Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Gated Spin Manipulation in Bipolar Rashba semiconductor: Janus TeSSe monolayer

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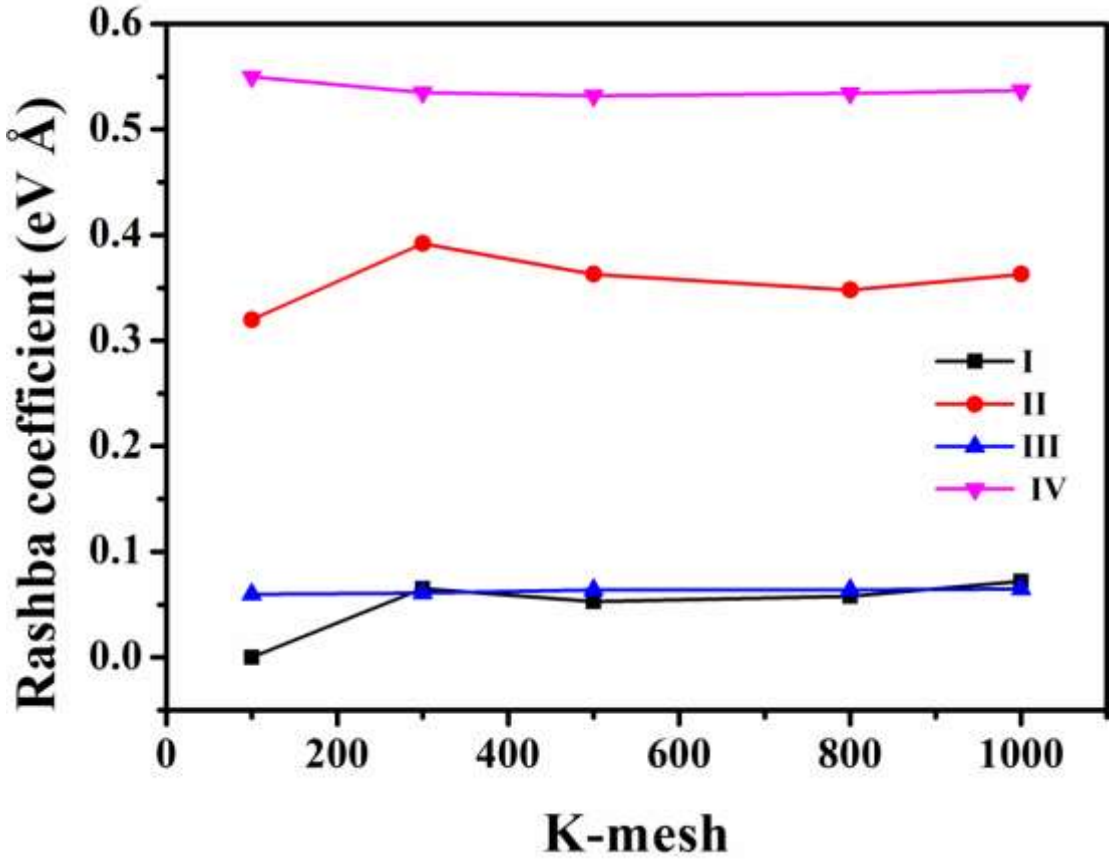

Fig. S1 Rashba coefficients Vs k-mesh. Several distinct constant energy surfaces near the Fermi level are labeled as I-IV (see Fig. 5(a) in the main text) with energies E = Ef + 0.40, -0.98, -1.1, and -1.3 eV, respectively.

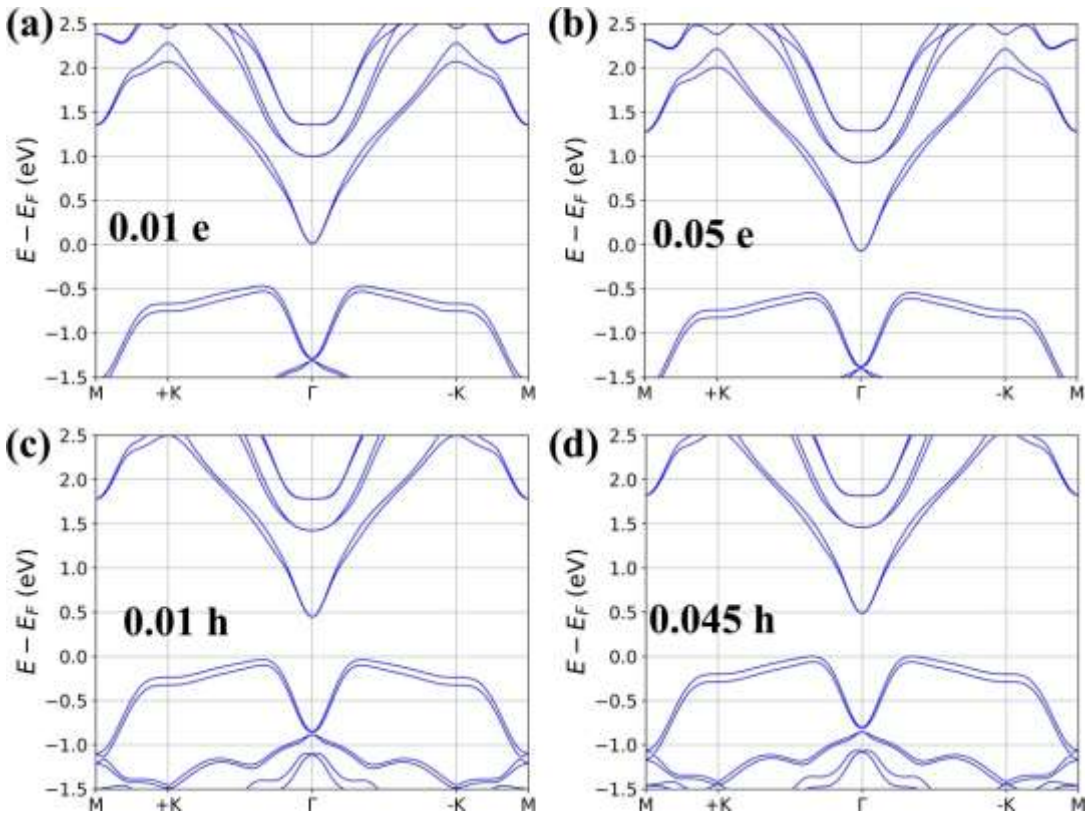

Fig. S2 Charge doping regulates the energy band, especially the Fermi level. Electron doping with (a) 0.01 e and (b) 0.05 e in the upper plane, hole doping with (c) 0.01 h and (d) 0.045 h in the lower plane.

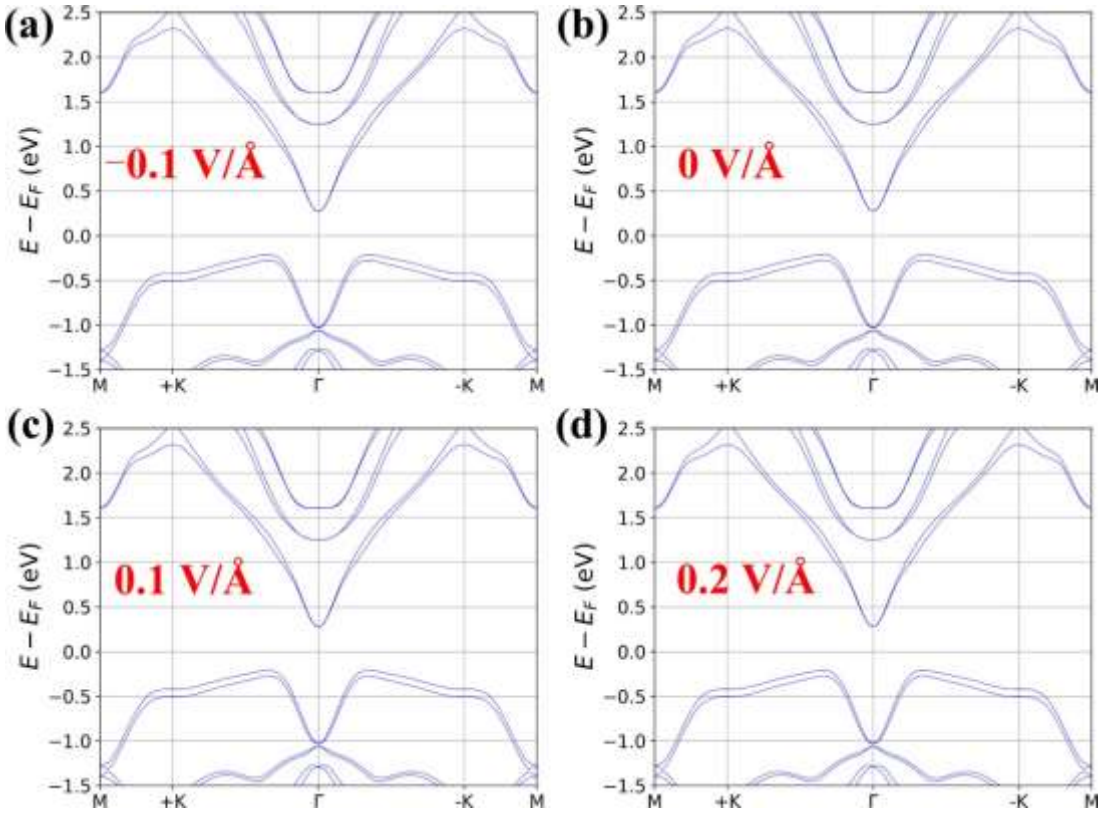

Fig. S3 The electric fields modulate the band structure curves. Representative electric fields are set as follows: E = -0.1 V/Å (a), 0.0 V/Å (b), 0.1 V/Å (c), and 0.2 V/Å (d).

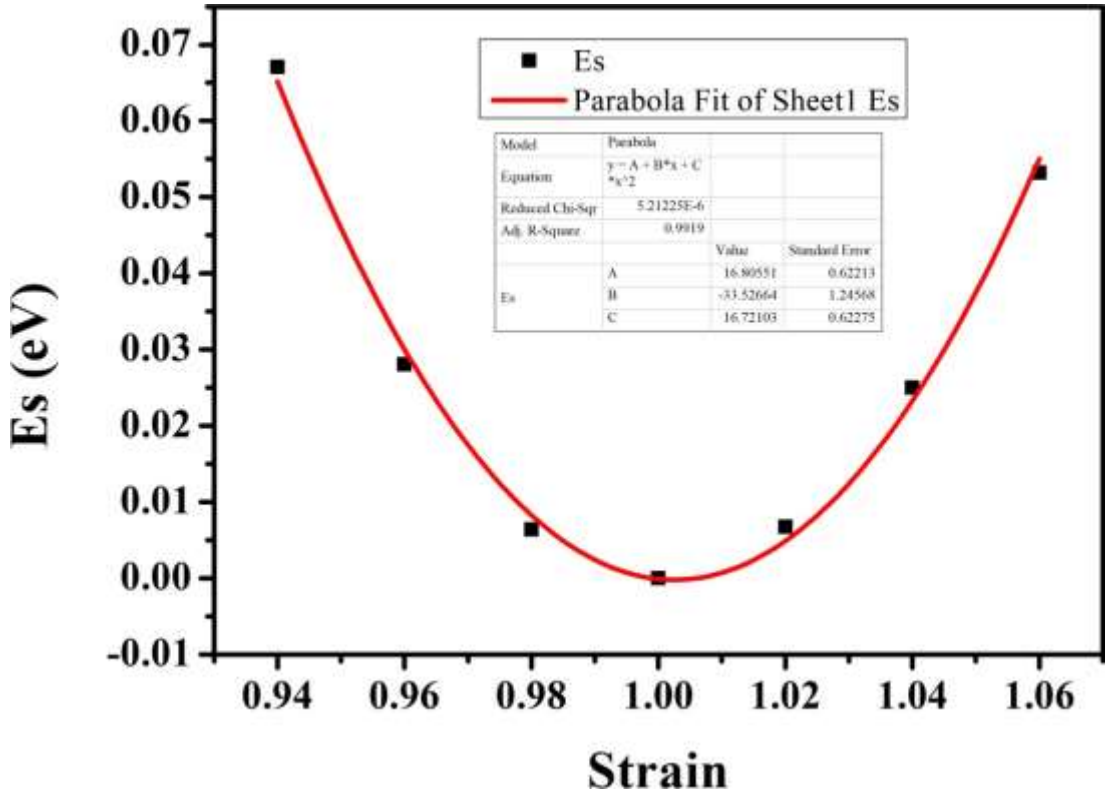

Fig. S4 The system energy (black square shape) varies with the applied strain. The solid red line represents the fitted curve of the relationship between energy and strain.

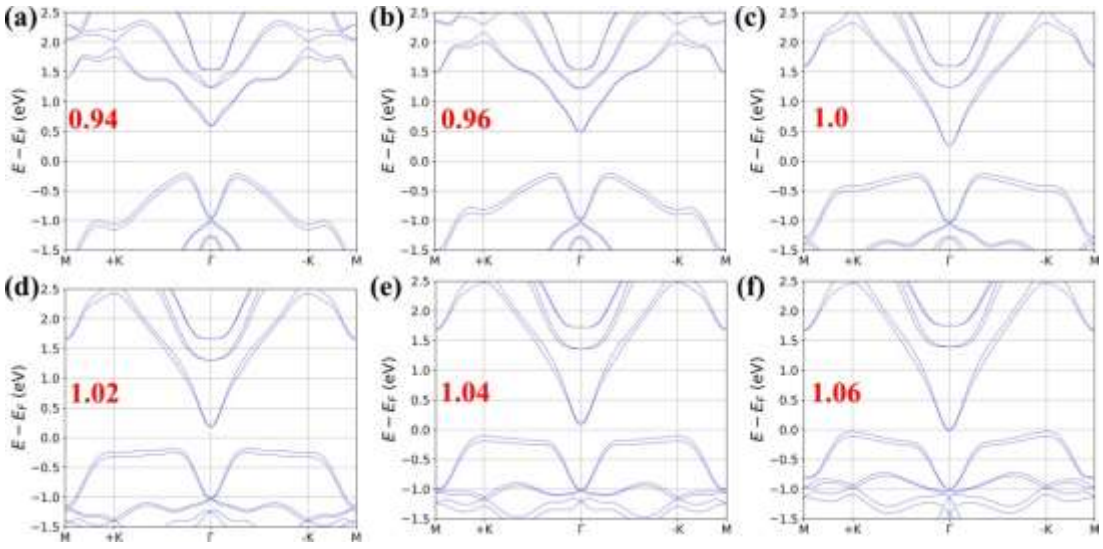

Fig. S5 The strain manipulates the electric band structures and bandgap. Electron band structure diagram with representative strain ε = (a) 0.94, (b) 0.96, (c) 1.0, (d)

1.02, (e) 1.04, and (f) 1.06, respectively.