*Electronic supplementary information (ESI) for*

# 1D group V-VI-VII ternary nanowires: moderate band gaps, easy to exfoliate from bulk, and unexpected ferroelectricity†

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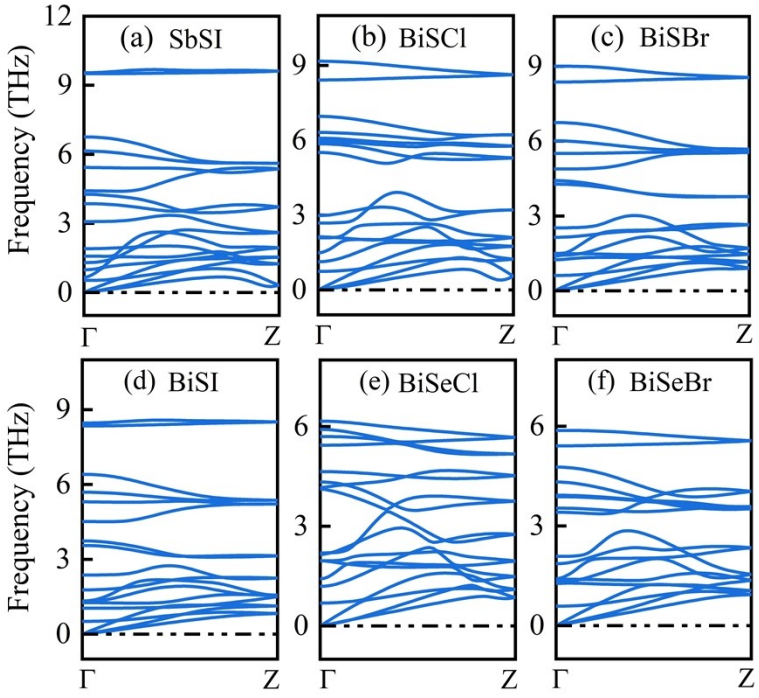


**Fig. S1.** The phonon dispersion spectra of partial 1D $X^{V}Y^{VI}Z^{VII}$ nanowires: (a) SbSI, (b) BiSCl, (c) BiSBr, (d) BiSI, (e) BiSeCl, and (f) BiSeBr.

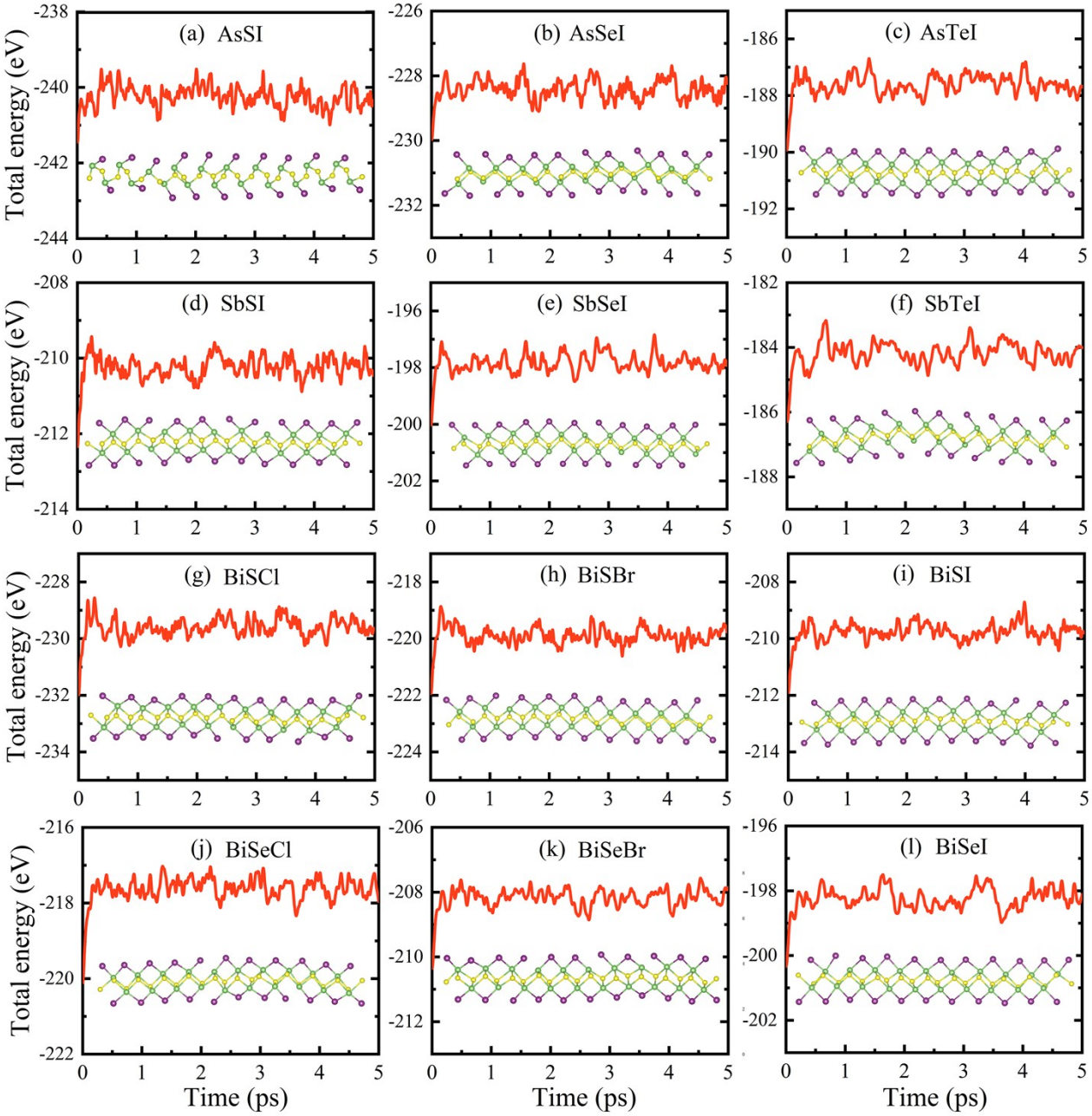


**Fig. S2.** The evolution of energies from AIMD simulations at 300 K of 1D $X^{V}Y^{VI}Z^{VII}$ nanowires. The insets present the snapshot of atomic structure after 5 ps.

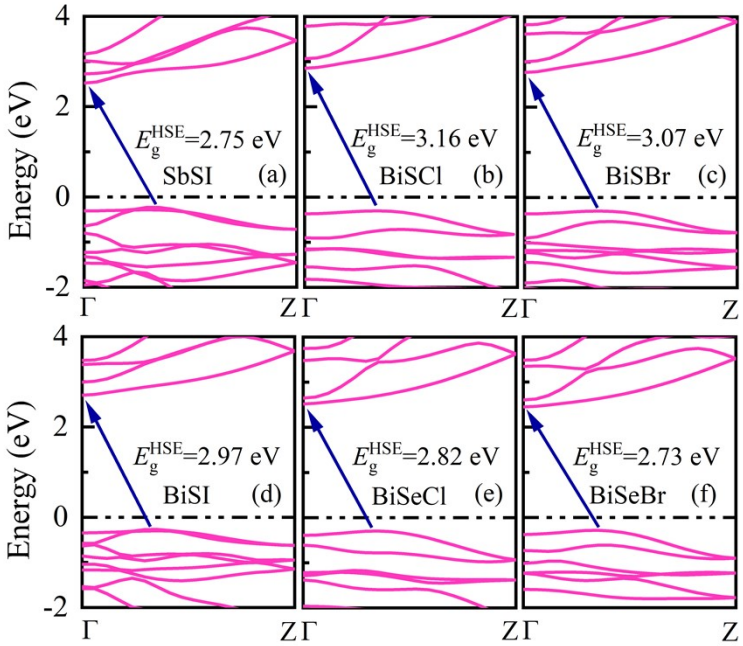


**Fig. S3.** The HSE06 band structures of partial 1D $X^{V}Y^{VI}Z^{VII}$: (a) SbSI, (b) BiSCl, (c) BiSBr, (d) BiSI, (e) BiSeCl, and (f) BiSeBr. The Fermi level is set to 0.

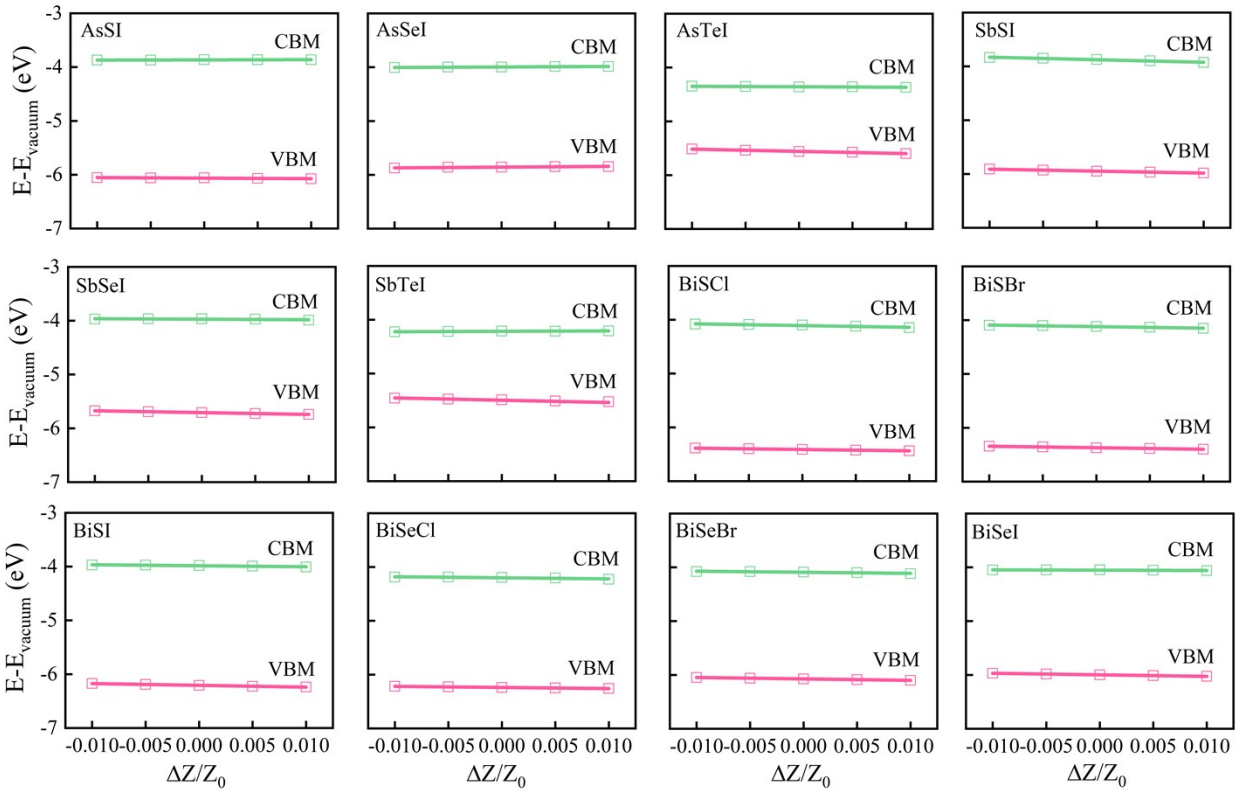


**Fig. S4.** Evaluations of band edges of nanowires 1D $X^{V}Y^{VI}Z^{VII}$ (X=As, Sb, Bi; Y=S, Se, Te; Z=Cl, Br, I) relative to vacuum level with respect to strains along the chain direction. The slope is the deformation potential $E_1$.

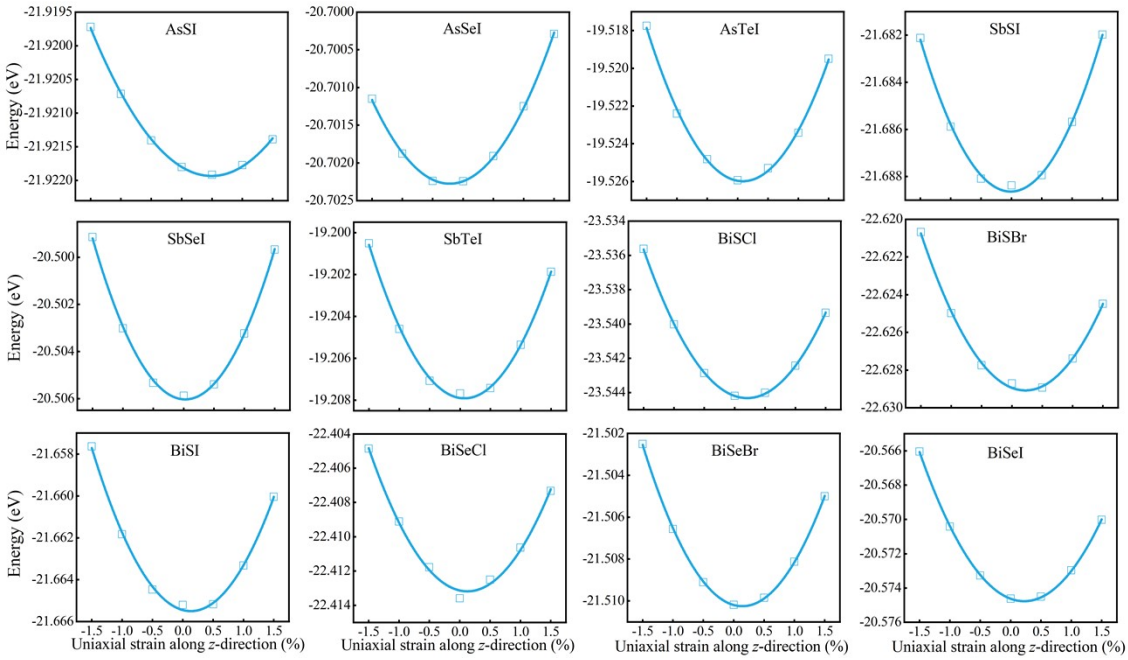


**Fig. S5.** The total energy of 1D $X^{V}Y^{VI}Z^{VII}$ (X=As, Sb, Bi; Y=S, Se, Te; Z=Cl, Br, I) nanowires as a function of the uniaxial strain applied along the chain direction.

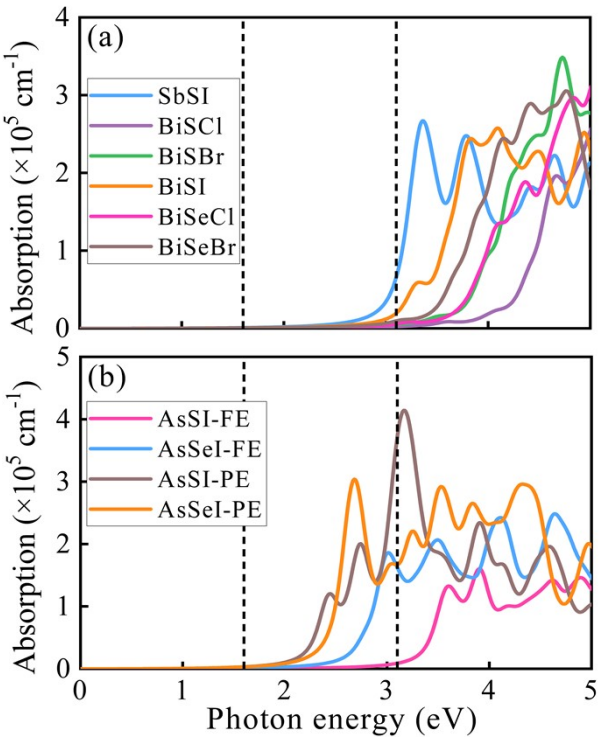


**Fig. S6.** (a) Calculated absorption coefficients of the partial 1D $X^{V}Y^{VI}Z^{VII}$ nanowires at the HSE06 level: SbSI, BiSCl, BiSBr, BiSI, BiSeCl, and BiSeBr. (b) The comparisons of absorption coefficients between the ferroelectric (FE) and paraelectric (PE) phases for 1D AsSI and AsSeI nanowires. The vertical dashed lines represent the visible region.