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Supplementary Information for

Prediction of single-layer $TiVI_6$ as a promising two-dimensional valleytronic semiconductor with spontaneous valley polarization

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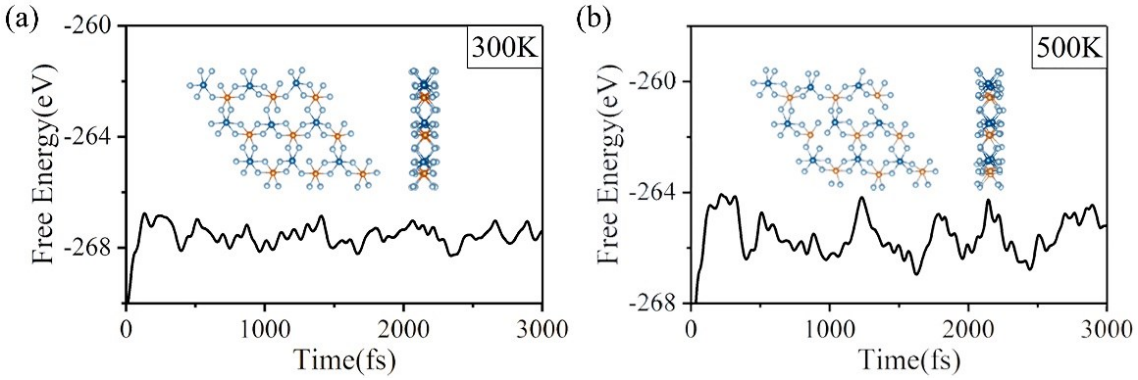

FIG. S1. The molecular dynamic (MD) simulation results of SL $TiVI_6$ at (a) 300K and (b) 500K. Insets are the top and side views of SL $TiVI_6$ structure after MD simulation. The well-preserved structures and small free-energy fluctuation indicate SL $TiVI_6$ remains stable at 300K and 500K.

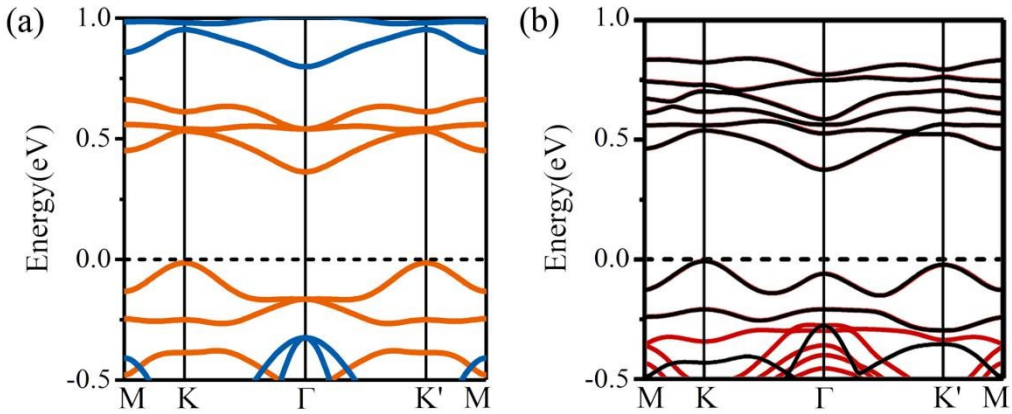

FIG. S2. Spin-polarized band structure of SL $TiVI_6$ (a) without and (b) with SOC based on PBE+U

and wannier function. The orange and blue lines in (a) correspond to spin-up and spin-down states, respectively. The black and red lines in (b) correspond to PBE+U and wannier function, respectively. The Fermi level is set to 0 eV.

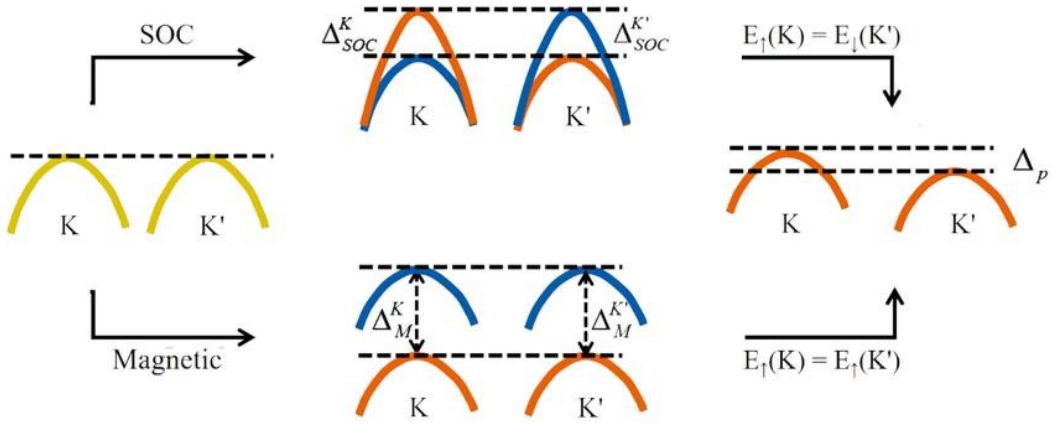

FIG. S3. Schematic diagram of the evaluation of top valance bands under SOC and magnetic exchange interaction.

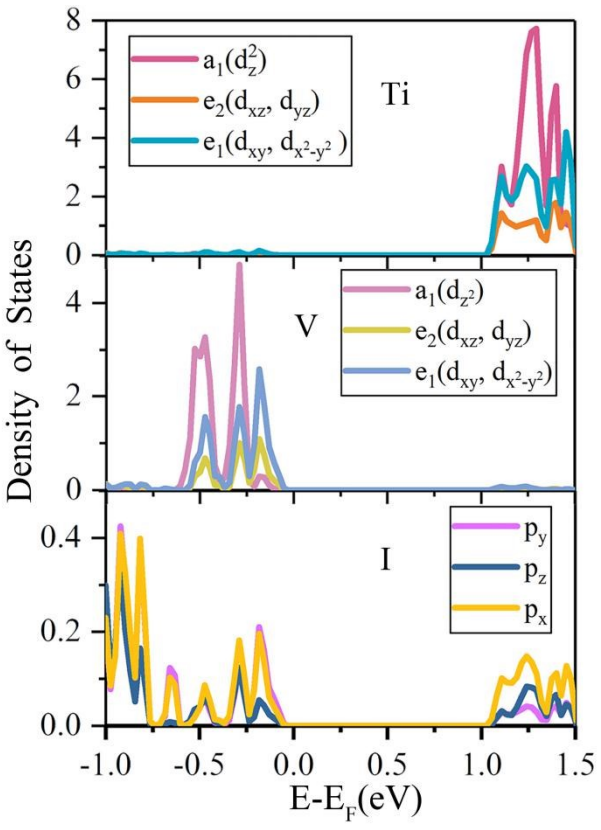

FIG. S4. Density of states of SL $TiVI_6$.

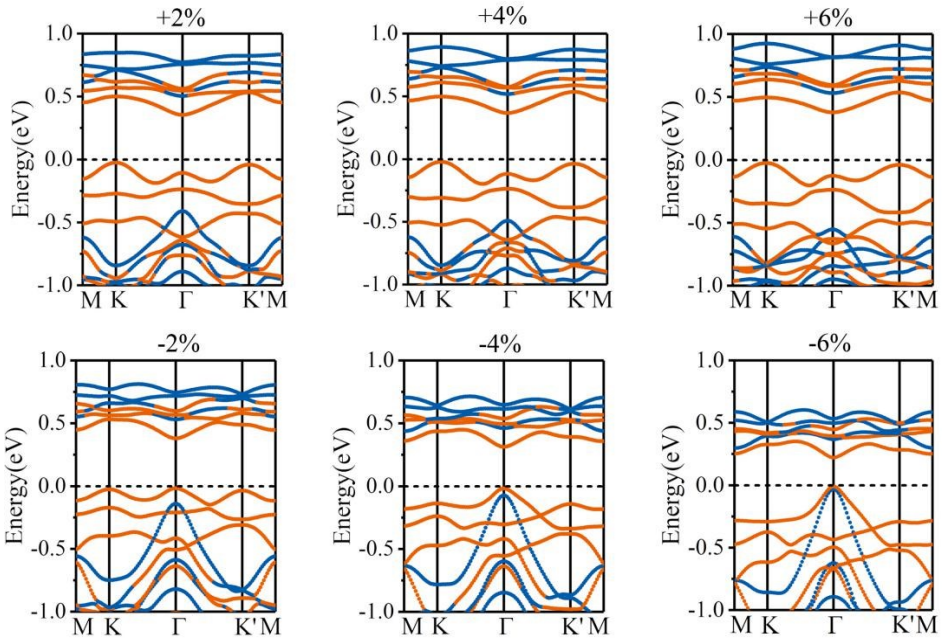

FIG. S5. Spin polarized band structure of SL $TiVI_6$ under various strains based on PBE+U. The orange and blue lines correspond to spin-up and spin-down states, respectively. The Fermi level is set to 0 eV.