

Supplementary Material for
Two-dimensional ferroelastic topological insulator with tunable topological edge
states in single-layer ZrAsX (X = Br and Cl)

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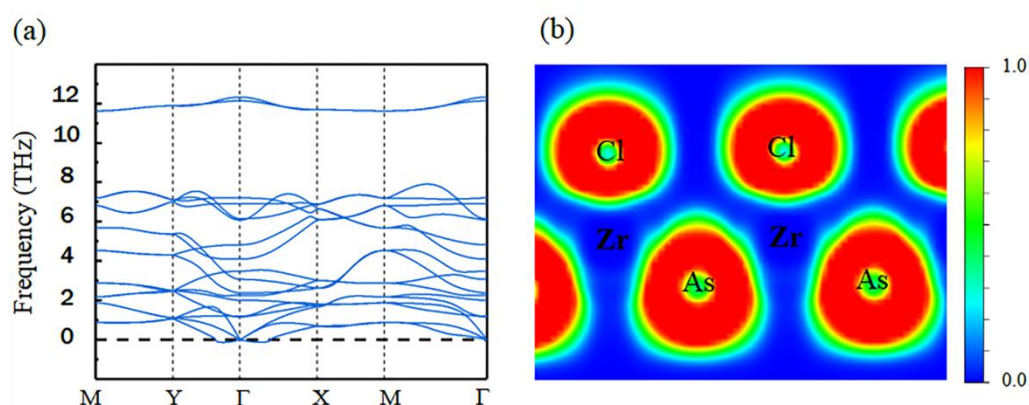


Figure S1. (a) Phonon spectra of single-layer ZrAsCl. (b) Map of electron localization function (ELF) on the plane perpendicular to the basal plane of SL ZrAsCl.

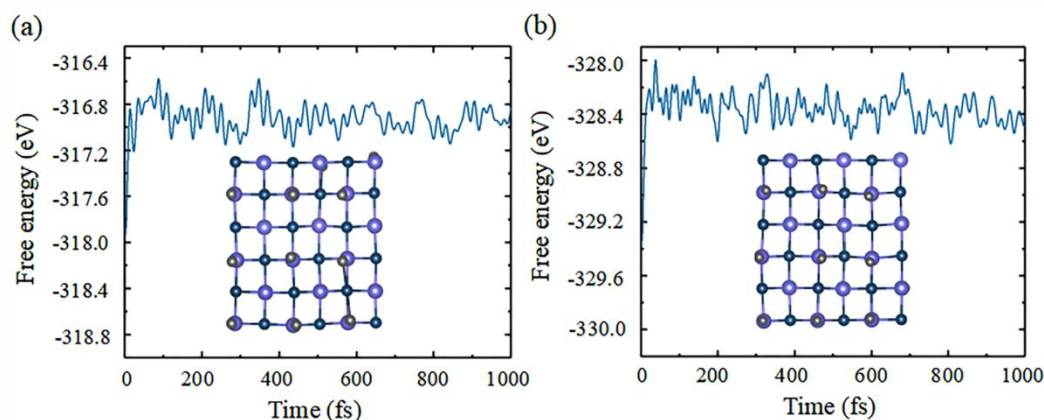


Figure S2. Time evolution of free energy during the molecular dynamics (MD) calculations of (a) ZrAsBr and (b) ZrAsCl with a 3×3 supercell at 300 K. The inset is the snapshot taken from the end of the MD calculations.

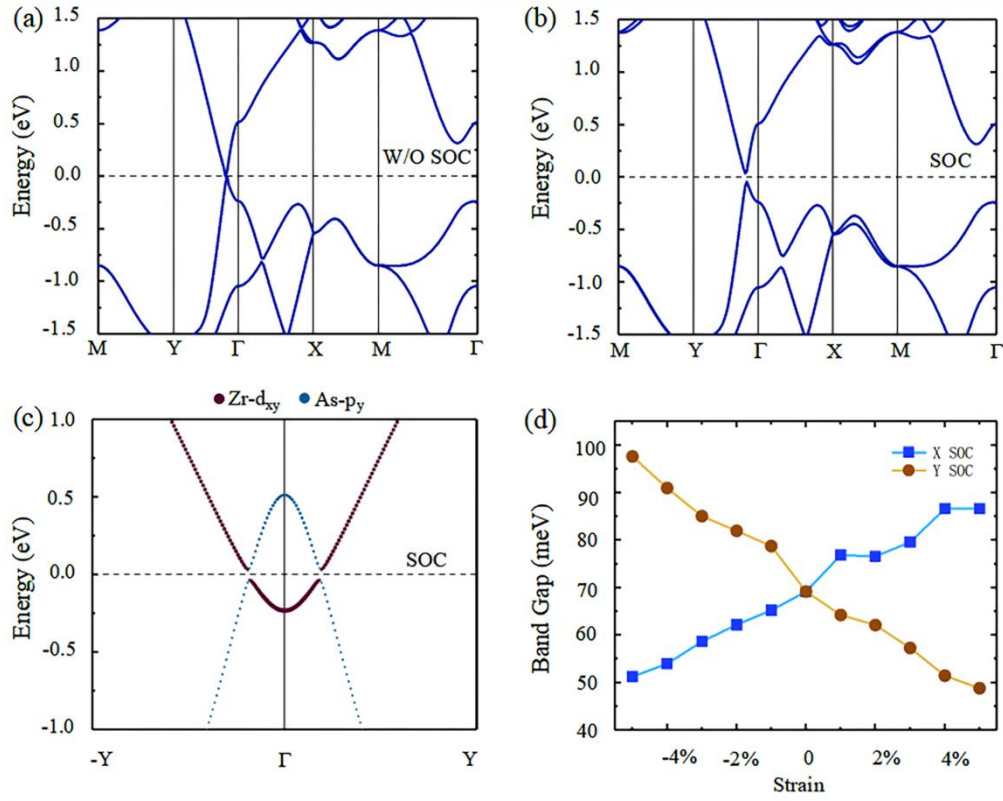


Figure S3. Band structures of single-layer ZrAsCl (a) without SOC and (b) with SOC. (c) Orbitaly resolved band structure of single-layer ZrAsCl. (d) Variation of the energy gaps for single-layer ZrAsCl versus the uniaxial along a- and b-axes.

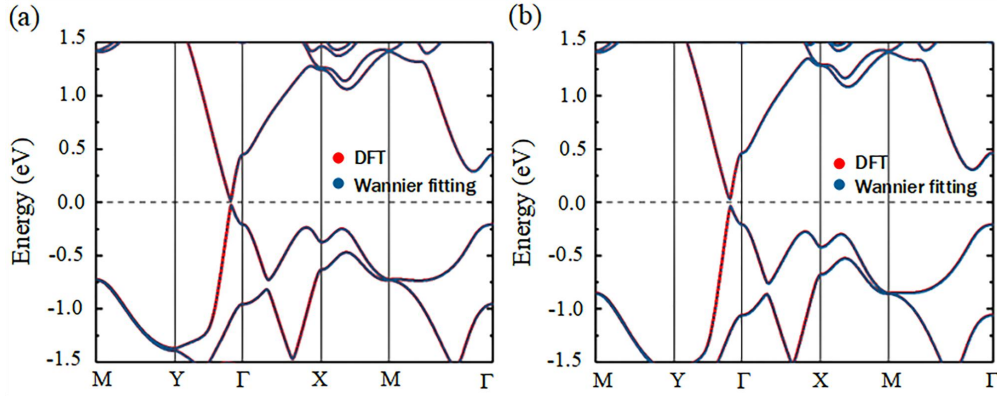


Figure S4. Wannier and first-principles band structures for (a) SL ZrAsBr and (b) SL ZrAsCl with spin-orbit coupling .

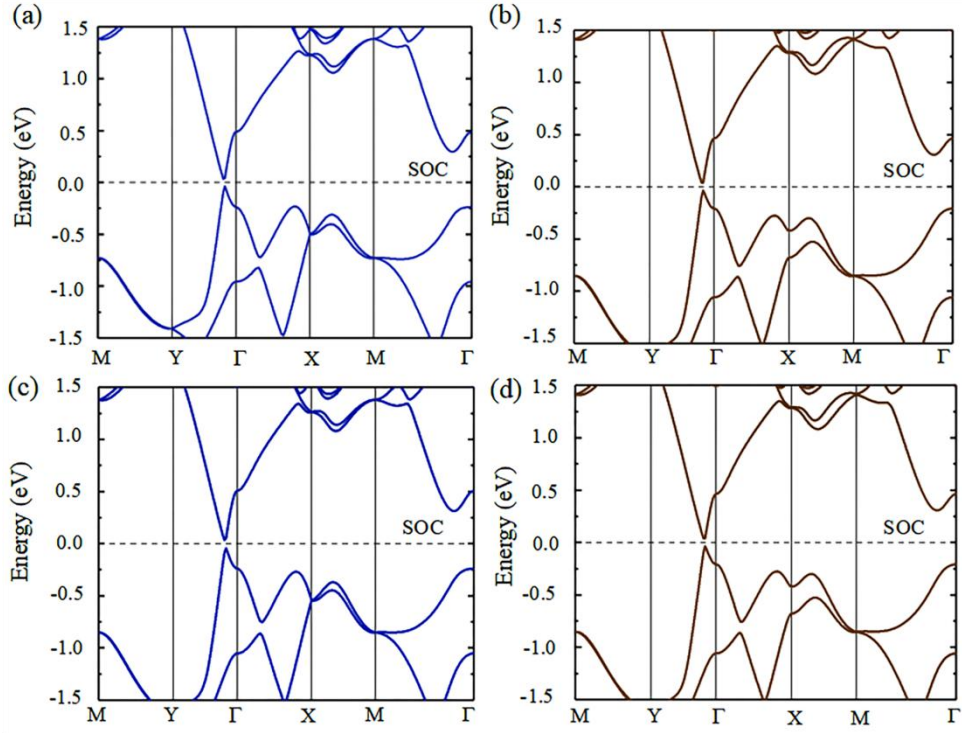


Figure S5. The calculated band structures of SL ZrAsBr from (a) VASP and (b) FLEUR with SOC, and that of SL ZrAsCl from (c) VASP and (d) FLEUR with SOC, indicating the consistency of the electronic properties computed within two codes.

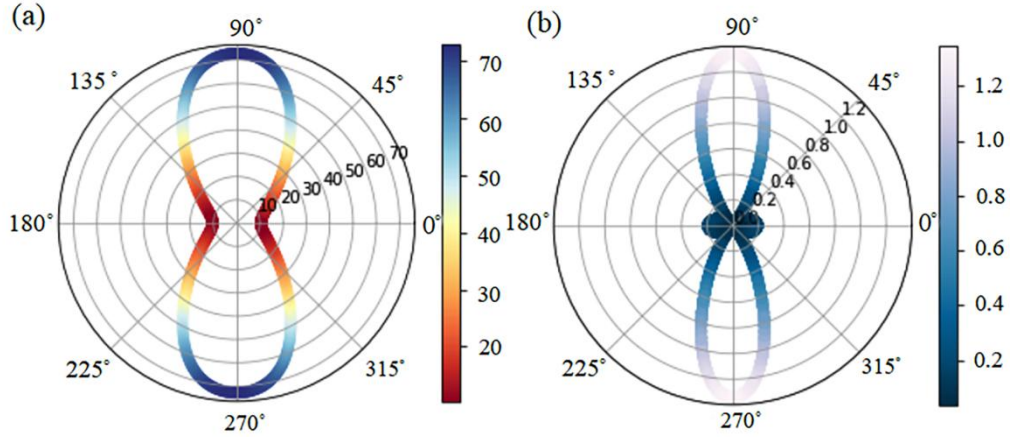


Figure S6. (a) Young's modulus and (b) Poisson's ration of single-layer ZrAsCl as a function of the angle θ . $\theta = 0^\circ$ corresponds to the a axis.

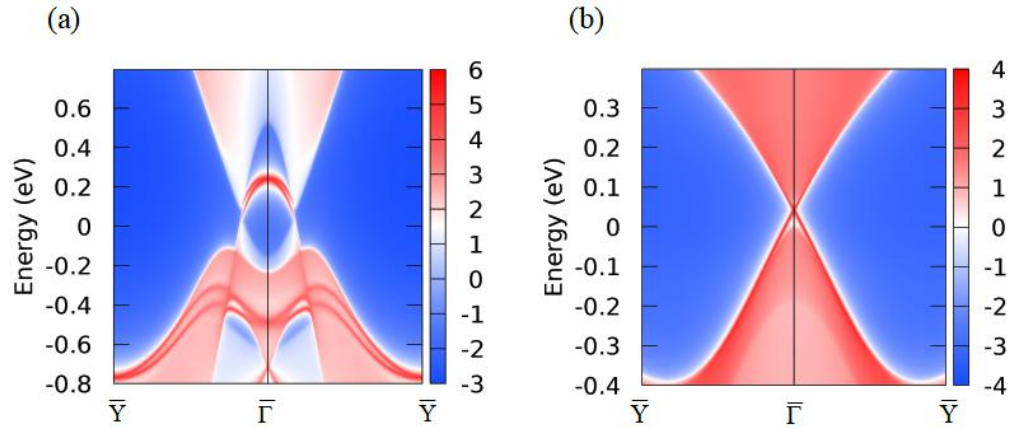


Figure S7. Local density of states of the semi-infinite ZrAsBr at ferroelectric states (a) F and (b) F' with SOC. The Fermi level is set to 0 eV.