Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Lone-pair-induced formation of intrinsic one-dimensional SbSX (X = Cl, Br, I) helix chain materials

Supporting Information

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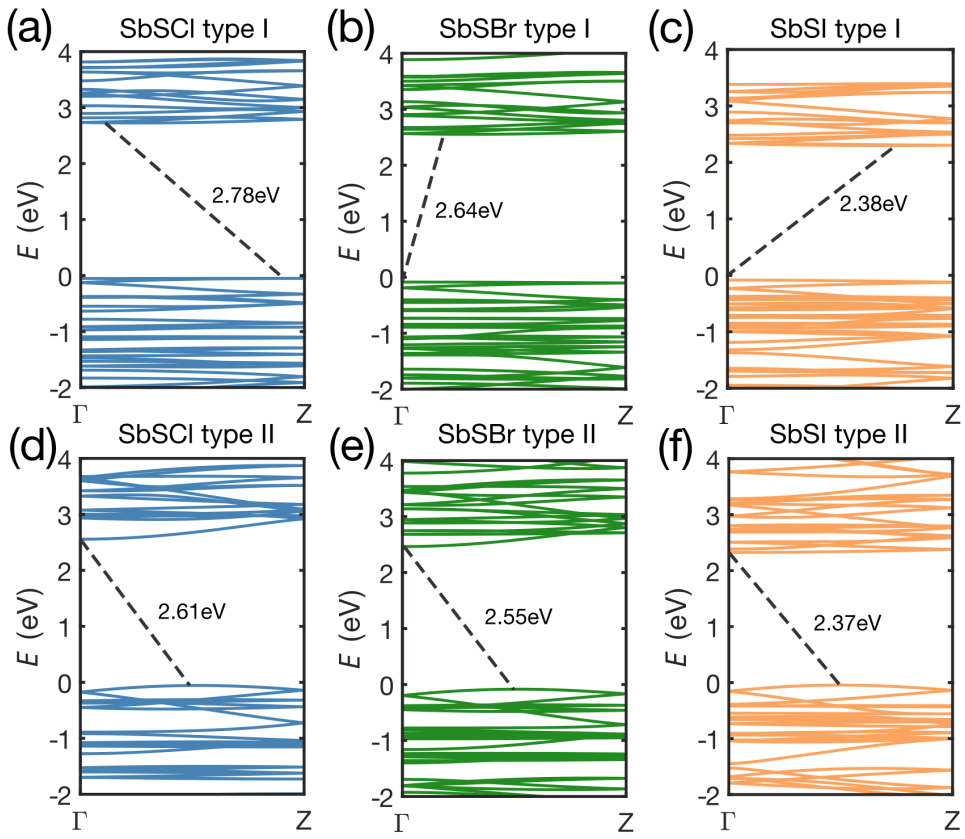

Figure S1. Electronic band structure of 1D SbSX (X = Cl, Br, I) helix-chains calculated with PBE functional.

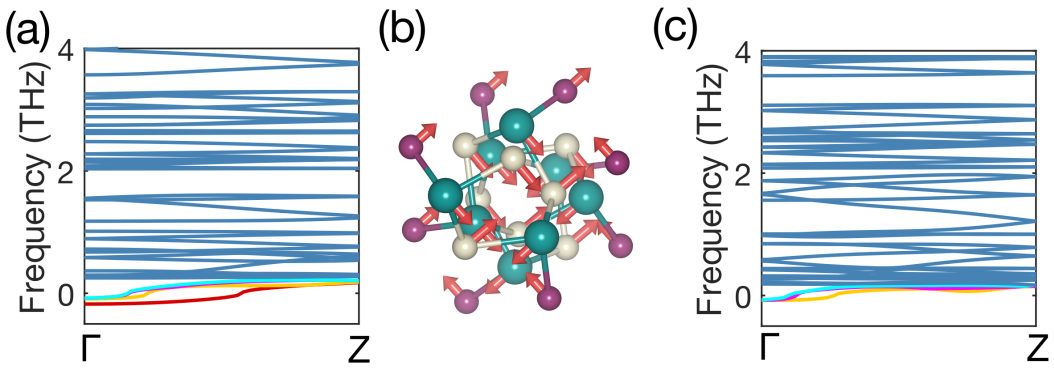

Figure S2. (a) Phonon spectra of SbSCl helix chain typee I phase. (b) Atomic displacement patterns corresponding to the torsional mode (the red line in (a)). (c) Phonon spectra of SbSCl helix chain typee II phase. The three non-red colorful lines indicate the three acoustic modes, and the red-line optical mode indicates the torsional mode.

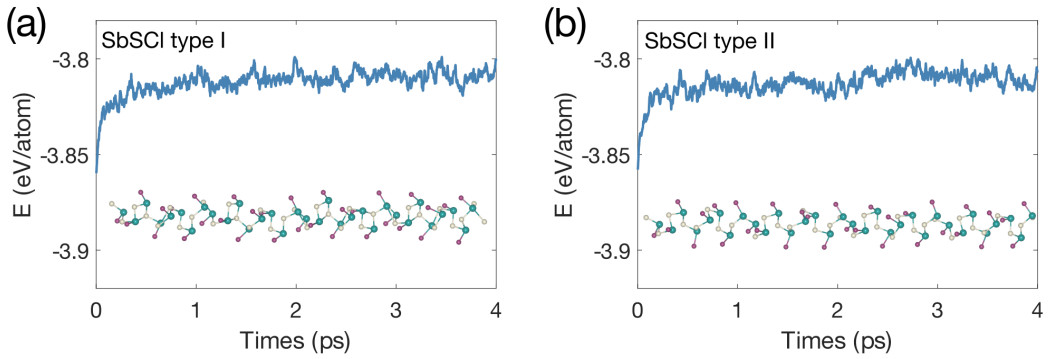

Figure S3. The evolution of energy of 1D SbSCl helix-chain type I phase (**a**) and type II phase (**b**) simulated with ab initio molecular dynamics at 300 K. The inset illustrates the final structures at 4 ps.

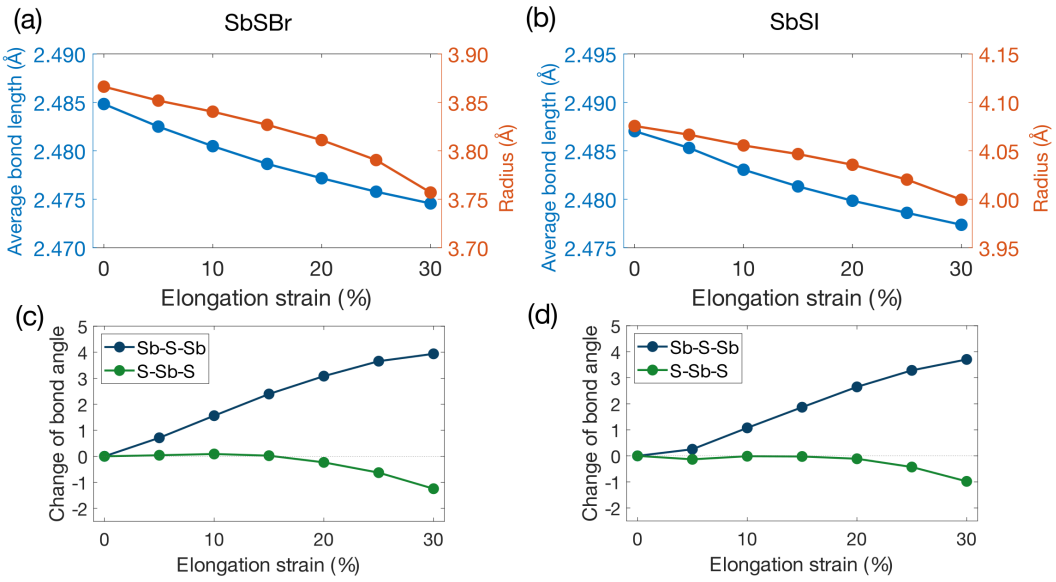

Figure S4. (**a**)(**b**) The average bond length and radius of 1D SbSBr and SbSI helix-chain type II phase as the function of elongation strains. (**c**)(**d**) Variation of average change of bond angle of Sb-S-Sb and S-Sb-S in 1D SbSBr and SbSI helix-chain type II phase under different elongation strains, compared to the equilibrium state.