Supporting Information for

Nonvolatile Electro-Mechanical Coupling in Two-Dimensional Lattices

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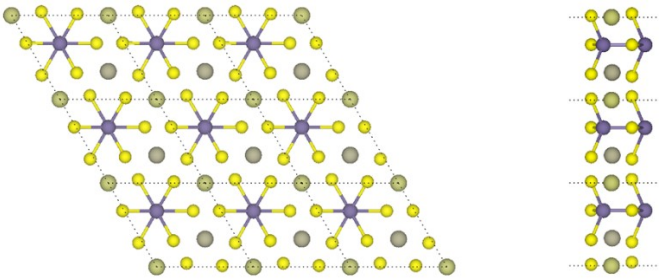

Fig. S1 Crystal structure of SL $ReIrGe_2S_6$ from top and side views.

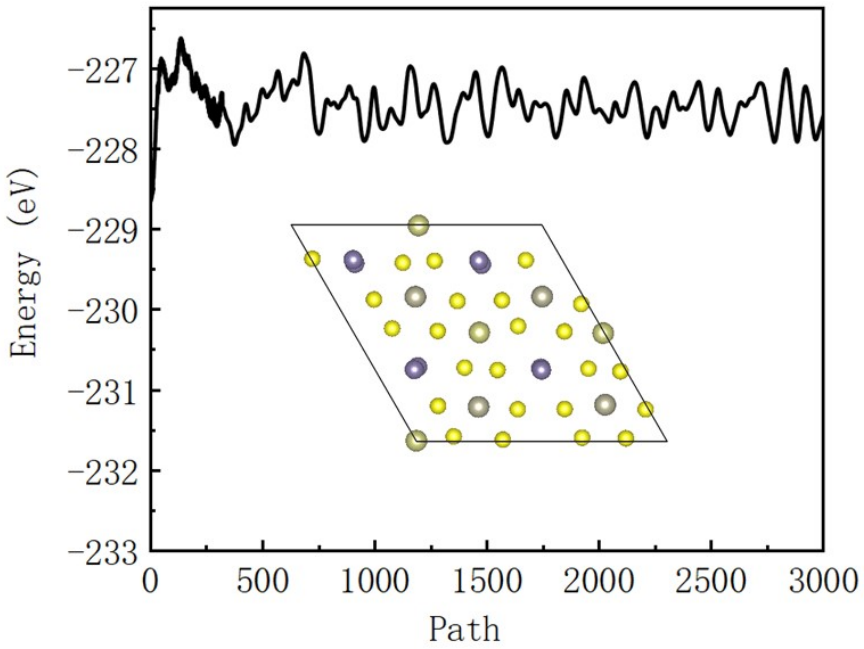

Fig. S2 Variation of total energy during AIMD (300 K, 3 ps) simulations. Inset is crystal structure of SL $ReIrGe_2S_6$ taken from the end of AIMD.

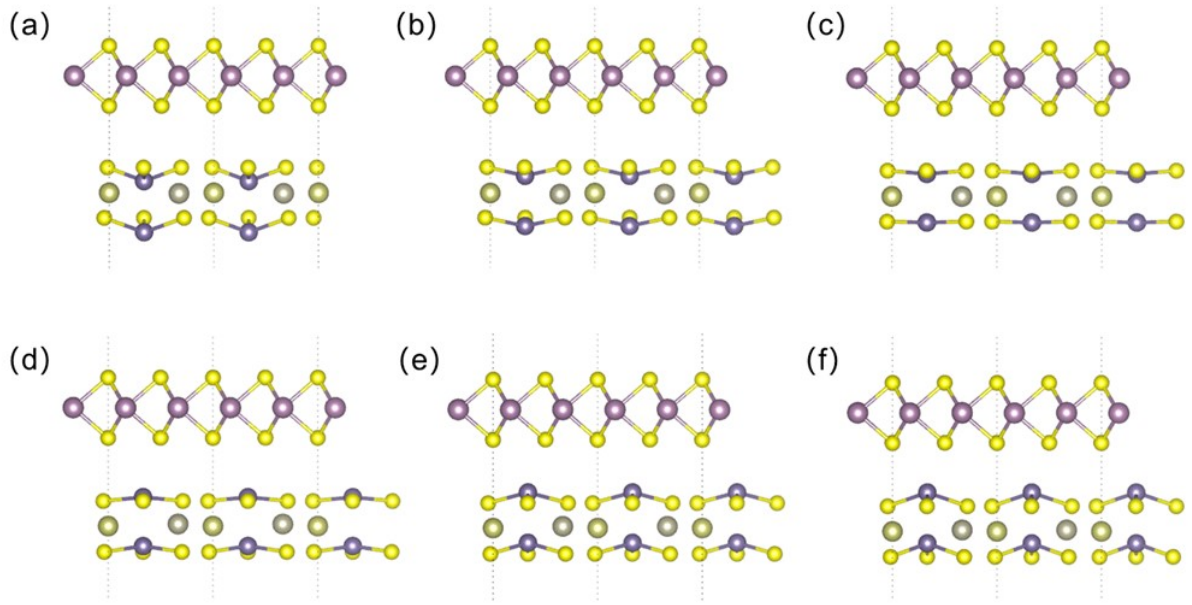

Fig. S3 Structure generation during CI-NEB for bilayer $MoS_2/ReIrGe_2S_6$. Yellow, blue, gray, brown, and purple spheres represent S, Ge, Re, Ir, and Mo atoms, respectively.

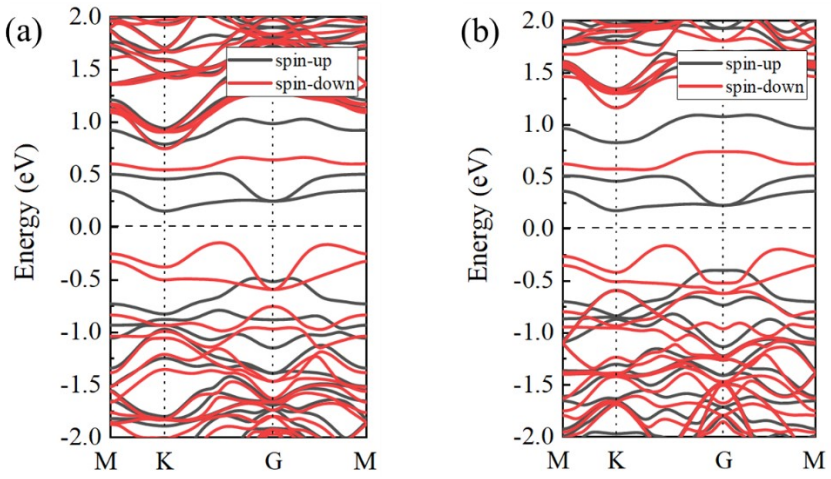

Fig. S4 (a-b) Band structures of MoS_2/$ReIrGe_2S_6$ bilayer with P↑ and P↓.

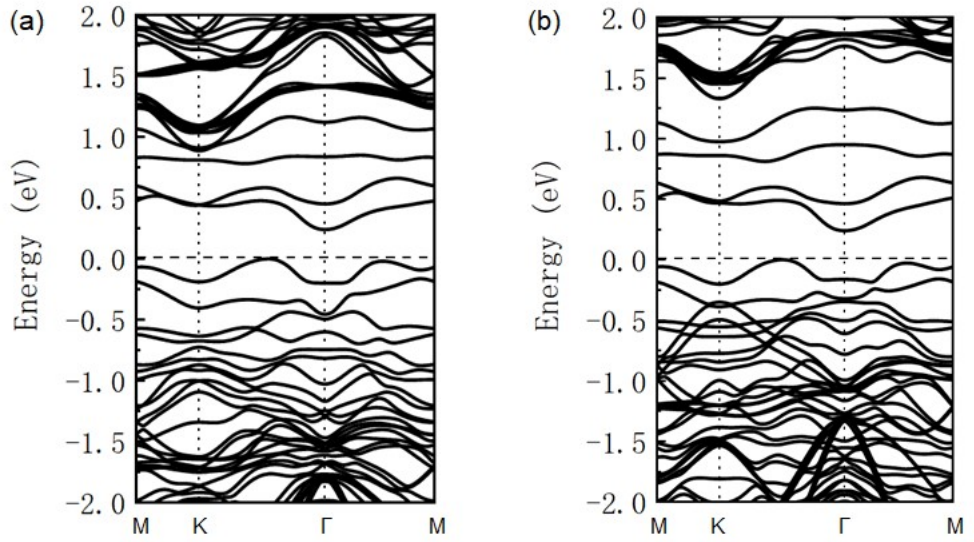

Fig. S5 (a-b) Band structures with SOC of $MoS_2/ReIrGe_2S_6$ bilayer with P↑ and P↓.

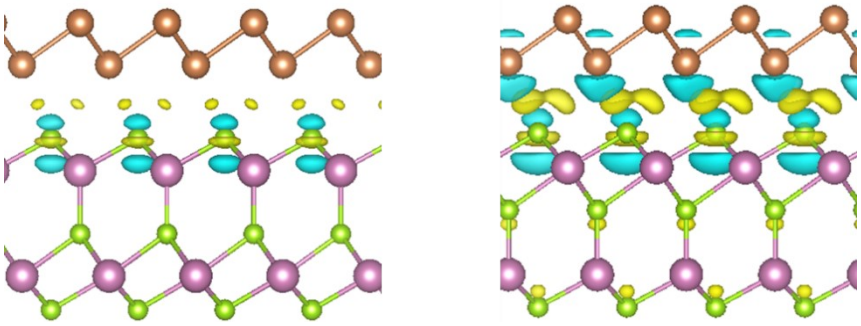

Fig. S6 The charge density difference of Sb/In_2Se_3 bilayer under P↑ and P↓. The isosurface value is set to 0.02 electrons per $Å^3$.

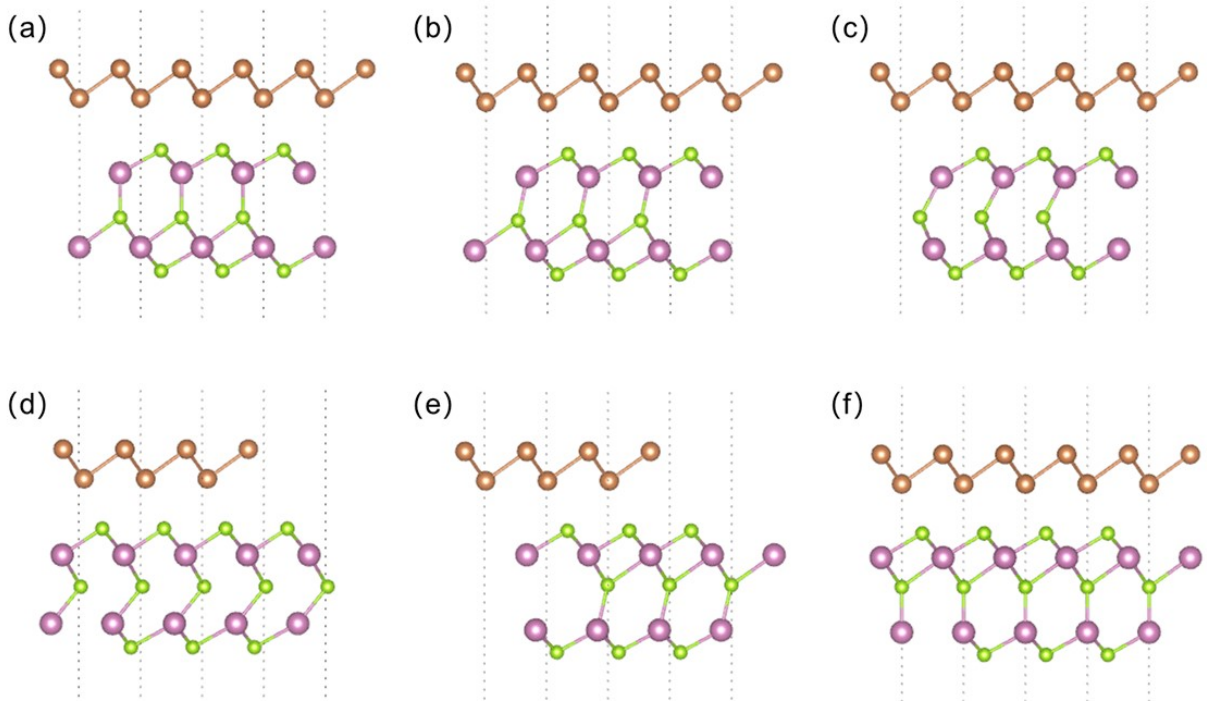

Fig. S7 Structure generation during CI-NEB for bilayer Sb/In_2Se_3. Brown, green, and purple spheres represent Sb, Se, and In atoms, respectively.

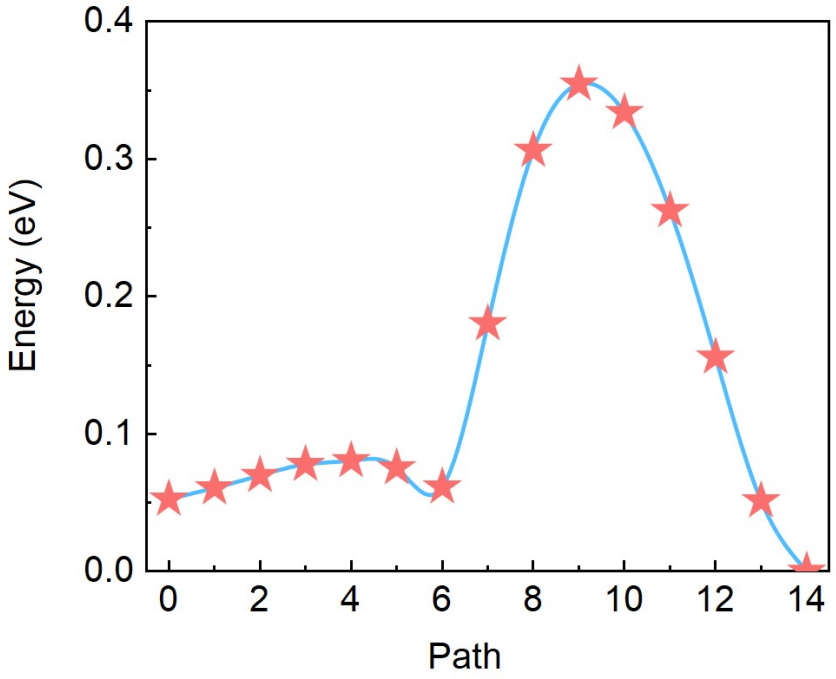

Fig. S8 Minimum energy pathway of FE switching as a function of step number within NEB for Sb/In_2Se_3 bilayer.

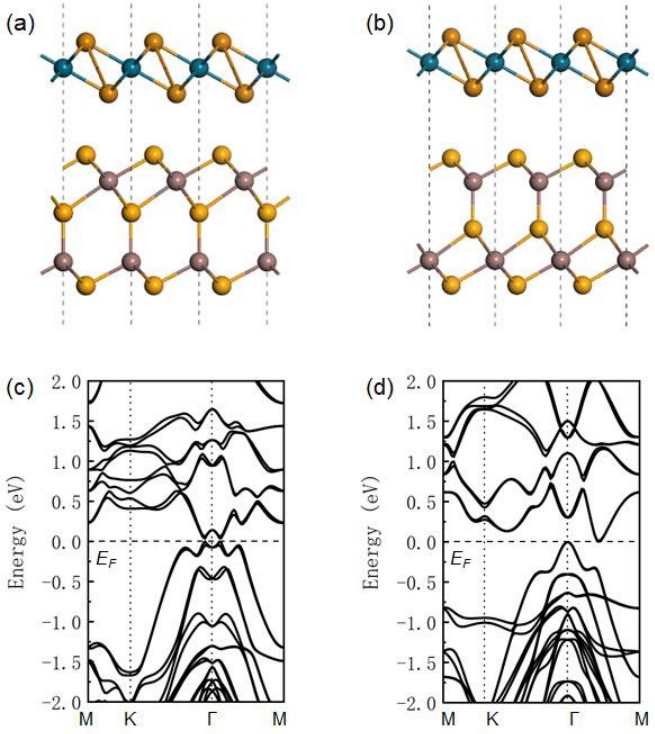

Fig. S9 (a-b) Crystal structures of $PdTe_2/In_2Se_3$ bilayer under P↑ and P↓ configurations. Orange, blue, yellow and brown spheres represent Te, Pd, Se and In atoms, respectively. (c-d) Band structures of $PdTe_2/In_2Se_3$ bilayer under P↑ and P↓ configurations.

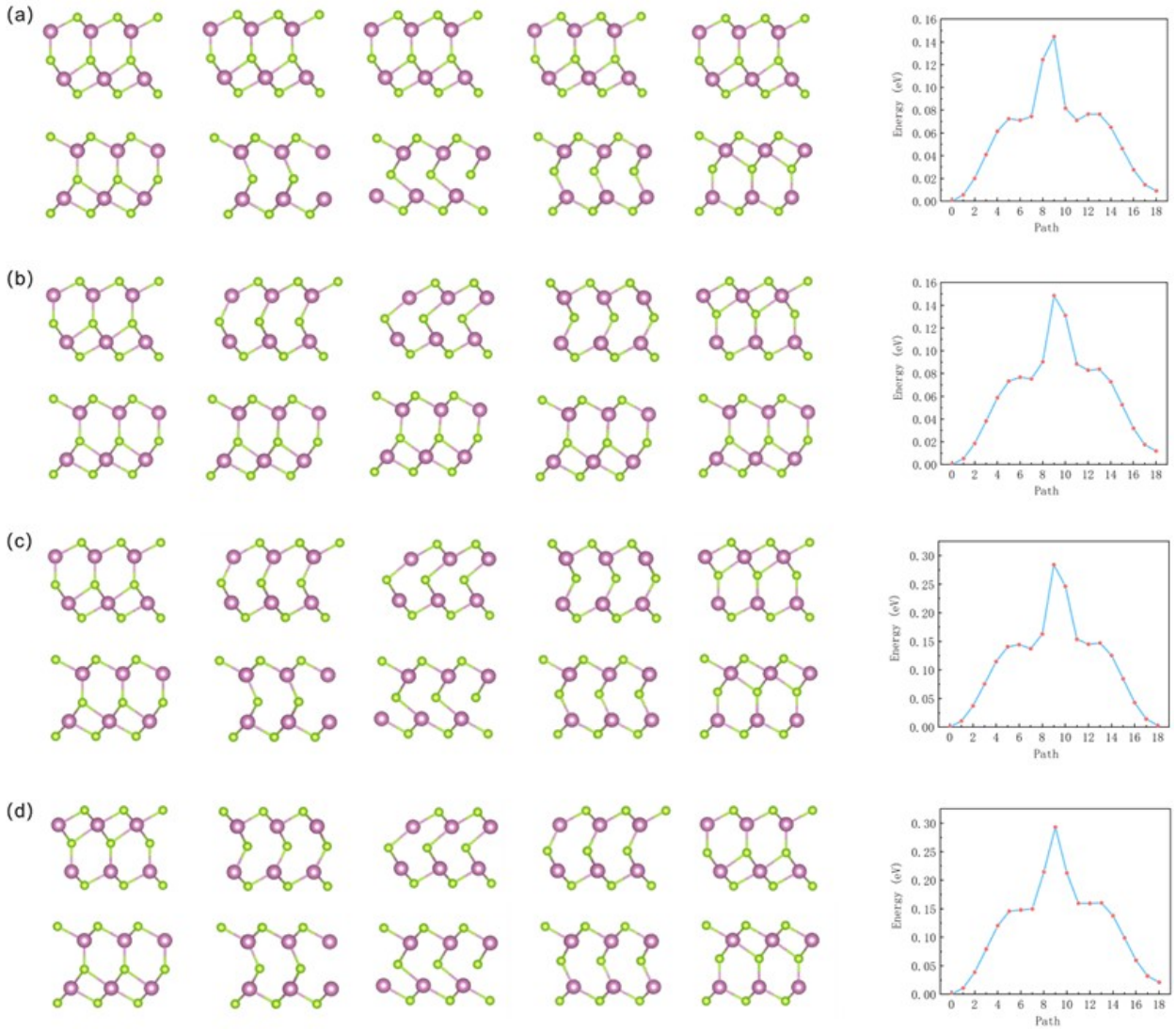

Fig. S10 Structure generation and Minimum energy pathway of FE switching for bilayer In_2Se_3. (a) From P↑↑ to P↑↓. (b) From P↑↑ to P↓↑. (c) From P↑↑ to P↓↓. (d) From P↓↑ to P↑↓. Green, and purple spheres represent Sb, Se, and In atoms, respectively.

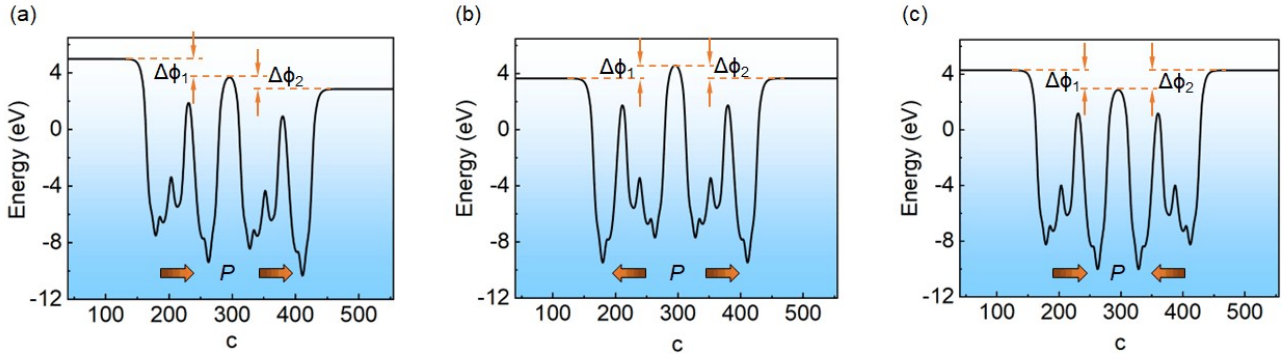

Fig. S11 Plane-averaged potential of bilayer In_2Se_3 along z direction under (a) P↑↑, (b) P↑↓ and (c) P↓↑configurations.