

Supporting Information for

**Penta-BCP Sheet with Strong Piezoelectricity and a Record High Positive
Poisson's Ratio**

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The coordinates and lattice parameters of the optimized geometry for penta-BCP in
the VASP-POSCAR format.

Penta-BCP			
1.0000000000000000			
3.7181999683000000		0.0000000000000000	0.0000000000000000
0.0000000000000000		3.6875998974000002	0.0000000000000000
0.0000000000000000		0.0000000000000000	21.0799007415999995
C	P	B	
2	2	2	
Direct			
0.2275573220106466	0.0084910296134737	0.4927373522990095	
0.7724426610073394	0.5084910294782858	0.5072626482250584	
0.4615985569580090	0.6860329068473163	0.4389086878008186	
0.5384014259841834	0.1860329069810689	0.5610913115137066	
0.1207179431704049	0.3611560725044214	0.4737279732646300	
0.8792820398694303	0.8611560725754330	0.5262720268967769	

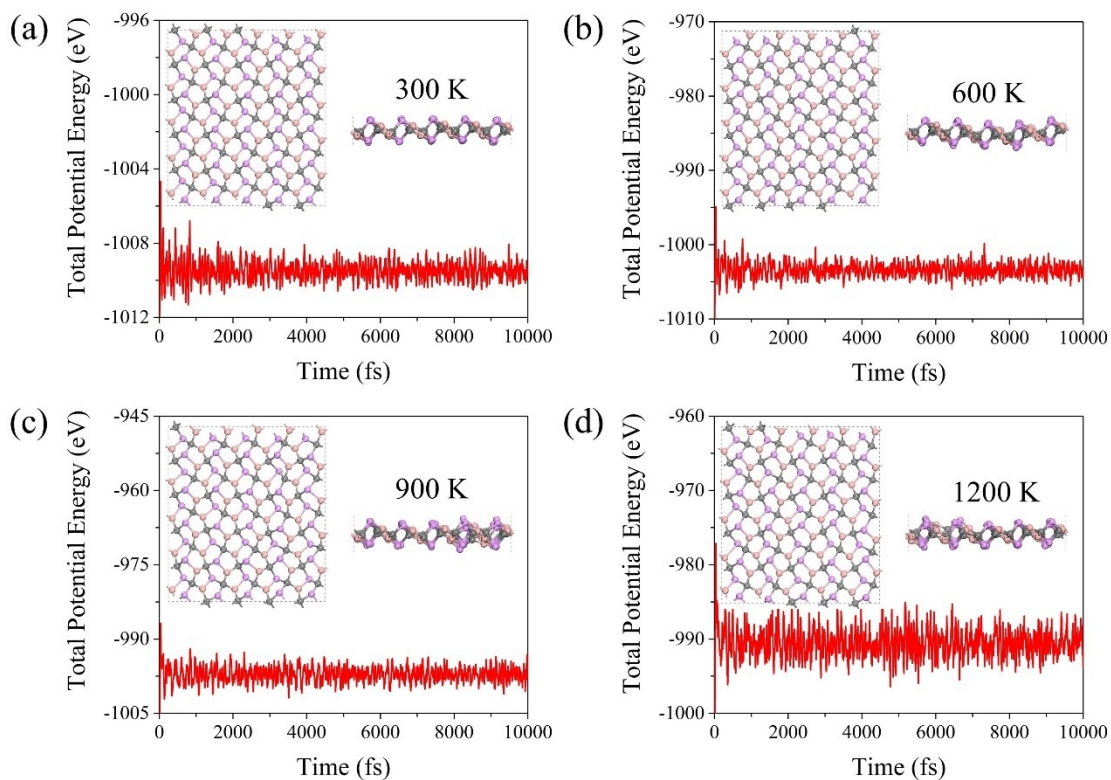


Fig. S1. Potential energy fluctuation with time during the AIMD simulation at (a) 300 K, (b) 600 K, (c) 900 K, and (d) 1200 K. The insets show the configuration of penta-BCP at the end of each simulation. The pink, gray, and purple spheres represent B, C, and P atoms, respectively.

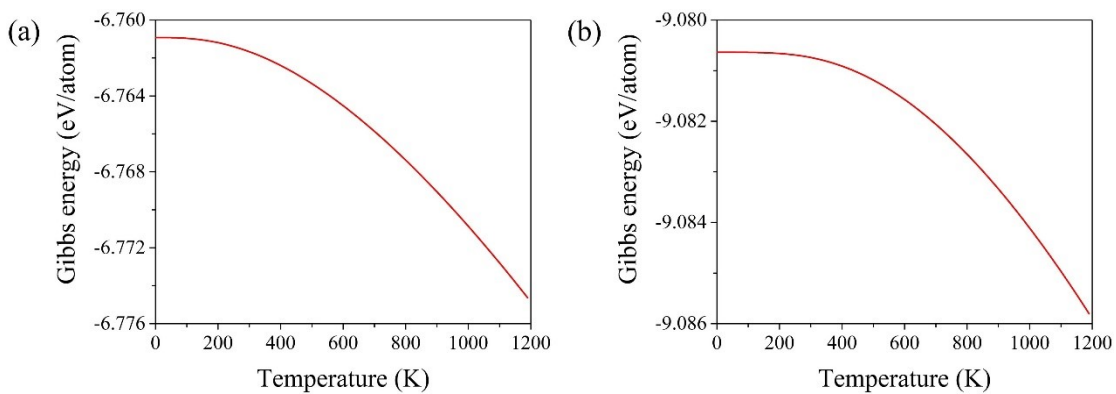


Fig. S2. Gibbs energy of (a) penta-BCP, and (b) diamond under different temperatures.

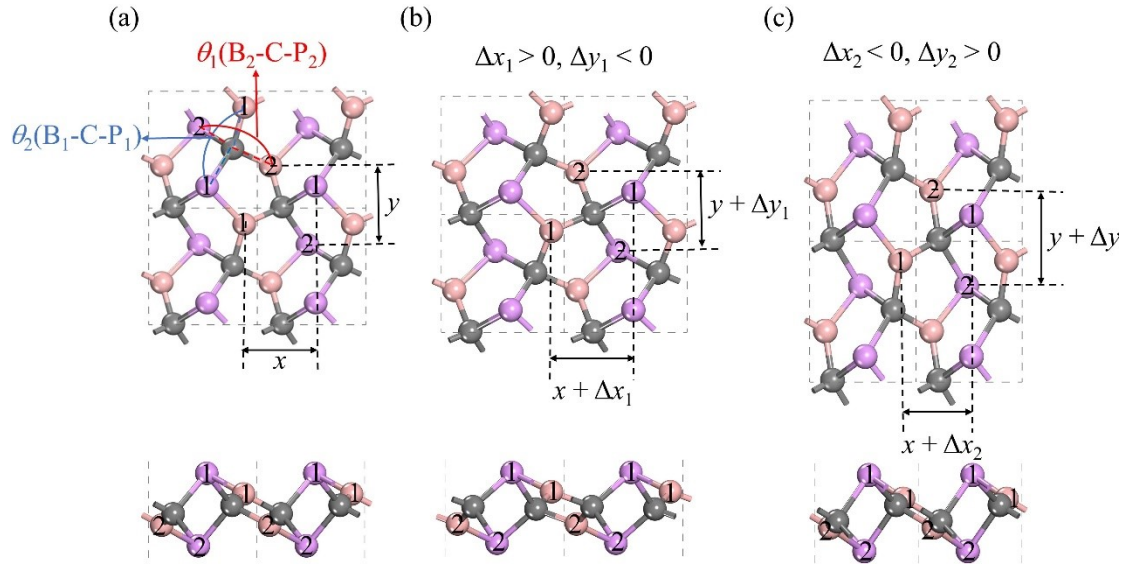


Fig. S3. (a) The length of the tetrahedral along the axial directions (x and y), and the bond angles $\theta(B_1-C-P_1)$ and $\theta(B_2-C-P_2)$ in the equilibrium state. (b) Schematic of the changes of the length (Δx_1 and Δy_1) under tensile strain along the $[100]$ direction, and (c) that (Δx_2 and Δy_2) along the $[010]$ direction. The pink, gray, and purple spheres represent B, C, and P atoms, respectively.

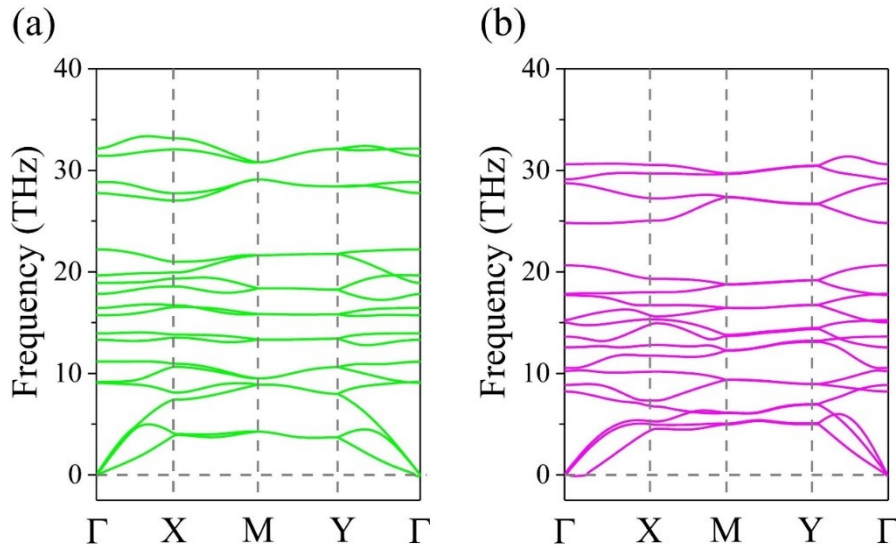


Fig. S4. (a, b) Phonon dispersion along the $[100]$ and $[010]$ direction of the penta-BCP under 10% uniaxial strain, respectively.

Table S1 Spontaneous polarization P_s (in 10^{-10} C/m) of penta-BCP with 2%, 4%, 6%, 8%, and 10% uniaxial tensile strains along the $[100]$ or $[010]$ directions.

Strain (%)	[100]	[010]
2%	4.56	4.78
4%	4.47	4.89
6%	4.37	5.00
8%	4.27	5.08
10%	4.17	5.16