Supplemental Materials

Extremely Promising Monolayer Materials with Robust Ferroelectricity and Extraordinary Piezoelectricity: δ-AsN, δ-SbN, and δ-BiN

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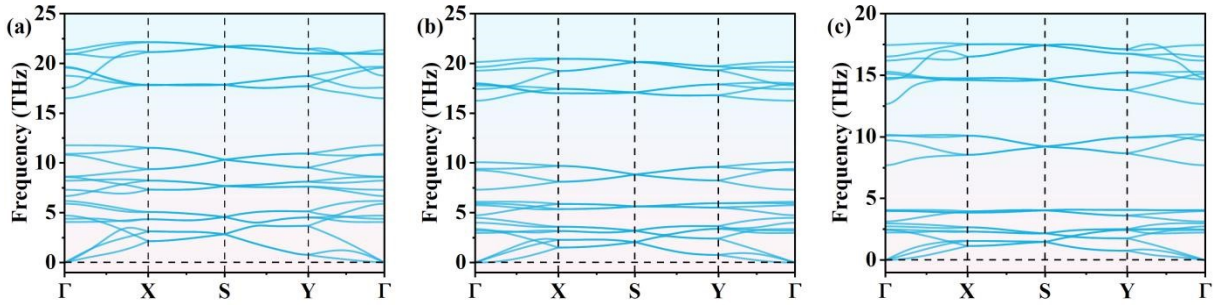

Fig. S1 Typical phonon dispersions of (a) δ-AsN, (b) δ-SbN, and (c) δ-BiN monolayer binary compounds.

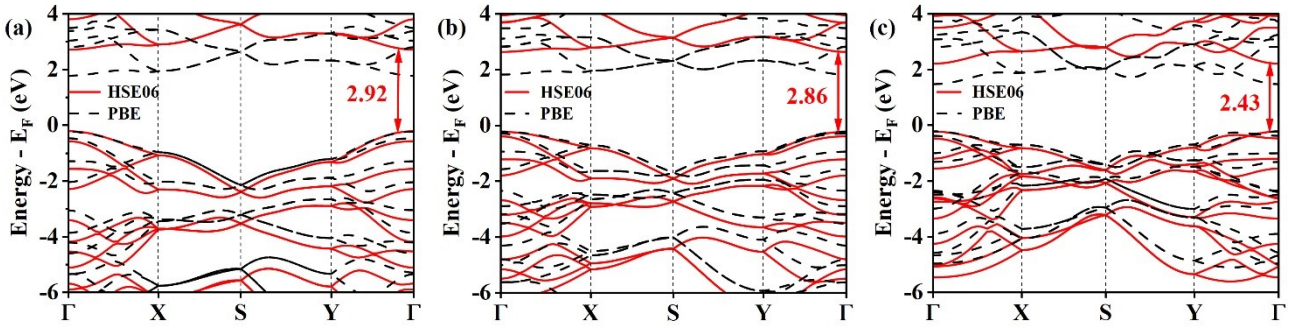

Fig. S2 Calculated DFT-PBE and HSE06 band structures of monolayer binary compounds of (a) δ-AsN, (b) δ-SbN and (c) δ-BiN at zero strain. The positions of band gaps are highlighted by red double-sided arrow and the Fermi level is set at zero.

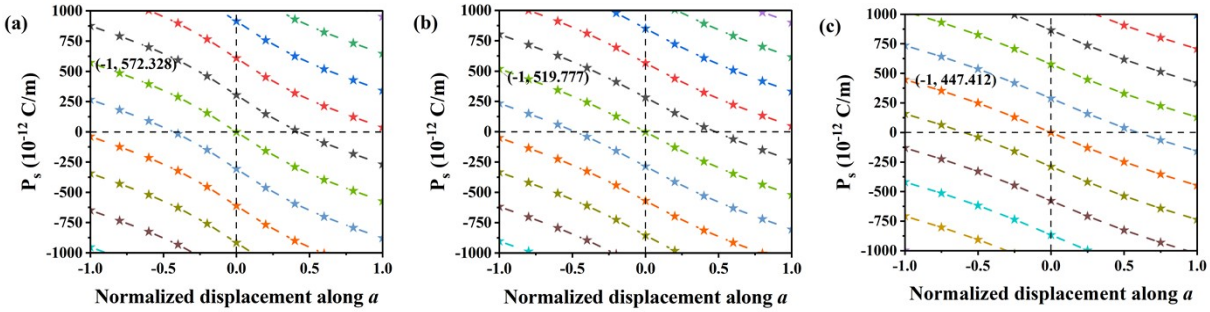

Fig. S3 The total polarization with spin-orbit coupling for (a) δ-AsN, (b) δ-SbN, and (c) δ-BiN monolayers as a function of normalized displacement.

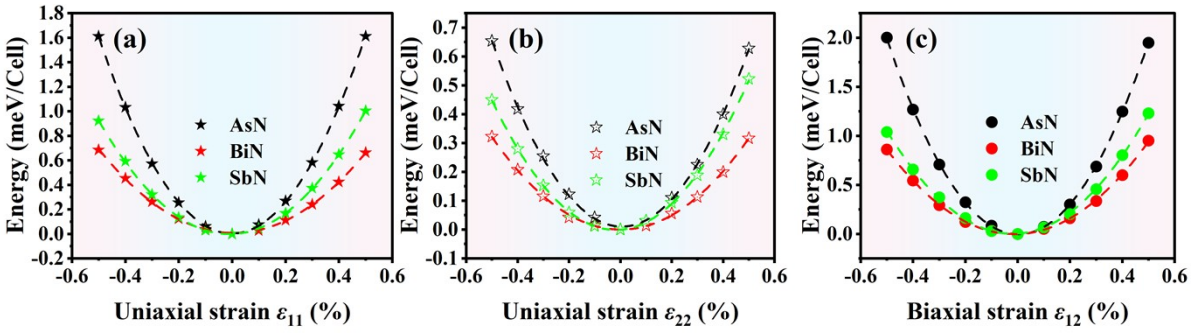

Fig. S4 Relaxed-ion elastic stiffness coefficients (a) C_{11}, (b) C_{22}, and (c) C_{12} of δ-AsN, δ-SbN, and δ-BiN are calculated by the energy-strain method. ($\varepsilon_{11} = \Delta a/a_0$; $\varepsilon_{22} = \Delta b/b_0$; $\varepsilon_{12} = \Delta a/a_0 = \Delta b/b_0$, a_0 and b_0 are lattice constants without strain applied)

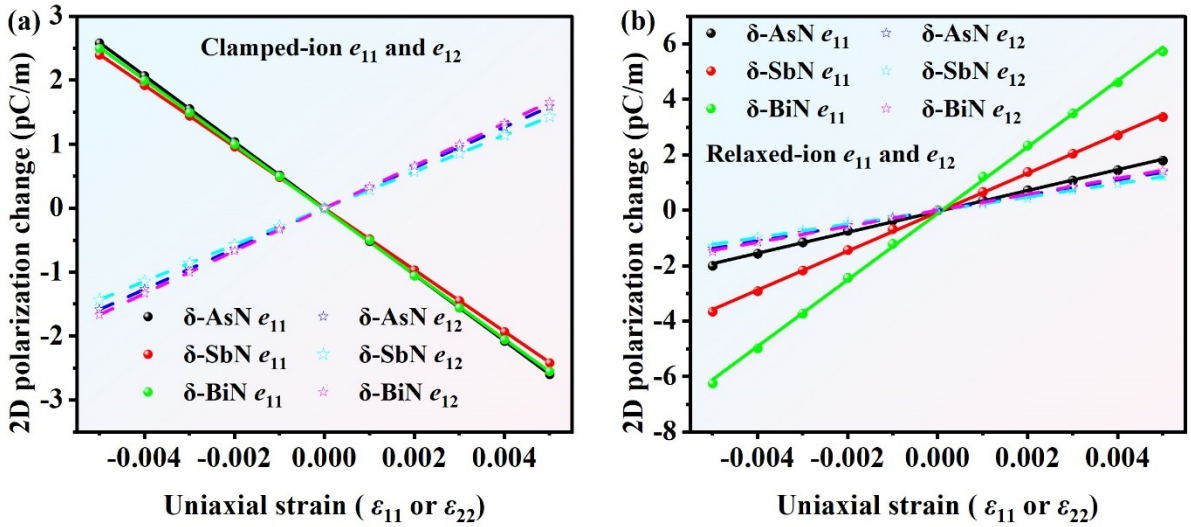

Fig. S5 (a) Clamped-ion piezoelectric coefficients e_{11} and e_{12} without spin-orbit coupling. (b) Relaxed-ion piezoelectric coefficients e_{11} and e_{12} with spin-orbit coupling.

Table S1 Energy comparison between δ-phase and α-phase of AsN, SbN, and BiN at GGA-PBE, meta-GGA, and HSE06 levels.

Materials	Methods	α-phase (eV/atom)	δ-phase (eV/atom)	ΔE (meV/atom)
AsN	GGA-PBE	-6.138	-6.156	18
	SCAN meta-GGA	-14.350	-14.367	17
	HSE06	-7.578	-7.596	18
SbN	GGA-PBE	-5.829	-5.877	48
	SCAN meta-GGA	-22.750	-22.801	51
	HSE06	-7.237	-7.296	56
BiN	GGA-PBE	-5.489	-5.504	15
	SCAN meta-GGA	-43.021	-43.035	14
	HSE06	-6.682	-6.712	30

Table S2 Lattice Parameters, Relaxed-Ion and Clamped-Ion Elastic Stiffness Coefficients C_{11}, C_{22}, and C_{12} for δ-AsN, δ-SbN, and δ-BiN Monolayers at the DFT-PBE Level. The C_{11}, C_{22}, and C_{12} are in units of N/m.

Material	Lattice Parameters			Relaxed-ion			Clamped-ion		
	a (Å)	*b* (Å)	*h* (Å)	C_{11}	C_{22}	C_{12}	C_{11}	C_{22}	C_{12}
δ-AsN	4.80	5.25	2.11	81.77	31.97	-6.69	142.12	117.85	27.48
δ-SbN	5.18	5.64	2.34	42.38	21.20	-6.88	120.68	105.24	26.68
δ-BiN	5.26	5.55	2.50	29.46	14.01	-1.90	115.79	107.34	25.76

Table S3 Piezoelectric Coefficients (e_{11}, e_{12}, $d_{11,}$ and d_{12}) for δ-AsN, δ-SbN, and δ-BiN Monolayers by Berry's Phase methods. The e_{11} and e_{12} are in units of 10^{-10} C/m, and d_{11} and d_{12} are in units of pm/V.

Material	Relaxed-ion				Clamped-ion			
	e_{11}	e_{12}	d_{11}	d_{12}	e_{11}	e_{12}	d_{11}	d_{12}
δ-AsN	3.76	2.75	5.39	9.73	-5.19	3.17	-4.37	3.71
δ-SbN	7.05	2.46	19.55	17.95	-4.81	2.86	-4.86	3.95
δ-BiN	12.42	2.88	43.87	26.50	-5.07	3.33	-5.35	4.39