

Supplementary Information

Valley Polarization and *p*-/*n*-Type Doping of Monolayer WTe₂ on Top of Fe₃O₄(111)

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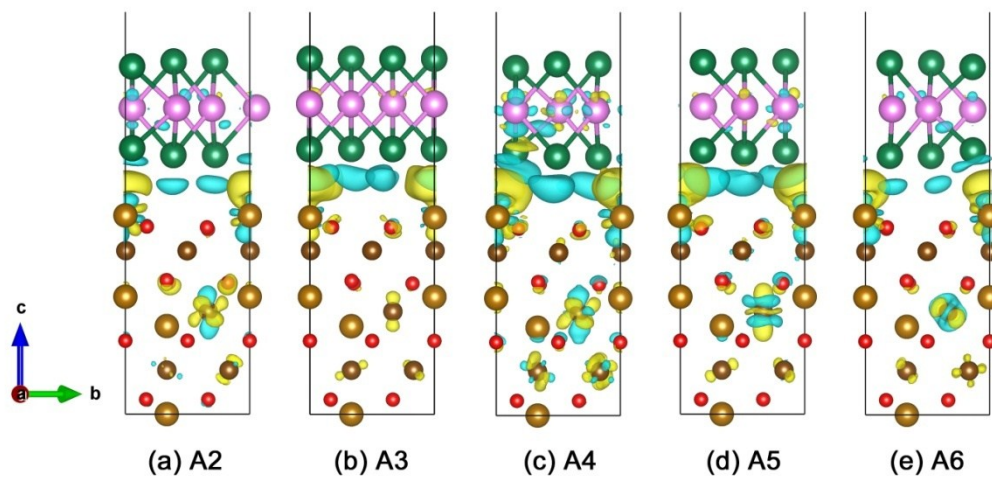


Fig. S1. Side views of charge density differences for A2-A6 models. The isosurface values for A2 and A6 models are 2 e/nm^3 and for A3-A5 models are 1 e/nm^3 . Yellow (blue) regions represent net charge gain (loss).

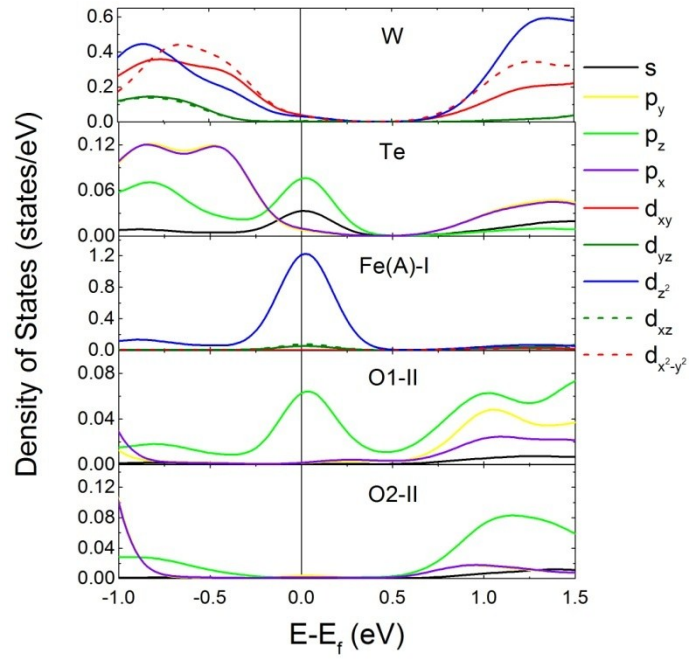


Fig. S2. The orbital-resolved DOS for W, Te, Fe(A)-I, O1-II and O2-II atoms in A4 model, respectively. Fermi energy is indicated by the vertical line and is set to zero.

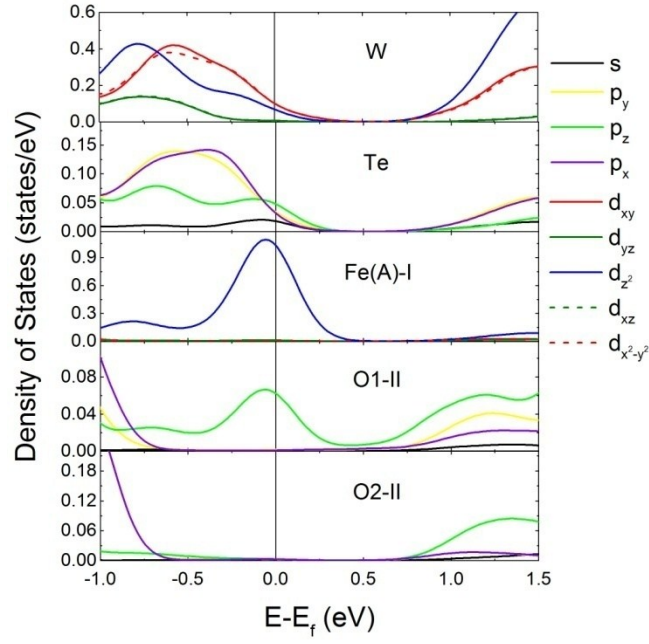


Fig. S3. The orbital-resolved DOS for W, Te, Fe(A)-I, O1-II and O2-II atoms in A5 model, respectively. Fermi energy is indicated by the vertical line and is set to zero.

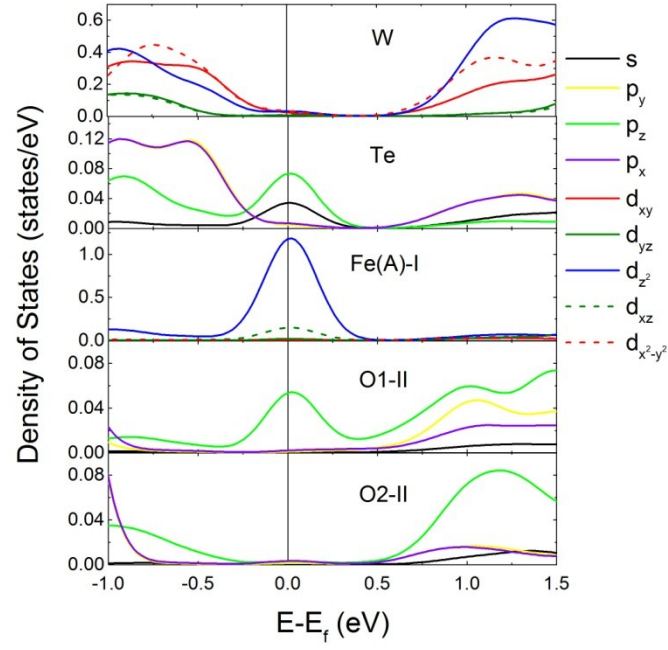


Fig. S4. The orbital-resolved DOS for W, Te, Fe(A)-I, O1-II and O2-II atoms in A6 model, respectively. Fermi energy is indicated by the vertical line and is set to zero.