Supplemental material

Control on magnetic anisotropy of a novel half-metallic Ir_2TeI_2 monolayer

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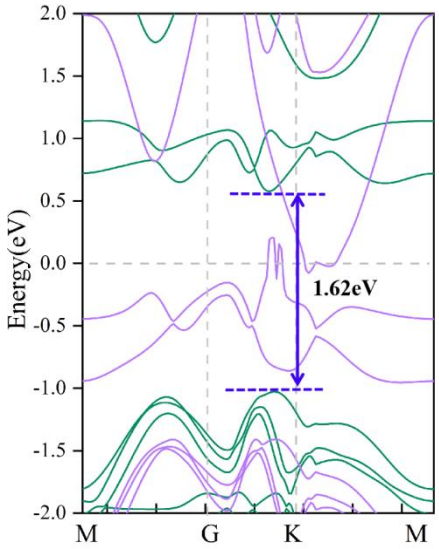

Fig. S1 The HSE band of Ir_2TeI_2 is shown in the figure. Blue and purple represent spin down and spin up, respectively. The spin down band gap is 1.62 eV, showing the semi-metal properties of spin polarization.

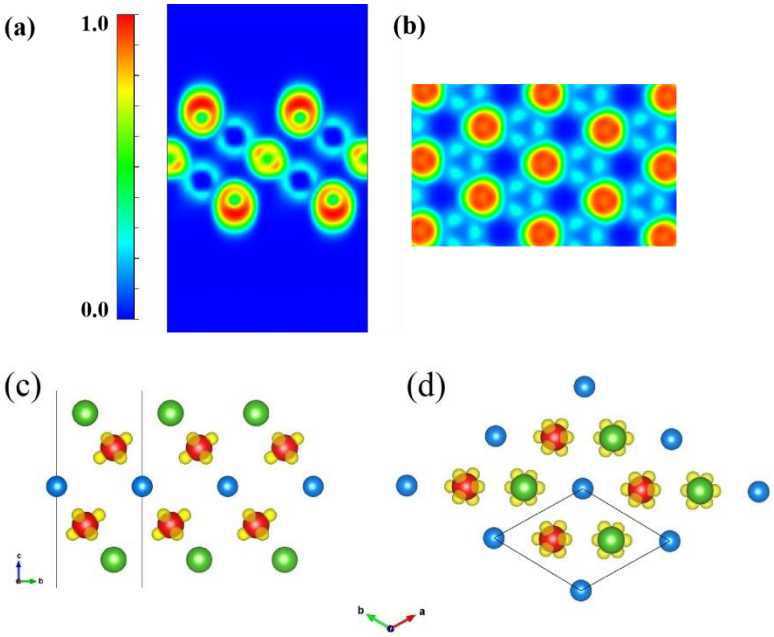

Fig. S2 The electron localization functions of the 2×2×1 Ir_2TeI_2 monolayer for FM state at ε = 0%. (a) section of (110) and (b) section of (001). The red and blue regions denote the electron accumulation and depletion, respectively. (c) and (d) give the schematic diagram of the spin charge density. Red represents Ir atom, blue and green represent Te atom and I atom respectively. The spin charge is mainly concentrated around Ir atom, indicating the source of magnetic moment.

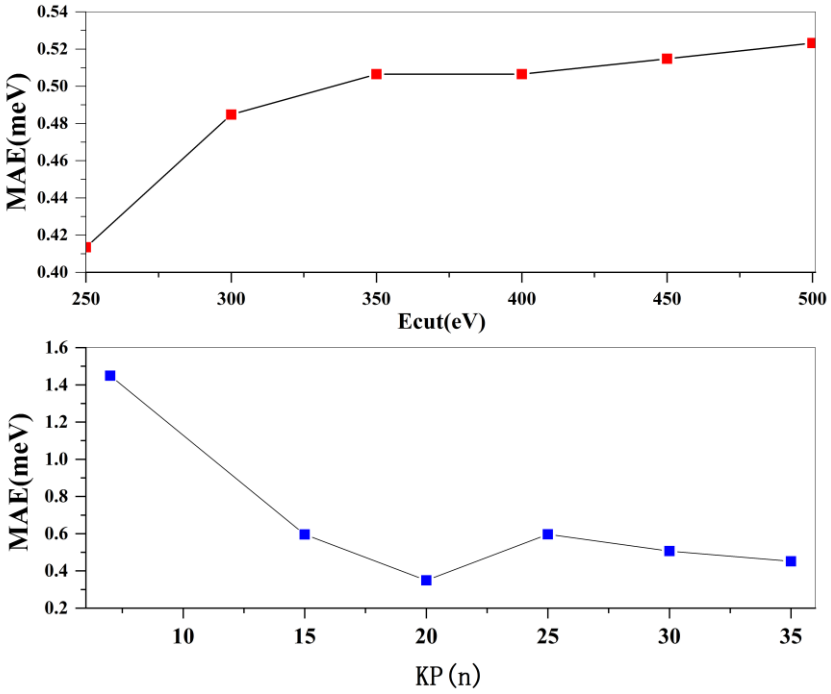

Fig. S3 The convergence test of K point and energy cutoff, MAE keeps a small float within the reasonable value range of K (7−35) and Ecut (350−500 eV).

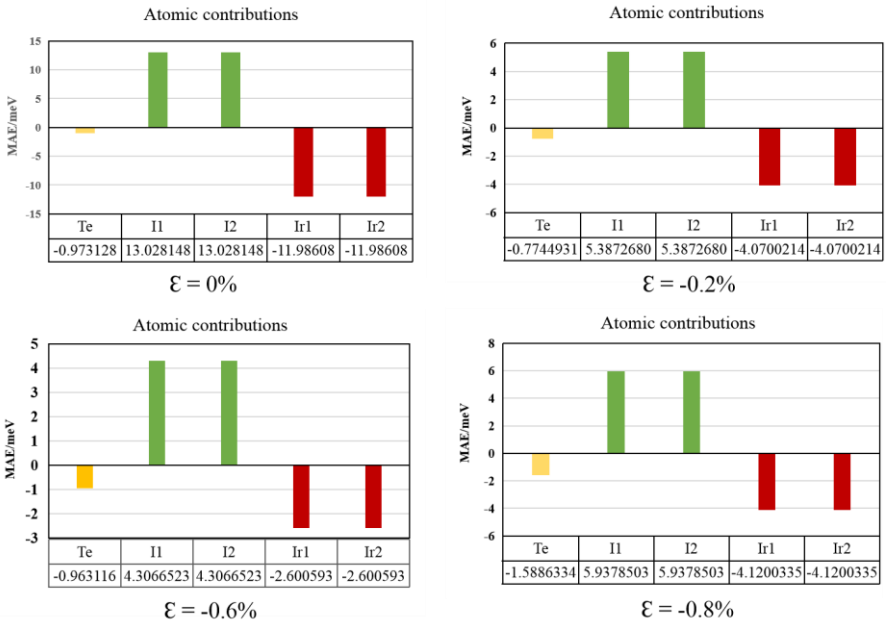

Fig. S4 Atomic contributions changes of MAE under strain function. The MAE comes mainly from the sum of the I atoms (positive) and the Ir atoms (negative), with the I atoms contributing more than the Ir atoms at compressive strains (0.2% – 0.6%).