

Stacking-insensitive ferroelectricity in layered ScPS₃: Lone-pair-driven polarization and strain-stabilized ferroelectricity against the antiferroelectric ground state

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Supporting information

Table S1. Structural parameters of monolayer ScPS₃. Energies are referenced to the FE state and given per two formula units (2 f.u.). The relaxed antiferroelectric (AFE) structure adopts a triclinic symmetry, resulting from the antiparallel arrangement of P-P dimers combined with the slight lattice distortion required to accommodate dimer buckling. This symmetry lowering is a physical consequence of structural relaxation, as confirmed by systematic checks of all symmetry operations.

Phase	Space group	Point group	a (Å)	b (Å)	ΔE (eV)	Ground state
PE	P $\bar{3}1m$ (No. 162)	D_{3d}	6.198	—	0.52	No
FE	P31m (No. 157)	C_{3v}	6.29	—	0	No
AFE	P $\bar{1}$ (No. 2)	C_i	6.32	10.95	-0.13	Yes

Table S2. Interlayer stacking configurations of bilayer ScPS₃ as a function of in-plane sliding displacement along different high-symmetry directions. The values 0, 1/3, 2/3, and 1 represent the normalized sliding displacement in units of the lattice constant, where 0 and 1 correspond to the initial and final equilibrium AB-stacked configurations, respectively.

Direction	0	1/3	2/3	1
$[1 \bar{1}]$	AB	AA	AB'	AB
$[1 0]$	AB	AC	AD	AB

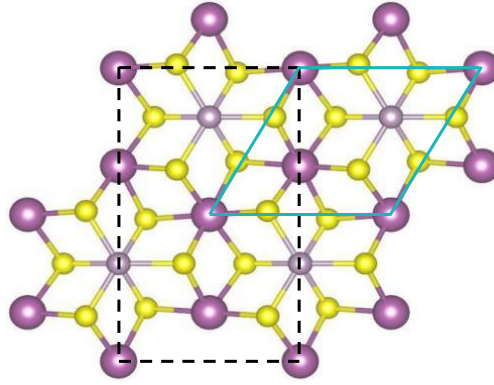


Fig. S1 Atomic structure of monolayer ScPS₃. The ferroelectric phase adopts a hexagonal unit cell, indicated by the blue solid line; the antiferroelectric phase uses a rectangular unit cell, marked by the black dashed line.

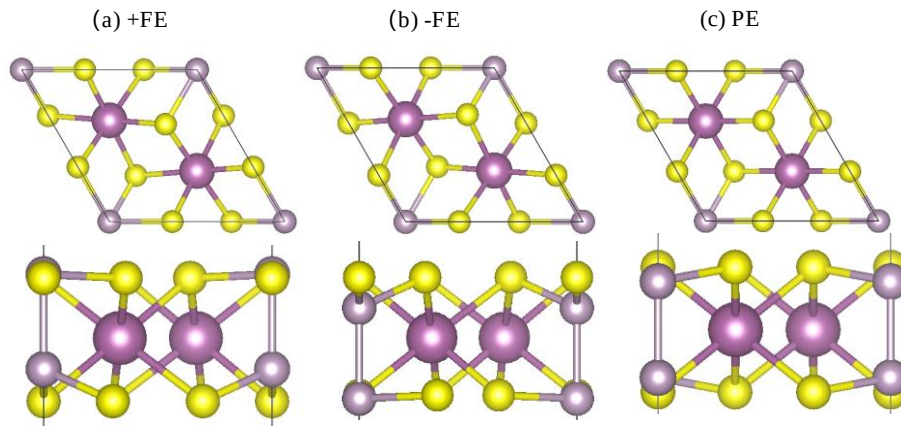


Fig. S2 Top and side views of monolayer ScPS₃. (a) ferroelectric with positive polarization; (b) ferroelectric with negative polarization; (c) paraelectric without polarization.

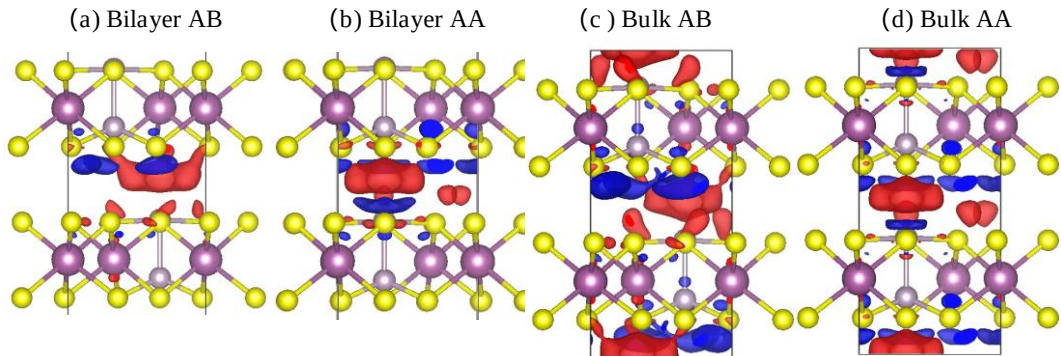


Fig. S3 Structures of bilayer and bulk ScPS₃ with AB and AA stacking sequence. The charge density difference with respect to free-standing monolayer counterparts is shown as red with $0.0003 \text{ e}/\text{\AA}^3$.

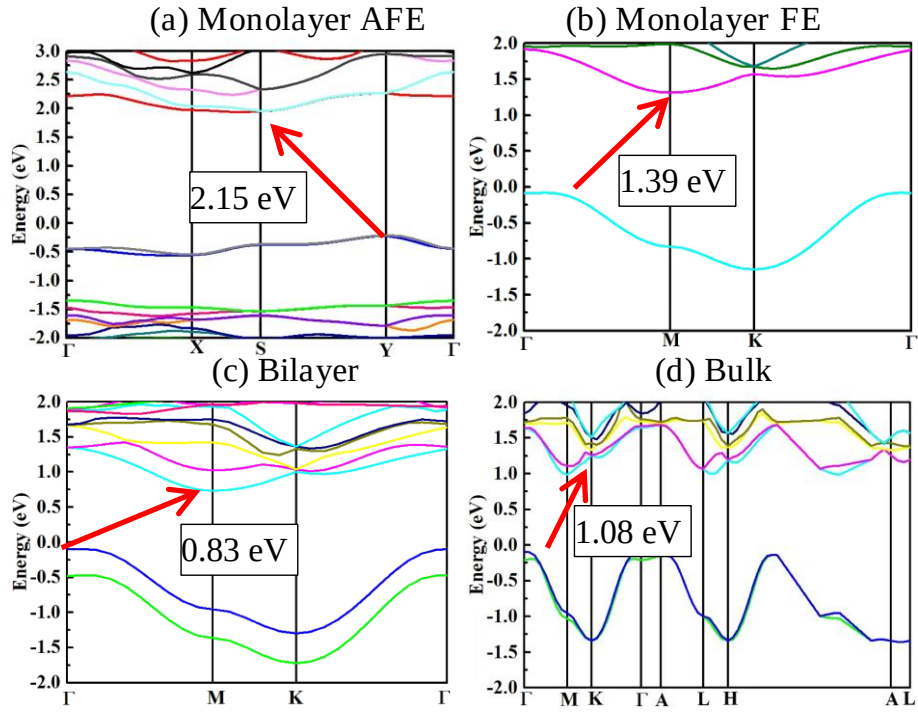


Fig. S4 The electronic band structures from HSE06 of (a) monolayer AFE, (b) monolayer FE, (c) bilayer and (d) bulk ScPS₃.

Table S3. P–P bond length l (in Å) and the layer thickness h of the FE and AFE phases under biaxial strains of -6% , 0 , and $+6\%$.

	strains	-6%	0	6%
FE	l	2.30	2.29	2.28
	h	3.26	2.98	2.76
AFE	l	2.31	2.27	2.25
	h	3.27	3.18	2.79