

Supporting Information

Piezochromic Effect and Low-pressure Superconductivity Discovered in Inorganic Halide Perovskite RbPbI₃

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Table S1. RbPbI₃ atomic positions of four stable structures at 0-100 GPa.

		Coordinates			
	<i>Atoms</i>	<i>Wyck.</i>	<i>x</i>	<i>y</i>	<i>z</i>
ppPv- <i>Pnma</i> (0 GPa)			a=10.2718 Å $\alpha=90^\circ$	b=4.7359 Å $\beta=90^\circ$	c=17.2976 Å $\gamma=90^\circ$
	Rb	4c	0.58055	0.25000	0.82556
	Pb	4c	0.33525	0.25000	0.44062
	I	4c	0.34435	0.25000	0.00686
	I	4c	0.97049	0.25000	0.88496
	I	4c	0.69645	0.25000	0.21768
ppPv- <i>Pnma</i> (I) (5 GPa)			a=7.9752 Å $\alpha=90^\circ$	b=5.073 Å $\beta=90^\circ$	c=16.4626 Å $\gamma=90^\circ$
	Rb	4c	1.07352	0.25000	0.8208
	Pb	4c	0.78359	0.25000	0.4439
	I	4c	0.85763	0.25000	0.04177
	I	4c	0.50008	0.25000	0.89006
	I	4c	1.18899	0.25000	0.23603
ppPv- <i>Pnma</i> (V) (20 GPa)			a= 6.5322 Å $\alpha=90^\circ$	b=5.1027 Å $\beta=90^\circ$	c=15.4785 Å $\gamma=90^\circ$
	Rb	4c	0.51283	0.25000	0.8397
	Pb	4c	0.32683	0.25000	0.4437
	I	4c	0.33923	0.25000	0.04398
	I	4c	0.00161	0.25000	0.86653
	I	4c	0.71879	0.25000	0.24444
<i>Pm</i> (80 GPa)			a=7.6996 Å $\alpha=90^\circ$	b=4.8445 Å $\beta=109.2692^\circ$	c=5.2376 Å $\gamma=90^\circ$
	Rb	1b	0.65882	0.50000	0.06823
	Pb	1b	0.44922	0.50000	0.45194
	I	1b	0.85000	0.50000	0.66872
	I	1b	0.26299	0.50000	0.85760
	I	1b	0.05094	0.50000	0.26532
	Rb	1a	0.06782	-0.00000	0.59025
	Pb	1a	0.86724	-0.00000	0.98253
	I	1a	0.47534	-0.00000	0.78269
	I	1a	0.25636	-0.00000	0.18192
	I	1a	0.66916	-0.00000	0.37803

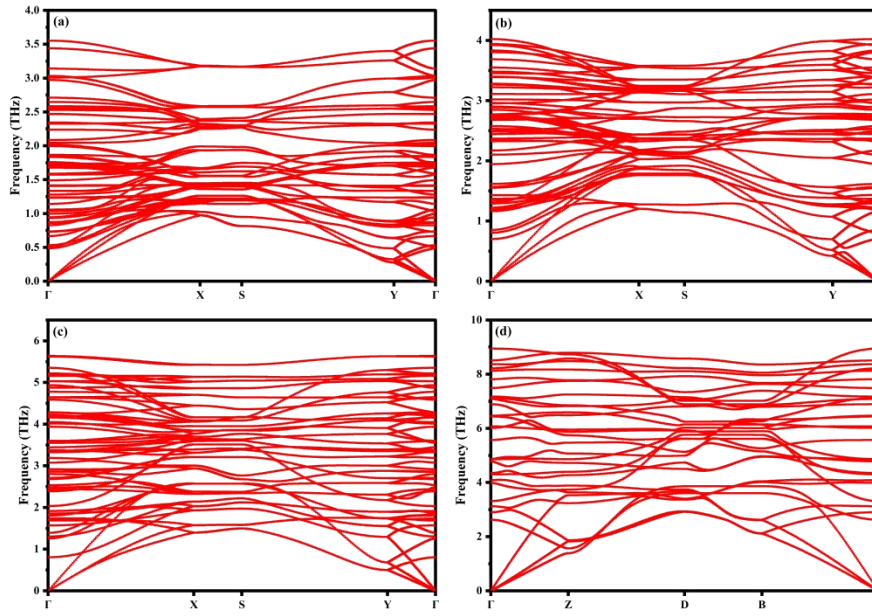


FIG. S1: Phonon spectrum of RbPbI_3 (a) $\text{ppPv-}Pnma$ (0 GPa), (b) $\text{ppPv-}Pnma(I)$ (5 GPa), (c) $\text{ppPv-}Pnma(V)$ (20 GPa), (d) Pm (80 GPa), respectively.

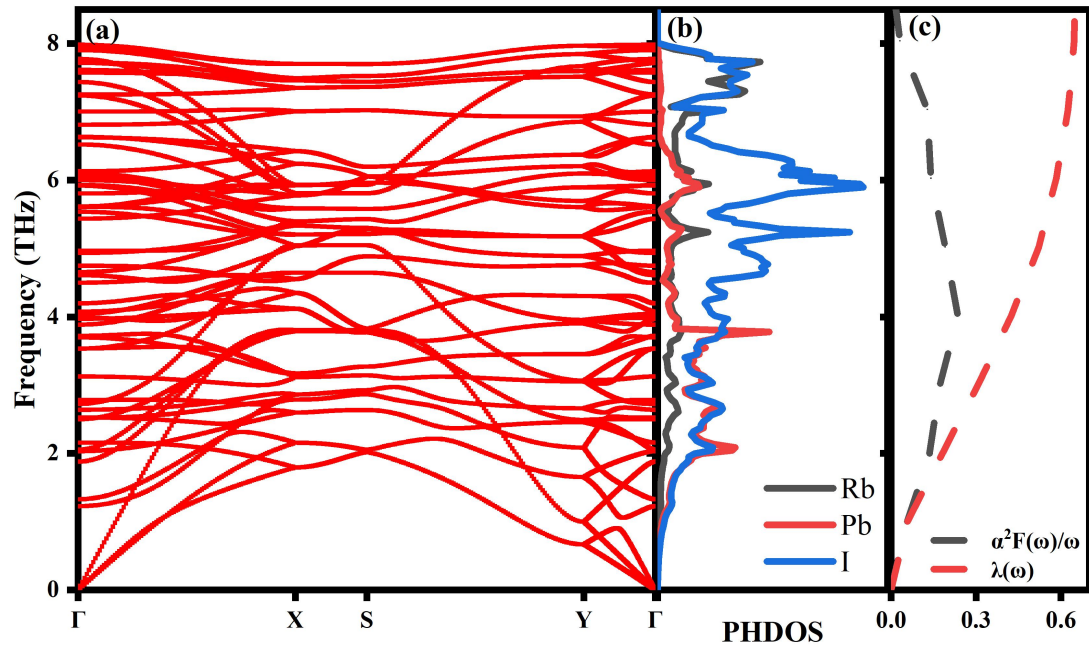


Fig. S2: Spectral function and electron-phonon coupling integral of the ppPv-Pnma(V) phase of RbPbI₃ at 60 GPa.