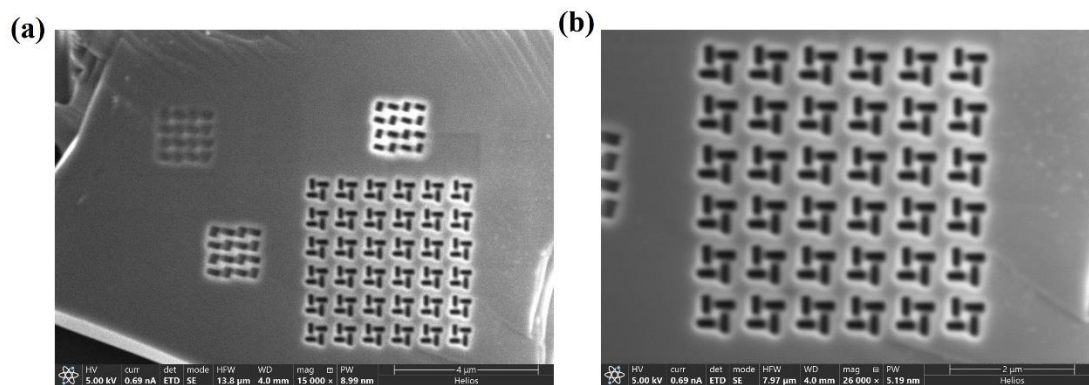


Figure S6. Scanning electron microscopy image in a single crystal of (DABCO)RbBr₃.

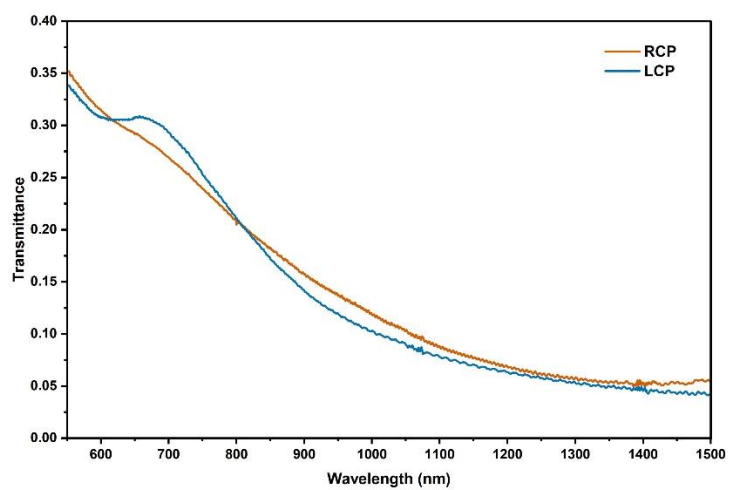


Figure S7. Transmittance under left-handed and right-handed circularly polarized light of (DABCO)RbBr₃.

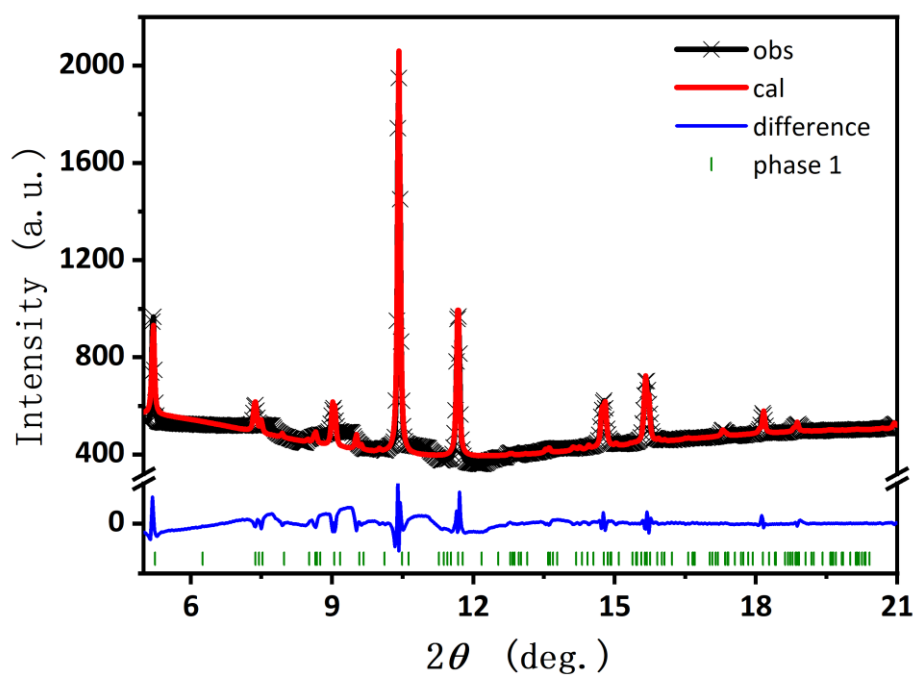


Figure S8. Refined X-ray diffraction pattern of (DABCO)RbBr₃

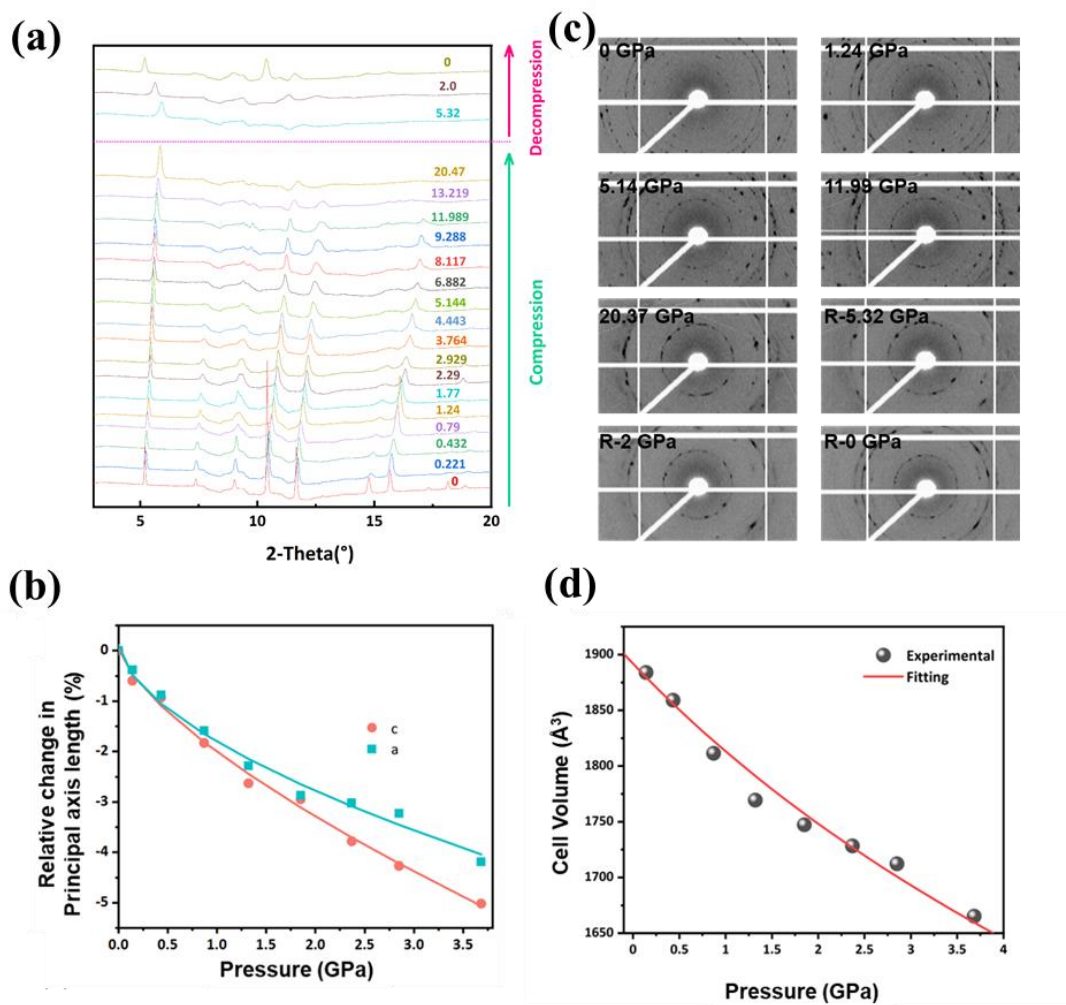


Figure S9. In-situ high-pressure XRD pattern (a) and diffraction rings (b) during compression at a selected pressure of (DABCO)RbBr₃. (DABCO)RbBr₃ cell parameters as a function of pressure: Axial compressibility (c) and changes in unit cell volume with pressure (d).

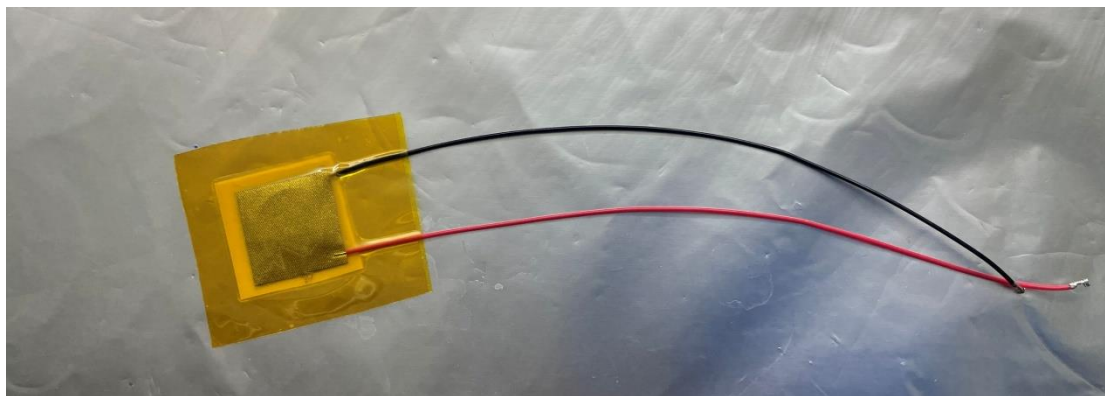


Figure S10. Piezoelectric energy harvesting device based on Cu/(DABCO)RbBr₃ composite film/Cu.



Figure S11. optical photograph of (DABCO)RbBr₃.

Table S1 Comparison of cell parameters of (DABCO)RbBr₃

	(DABCO)RbBr ₃	
Formula	(C ₆ H ₁₄ N ₂)RbBr ₃	
Mr (g mol ⁻¹)	439.36	
Space group	<i>P</i> 322 ₁	
Crystal system	hexagonal	
a (Å)	9.6444 (6)	
b (Å)	9.6444 (6)	
c (Å)	23.254(12)	
V (Å ³)	1873.2(7)	
Z	6	
F(000)	1236.0	
Dc (gcm ⁻³)	2.337	
μ (mm ⁻¹)	13.522	
R _{int}	0.0652	
Limiting indices	-11 ≤ h ≤ 12 -19 ≤ k ≤ 19	
GOF on F ²	1.025	
R ₁ , wR ₂ [I > 2σ(I)] ^a	0.0203	0.0470

^a $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; ^b $R_w = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma w(F_o^2)^2]^{1/2}$.

Table S2 The elastic constant matrix C_{ij} of (DABCO)RbBr₃

C_{ij} (GPa)	(DABCO)RbBr ₃
C_{11}	34.87125
C_{33}	31.646
C_{44}	11.61975
C_{12}	16.608
C_{13}	16.7602
C_{14}	0.0792

Table S3 The piezoelectric output performance of common lead-free hybrid piezoelectric composite film materials.

Materials	Force (N)	Voltage (V)	Power density ($\mu\text{W}/\text{cm}^2$)	Refs.
(DABCO)RbBr ₃	2	8.5	2.6	this work
R-(MP)CdCl ₄	2	2.57	0.55	43
S-(APP) ₂ CoBr ₄	2	10.21	3.07	44
(BTMA) ₂ CoBr ₄	2.5	19.7	11.72	45
(BPMBDMA)(Bi ₂ Br ₉)	21	24.6	13.65	46
(Me ₃ NCH ₂ CH ₂ OH)CdCl ₃	40	55.2	70.9	47
(DPDP)PF ₆	15	8.5	1.74	48

Reference

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