

Supplementary Information

Structural evolution, superconductivity, and high carrier mobility in anti-perovskite Ca_3BiX (X=H, N, P): First-principles calculations

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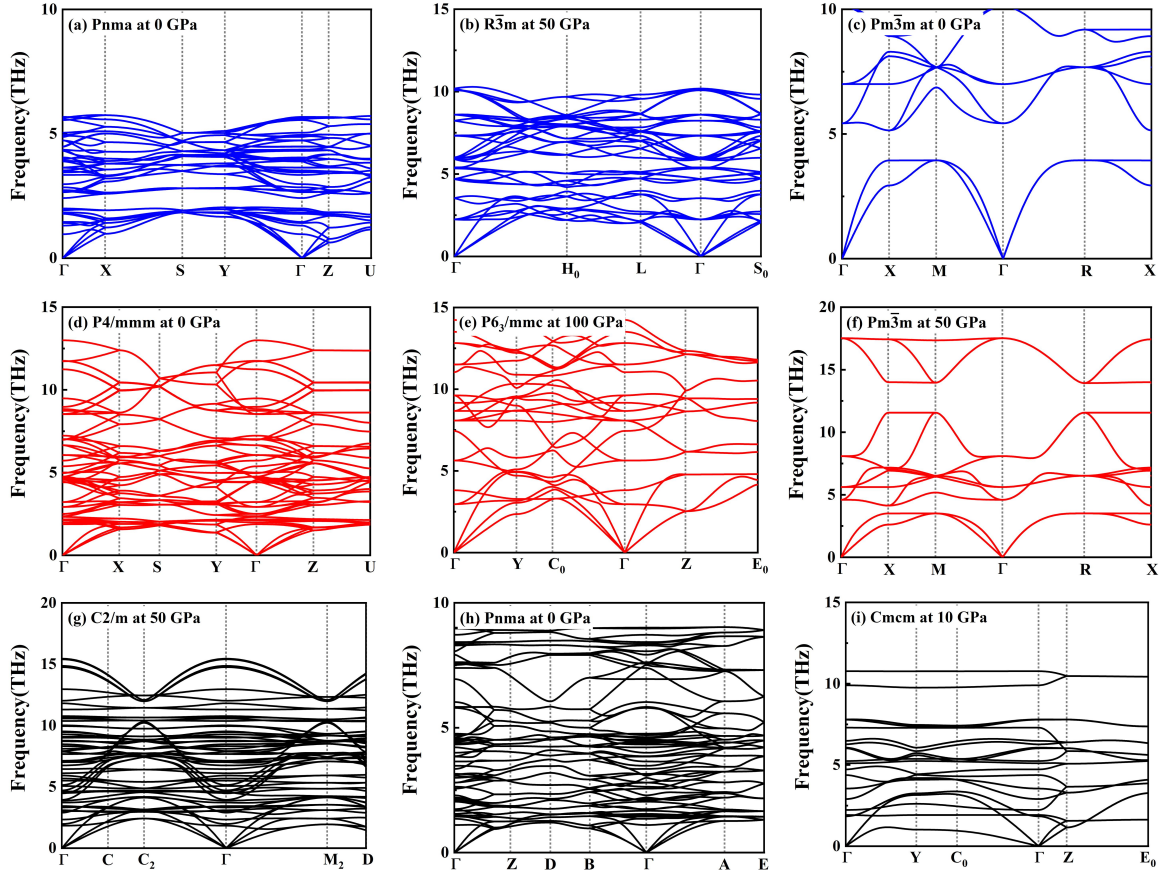


Fig. S1 Phonon dispersion curves of Ca_3BiH in the (a) Pnma (0 GPa), (b) $\text{P6}_3/\text{mmc}$ (50 GPa), and (c) $\text{Pm}\bar{3}\text{m}$ (50 GPa); Ca_3BiN in the (d) $\text{P4}/\text{mmm}$ (0 GPa), (e) $\text{P6}_3/\text{mmc}$ (100 GPa), and (f) $\text{Pm}\bar{3}\text{m}$ (50 GPa); and Ca_3BiP in the (g) $\text{C2}/\text{m}$ (100 GPa), (h) Pnma (5 GPa), and (i) Cmcm (10 GPa).

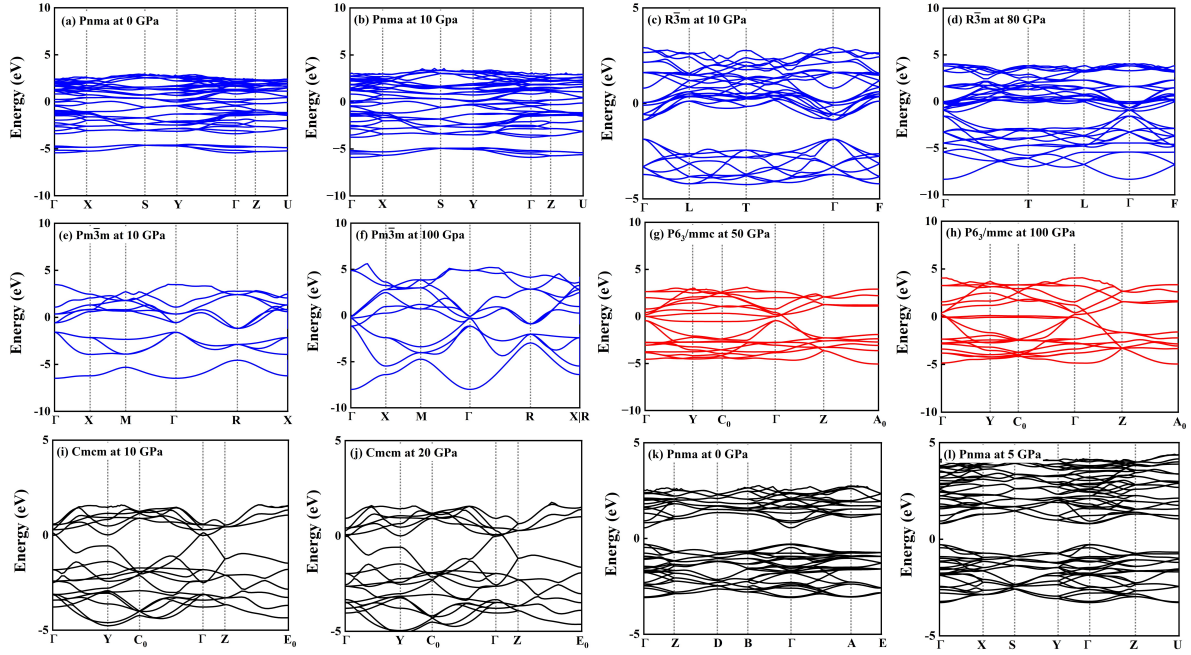


Fig. S2 Band structures of Ca_3BiH of Pnma at (a) 0 GPa, (b) 10 GPa, $\bar{R}3m$ at (c) 10 GPa, (d) 80GPa, $\bar{P}m\bar{3}m$ at (e) 10 GPa, (f) 100 GPa, Ca_3BiN of $P6_3/mmc$ at (g) 50 GPa, (h) 100 GPa, and Ca_3BiP of Cmc at (i) 10 GPa, (j) 20 GPa, Pnma at (k) 0 GPa, (l) 5GPa.

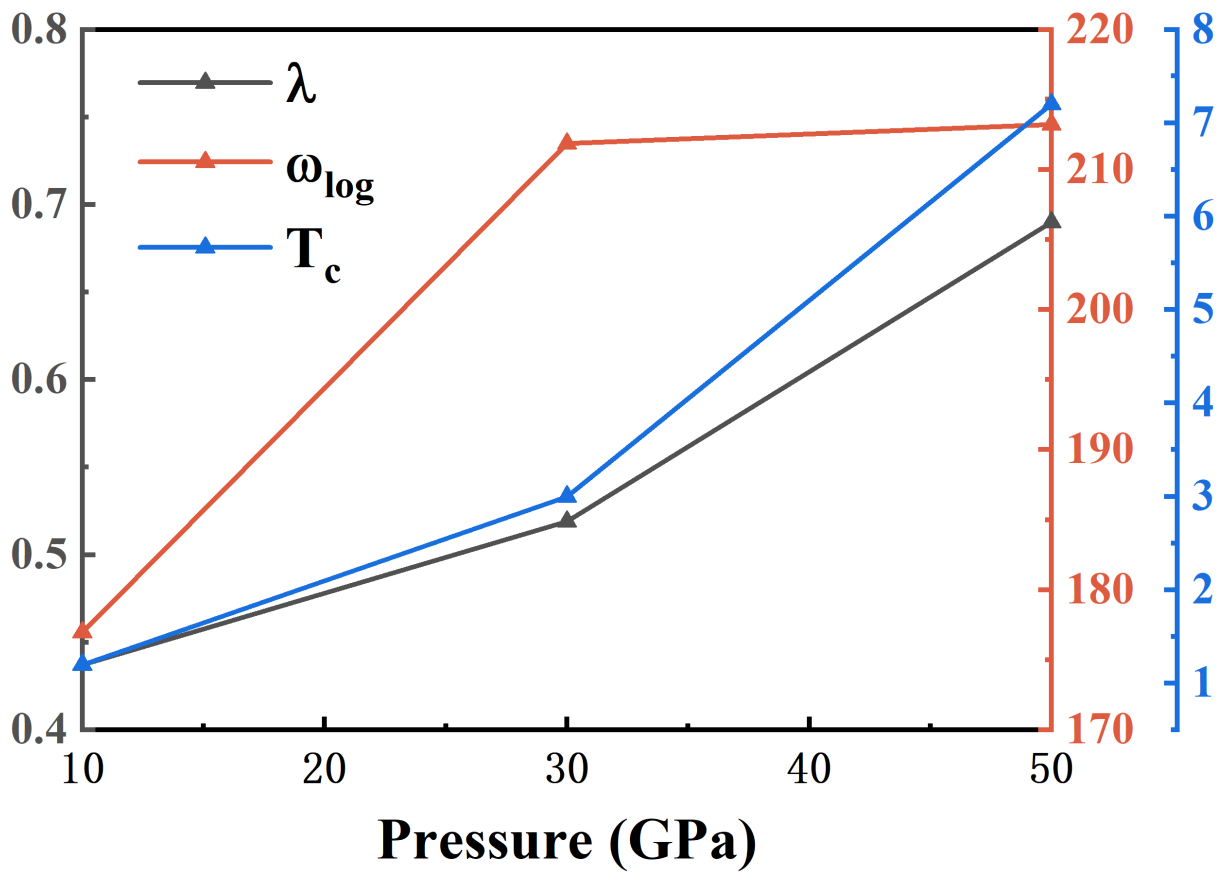


Fig. S3 The λ , ω_{\log} , and T_c values for $Pm\bar{3}m$ at 10, 30, and 50 GPa.

Table S1 The band gap values corresponding to the stable phases of Ca_3BiP ($X = \text{H, N, P}$) in Fig. 3 and Fig. S2.

Anti-perovskite	Space group	Pressure (GPa)	Band gap value (eV)
Ca_3BiH	Pnma	0	Metal
		10	Metal
	$R\bar{3}m$	10	Metal
		80	Metal
	$\text{Pm}\bar{3}m$	10	Metal
		100	Metal
Ca_3BiN	$\text{P4}/mmm$	0	0.3528
		70	Metal
	$\text{P6}_3/mmc$	50	Metal
		100	Metal
	$\text{Pm}\bar{3}m$	0	0.3731
		70	Metal
Ca_3BiP	$\text{C2}/m$	10	0.1316
		100	Metal
	Pnma	0	0.8444
		5	1.0799
		10	Metal
		20	Metal
Cmcm	10	Metal	
	20	Metal	

Table S2 The effective carrier mass $m^*(m_0)$, deformation potential $E_a(\text{eV})$, and carrier mobility $\mu_a(\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1})$ of electrons and holes in the Pnma phase of Ca_3BiP along the x, y, and z directions.

Carrier	m_{xx}^*	m_{yy}^*	m_{zz}^*	E_{xx}	E_{yy}	E_{zz}	μ_{xx}	μ_{yy}	μ_{zz}
Electronic	0.101	0.133	0.144	3.36	10.81	6.63	71520.09	4617.19	9898.10
Hole	0.652	0.106	1.022	2.25	10.06	3.73	1503.79	9397.67	233.12