Electronic Supplementary Information for

Valley polarization and magnetic anisotropy of two-dimensional $Ni_2Cl_3I_3/MoSe_2$ heterostructure

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A. Band structure of $Ni_2Cl_3I_3/MoSe_2$

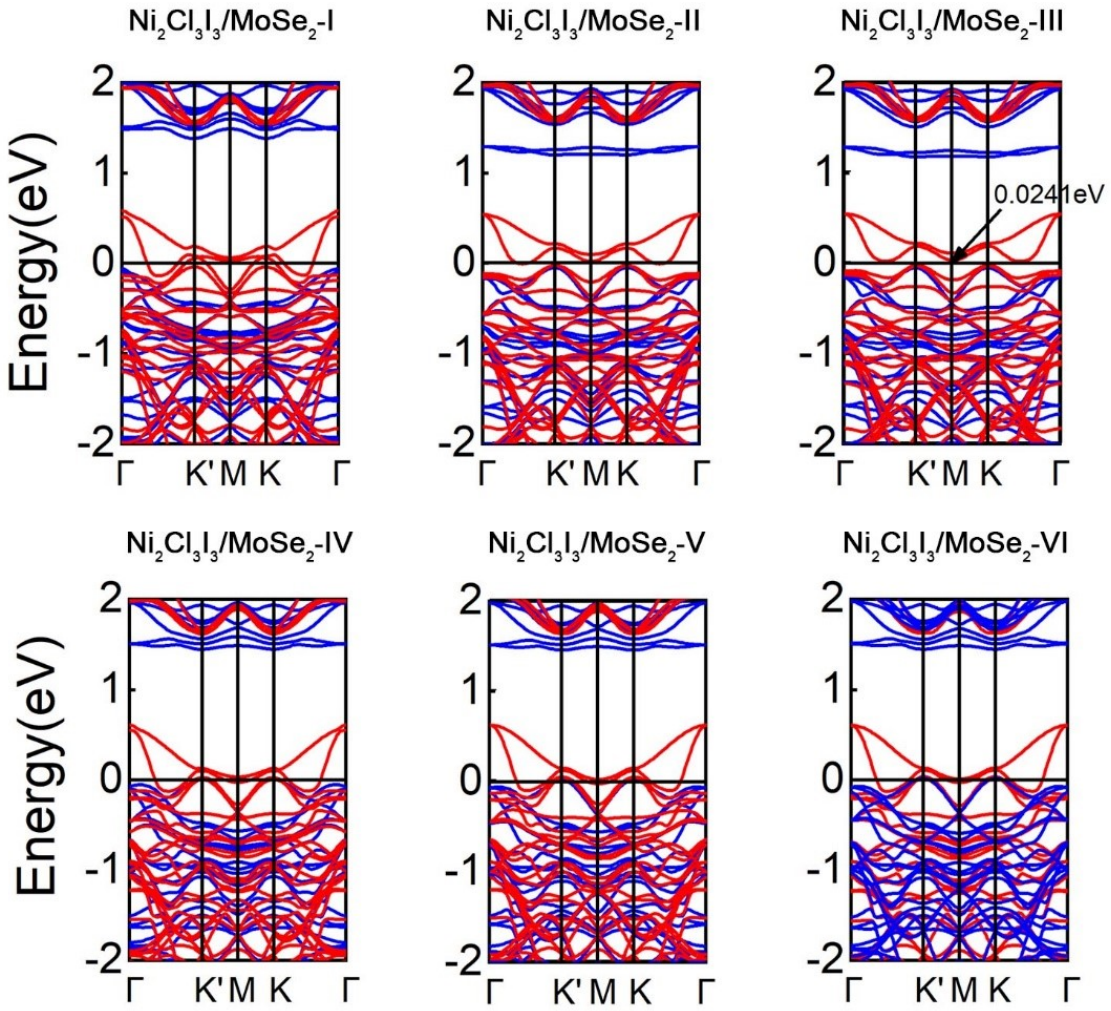

Fig. S1. The band structure of $Ni_2Cl_3I_3/MoSe_2$ using the PBE+*U*.

B. MAE of $Ni_2Cl_3I_3/MoSe_2$-I after applying biaxial strain

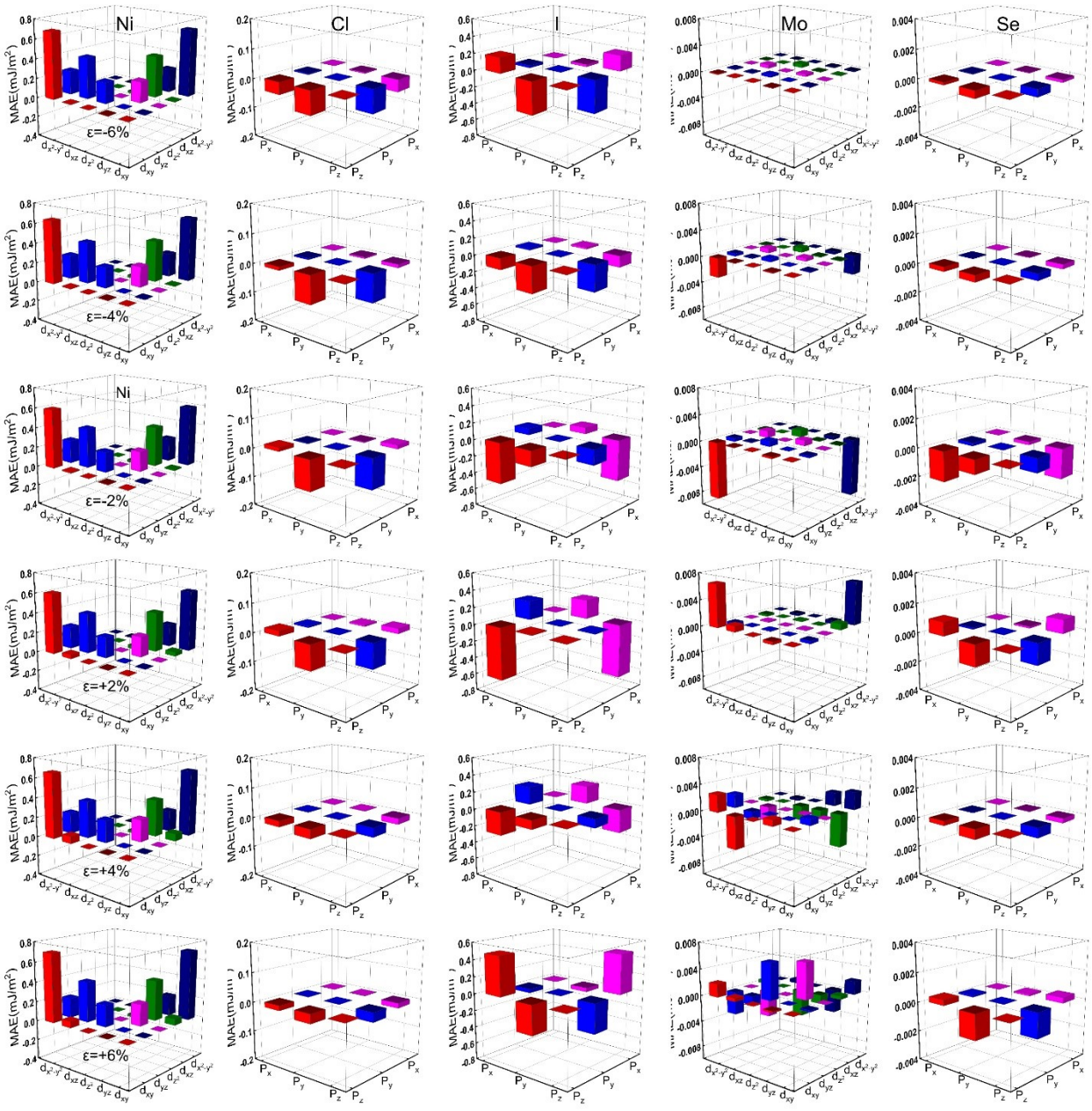

Fig. S2. The MAE of $Ni_2Cl_3I_3/MoSe_2$-I after applying biaxial strain.

C. MAE of $Ni_2Cl_3I_3/MoSe_2$- III after applying biaxial strain

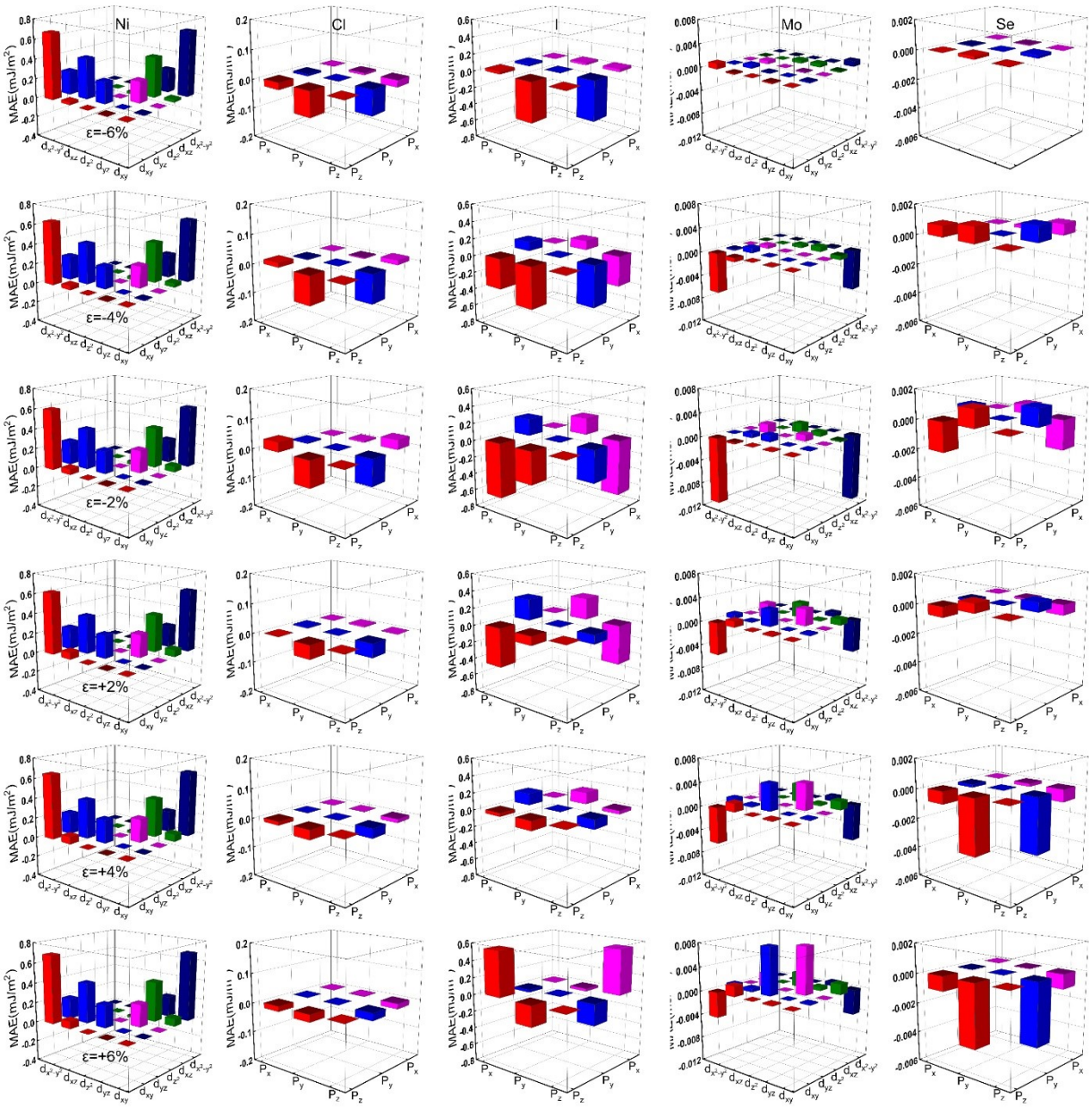

Fig. S3. The MAE of $Ni_2Cl_3I_3/MoSe_2$- III after applying biaxial strain.

D. The planar average of electrostatic potential after applying biaxial strain

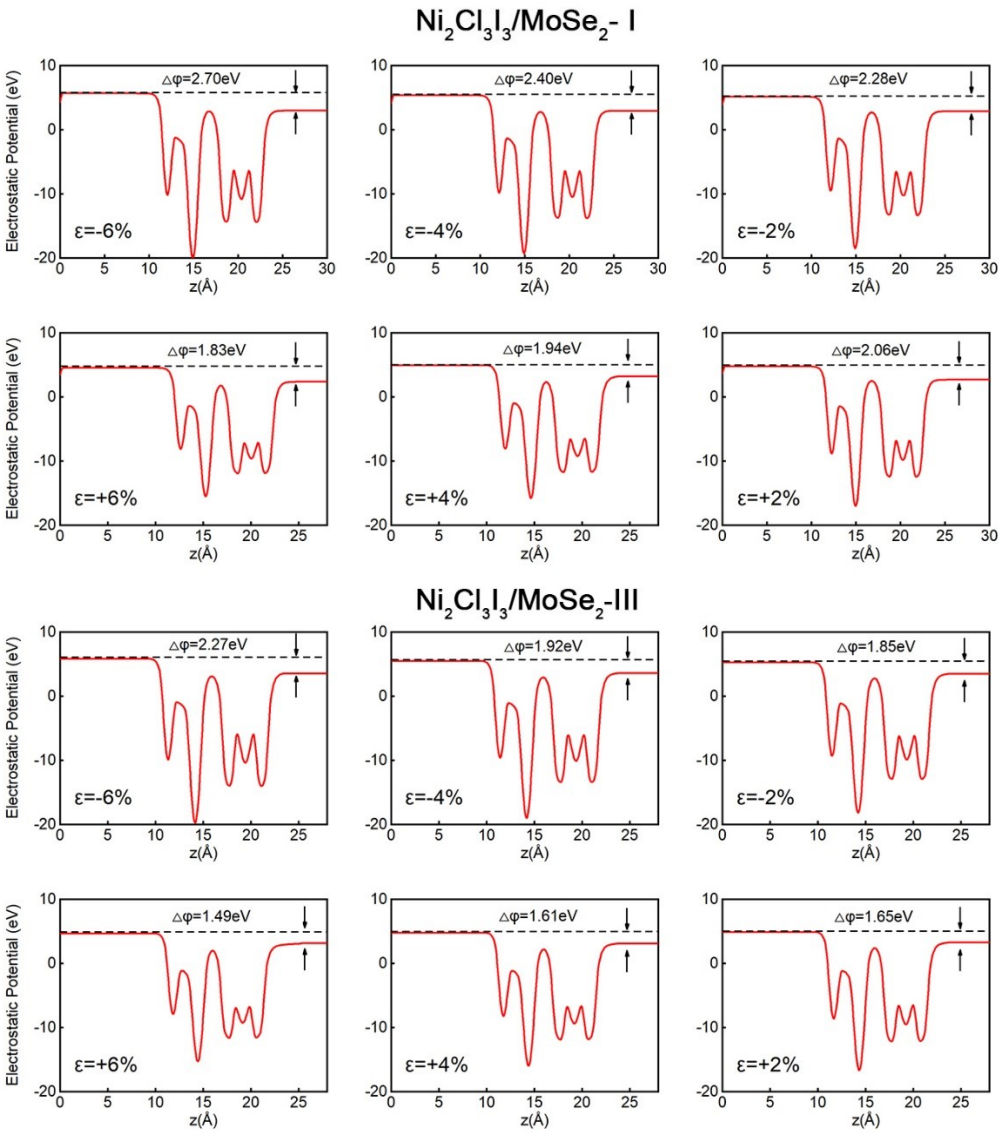

Fig. S4. The planar average of electrostatic potential of $Ni_2Cl_3I_3/MoSe_2$-I and III after applying biaxial strain.

E. The Phonon spectra

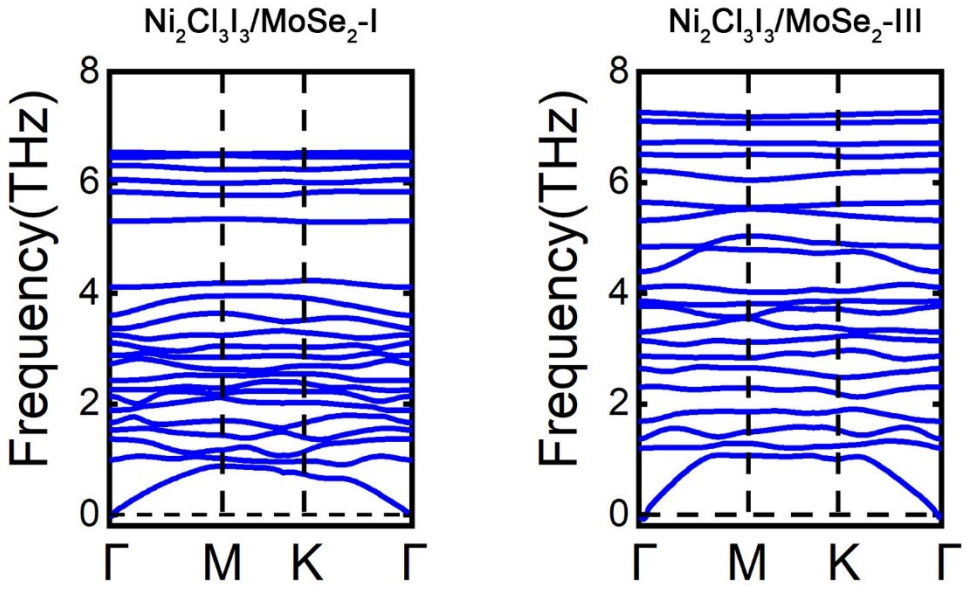

Fig. S5. The Phonon spectra of $Ni_2Cl_3I_3/MoSe_2$-I and III.