

Supplementary Information

Tunable valley polarization and magnetic anisotropy by polarization reversal in $\text{Ni}_2\text{Cl}_3\text{I}_3/\text{AgBiP}_2\text{S}_6$ heterojunction

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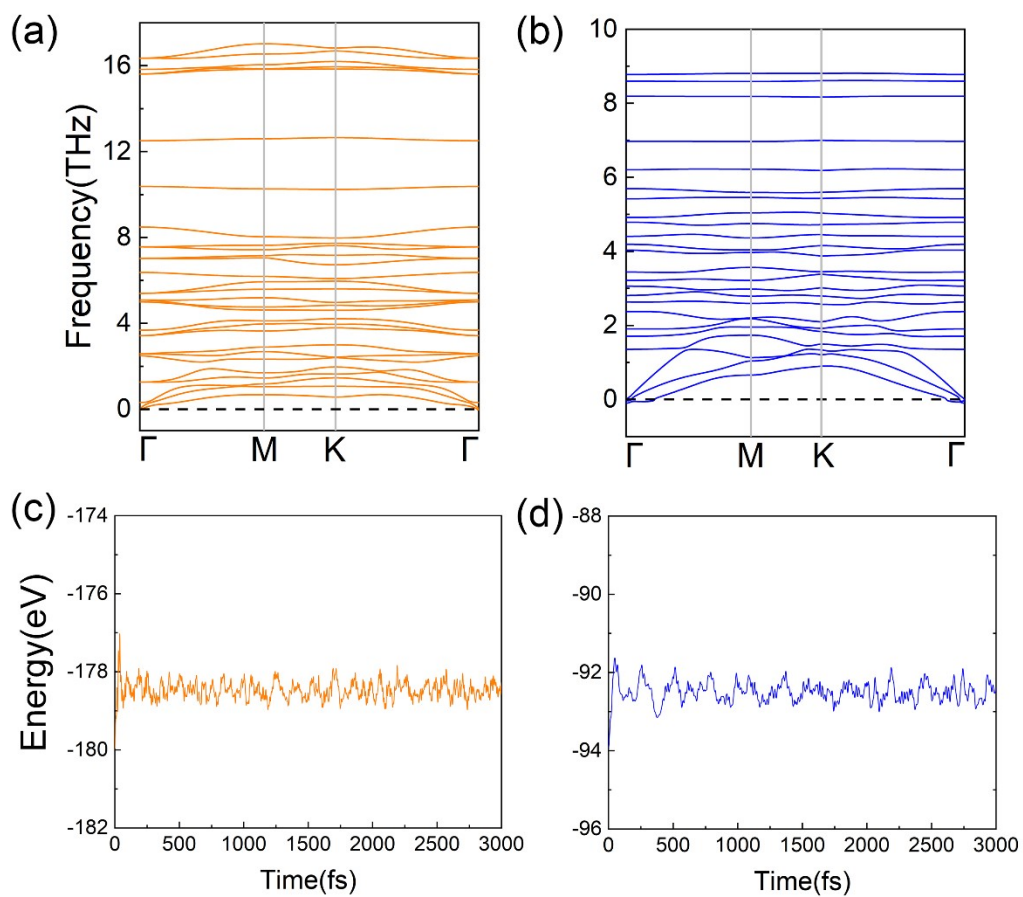


Fig. S1 Phonon spectrum of (a) AgBiP₂S₆ and (b) Ni₂Cl₃I₃. Variations of the total potential energy of (c) AgBiP₂S₆ and (d) Ni₂Cl₃I₃ in AIMD simulations at 300 K.

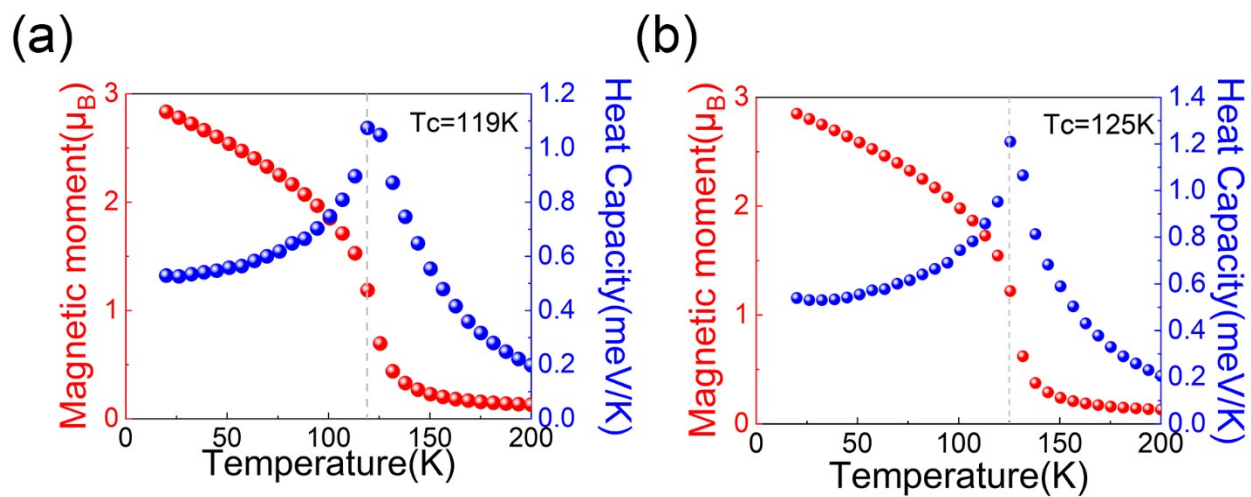


Fig. S2 The magnetic moment and heat capacity as functions of temperature for (a) $\text{Ni}_2\text{Cl}_3\text{I}_3$ and (b)

$\text{Ni}_2\text{Cl}_3\text{I}_3/\text{AgBiP}_2\text{S}_6$.

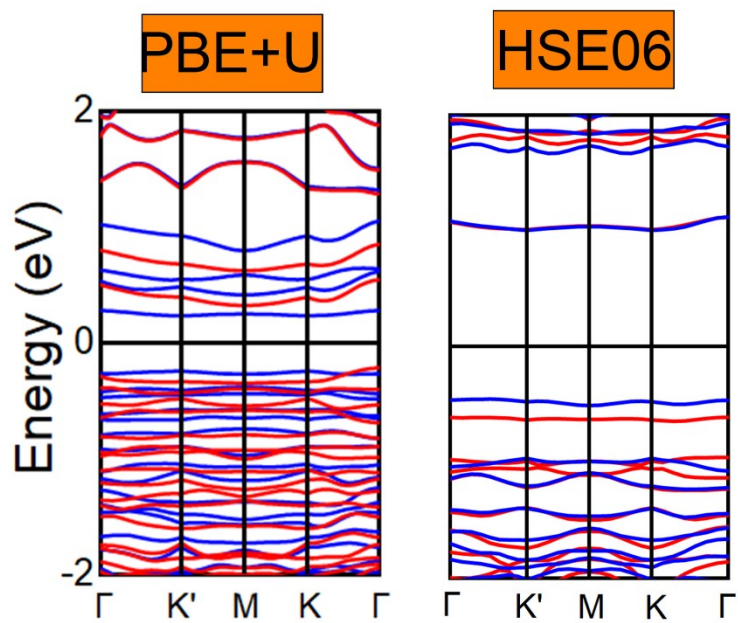


Fig. S3 The band structures of $\text{Ni}_2\text{Cl}_3\text{I}_3/\text{AgBiP}_2\text{S}_6$ calculated by the (a) PBE+ U and (b) HSE06.

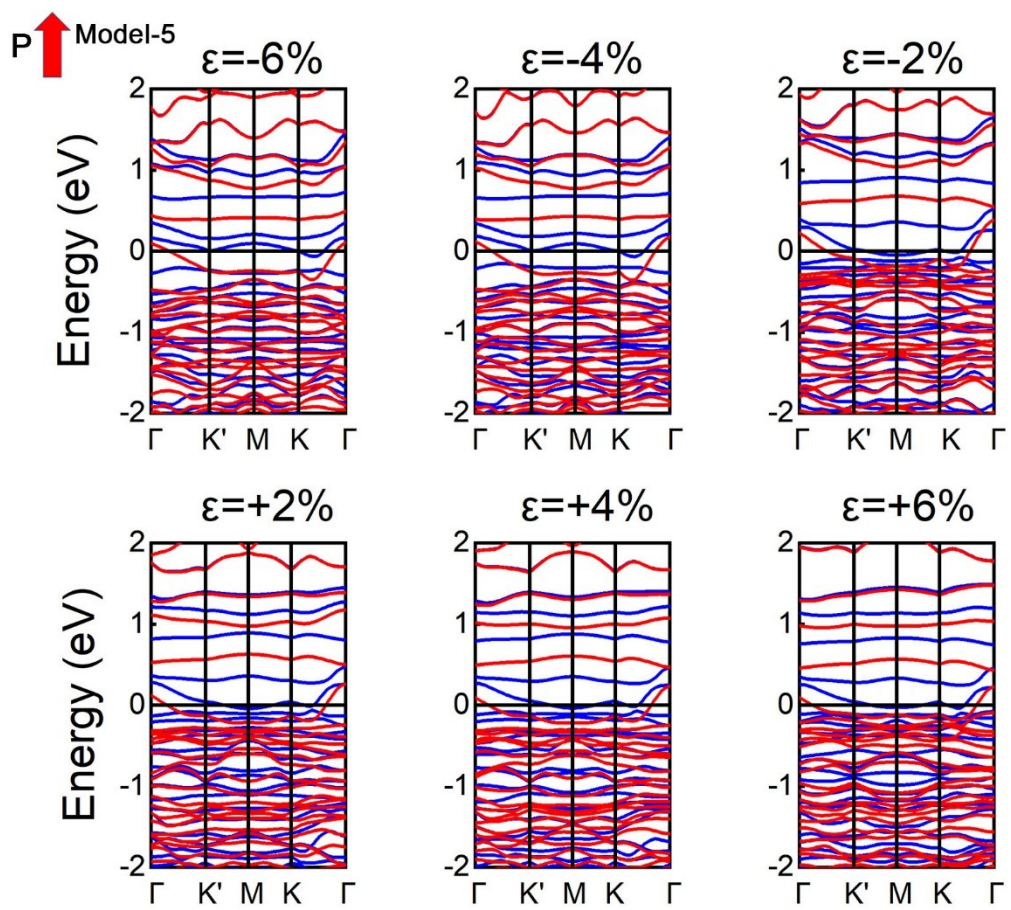


Fig. S4 The band structures of $\text{Ni}_2\text{Cl}_3\text{I}_3/\text{AgBiP}_2\text{S}_6$ using the $\text{PBE}+U$ after applying biaxial strain.

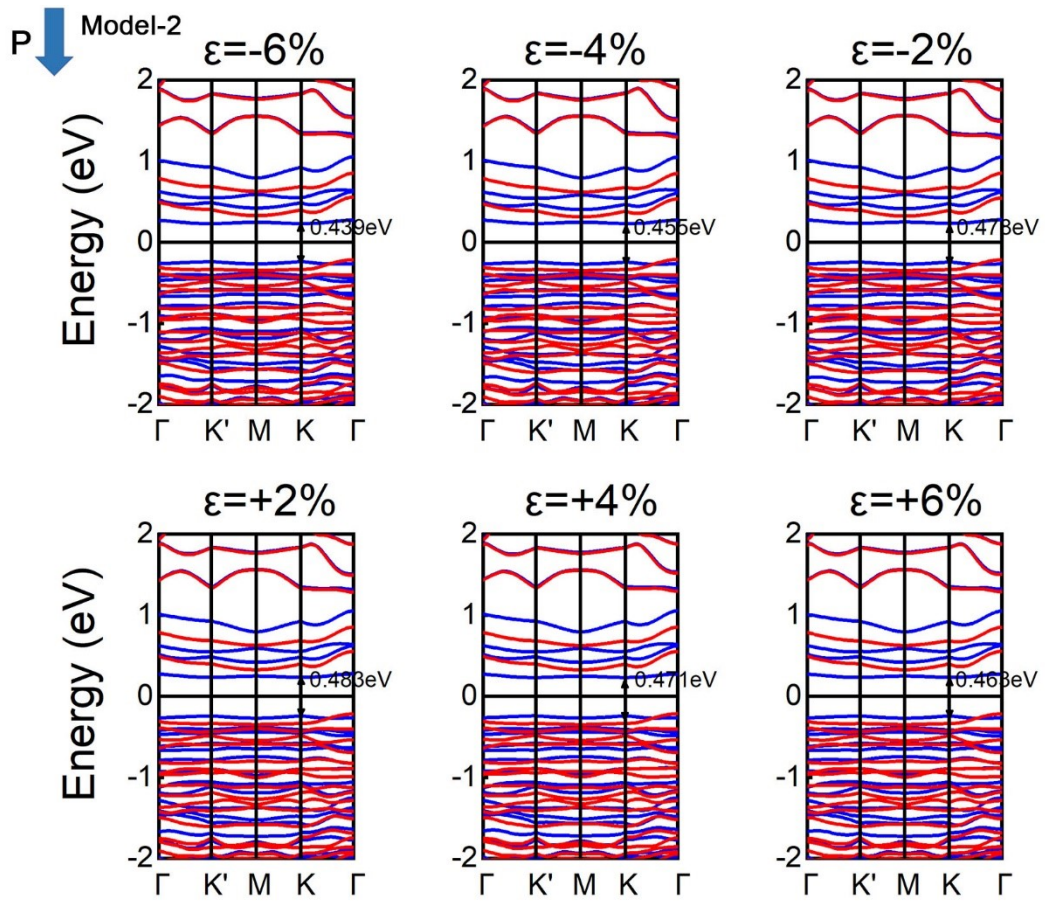


Fig. S5 The band structures of $\text{Ni}_2\text{Cl}_3\text{I}_3/\text{AgBiP}_2\text{S}_6$ using the PBE+ U after applying biaxial strain.

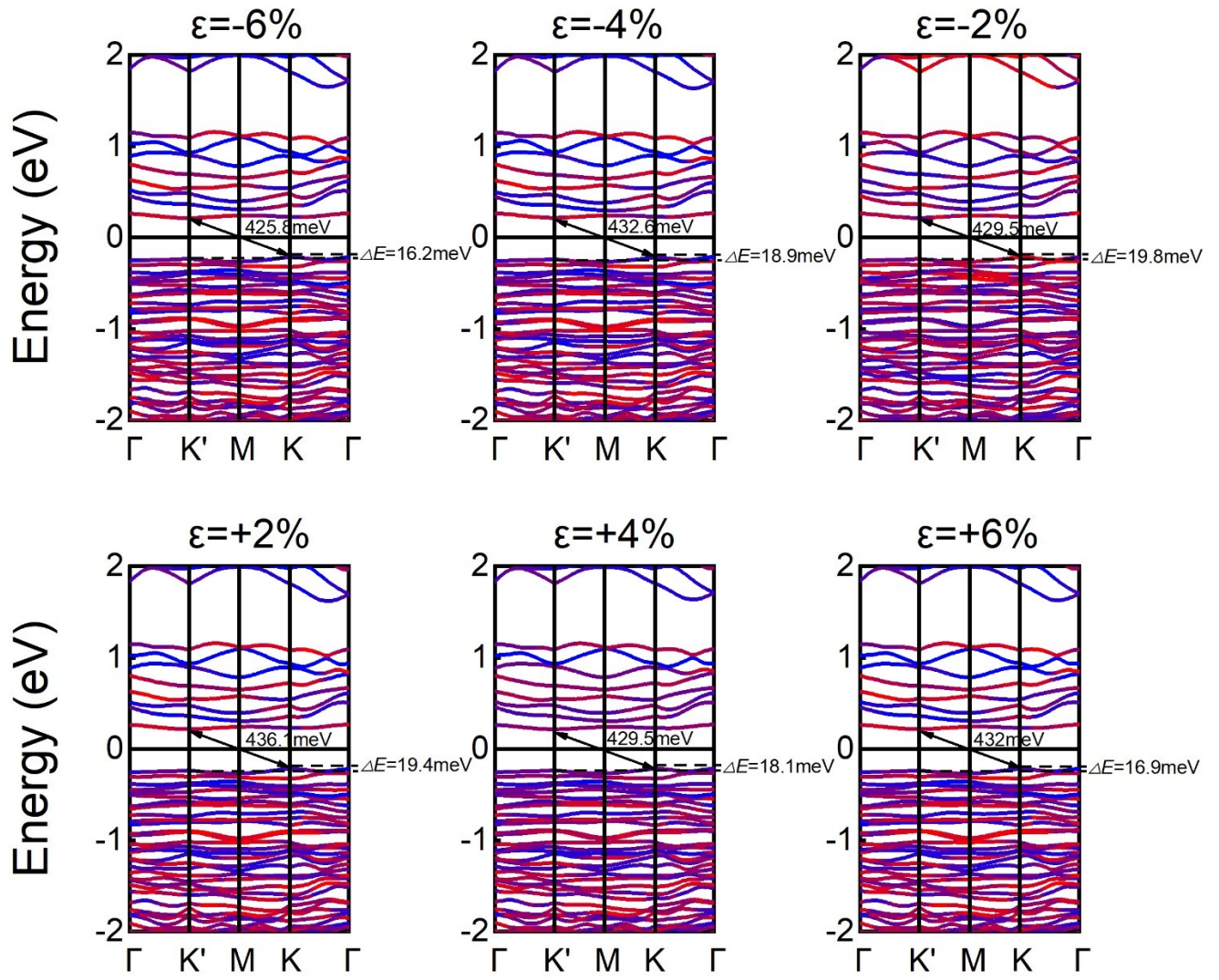


Fig. S6 The band structures of $\text{Ni}_2\text{Cl}_3\text{I}_3/\text{AgBiP}_2\text{S}_6$ after applying biaxial strain and SOC.

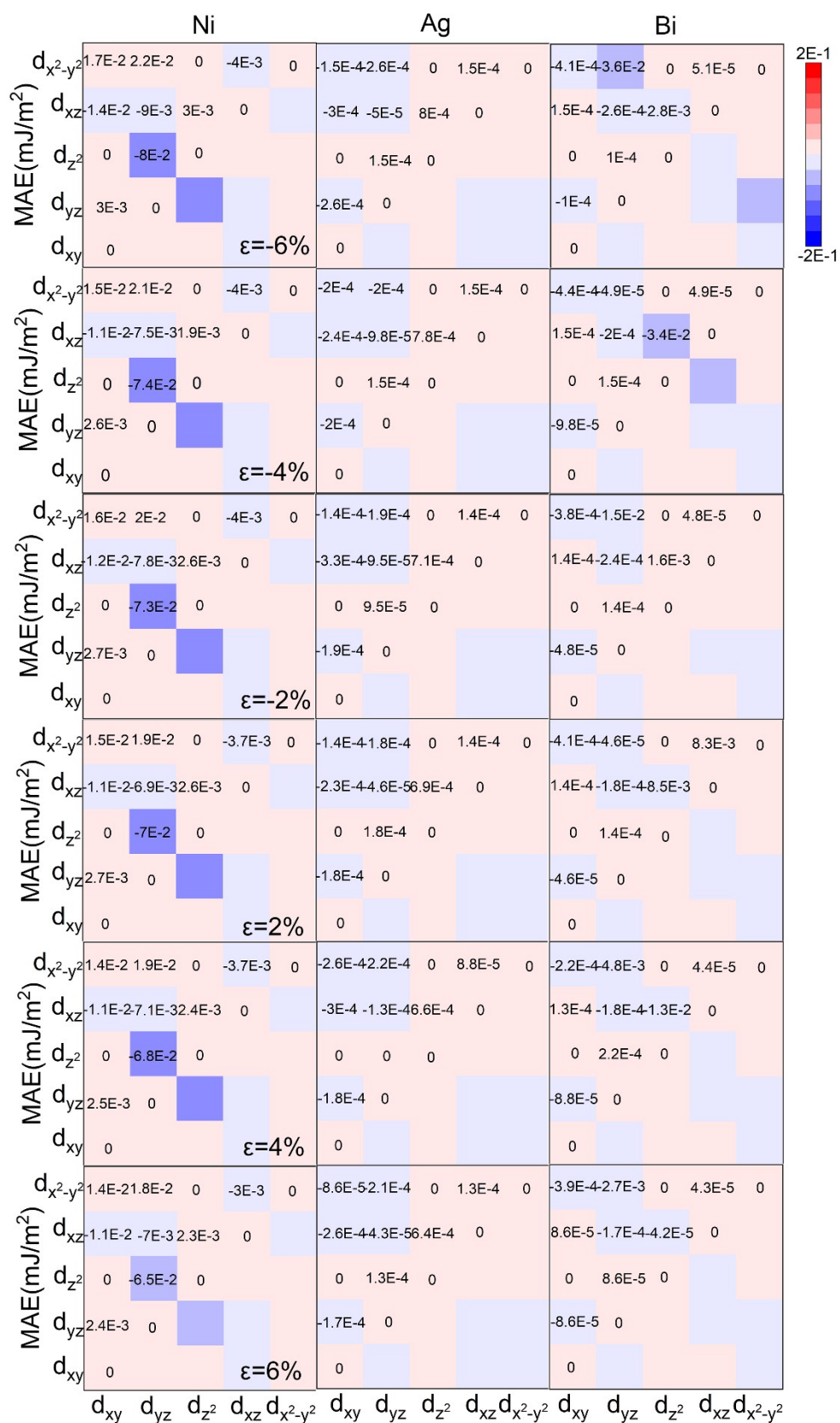


Fig. S7 The MAE of Ni, Ag and Bi atoms in model-2↓ after applying biaxial strain.