

Electronic Supplementary Information

**Phase Transitions and Ferroelasticity/Multiferroicity in Bulk and Two-dimensional Silver and Copper Monohalides**

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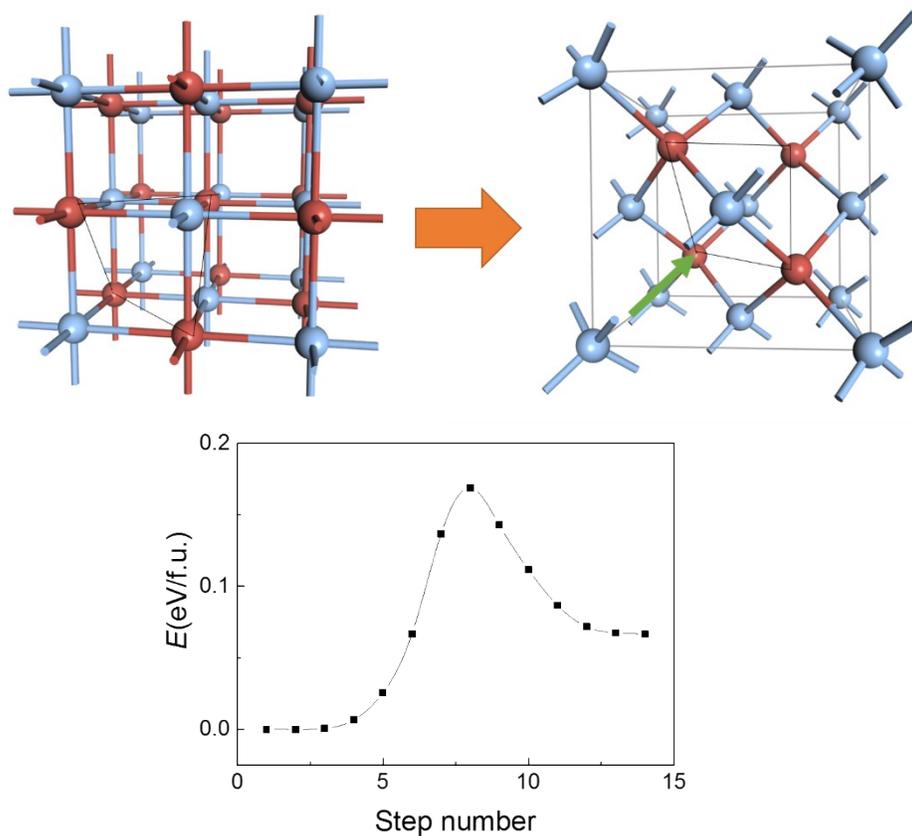


Figure S1. Computed pathway of transformation of RS into ZB phase by simultaneously displacing all halide anions in RS structure by the vector  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ .

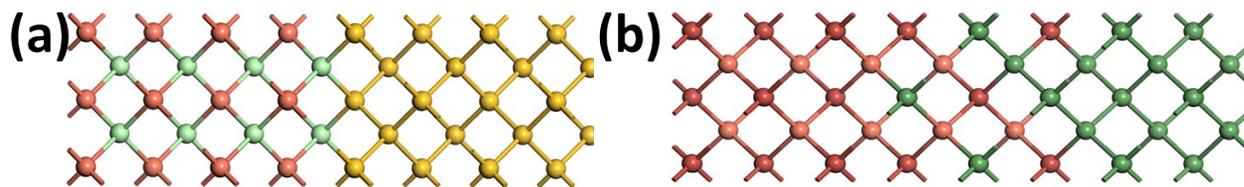


Figure S2. Two typical models of chemical multi-junction: (a) CuCl/Si and (b) CuBr/Cu<sub>1-x</sub>Br<sub>1-x</sub>Ge<sub>x</sub>/Ge.

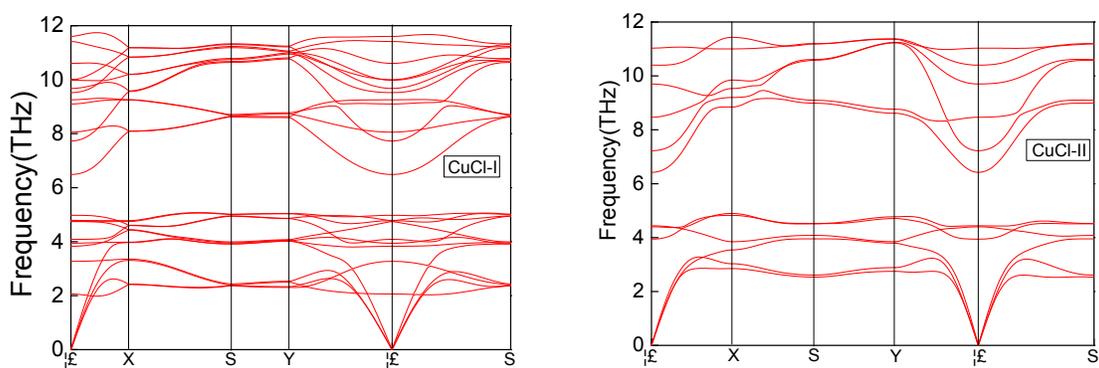


Figure S3. Phonon dispersion of 2D polymorph I and II of CuCl calculated by using Phonopy.

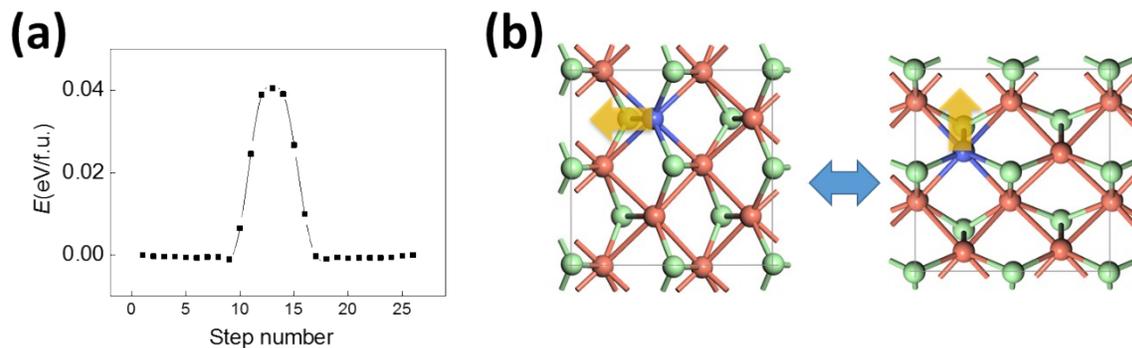


Figure S4. (a) The switching pathway for 2D CuCl polymorph II, and (b) 90 degree ferromagnetic switching induced by 90 degree ferroelectric switching (ferroelastic switching) upon doping of Ni ions.