Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Two-dimensional FeTe2 and predicted Janus FeXS (X: Te and Se) monolayers with intrinsic half-metallic character: Tunable electronic and magnetic properties via strain and electric field

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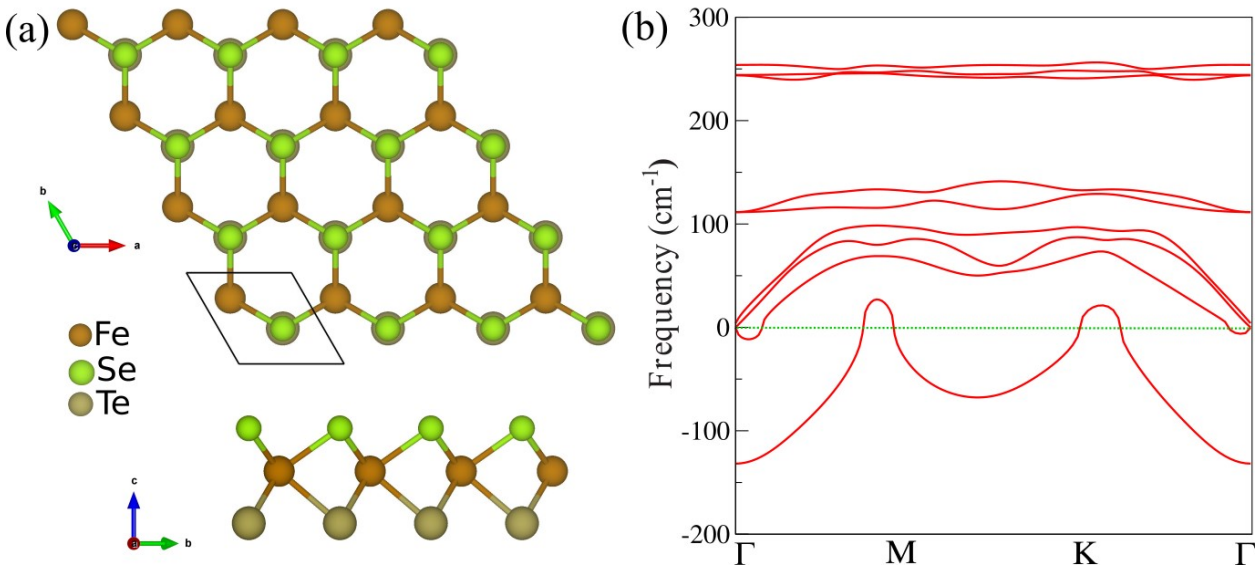

Figure S1: (a) Atomic structure and (b) phonon band of FeTeSe monolayers. The primitive unit cell is indicated by a black parallelogram.

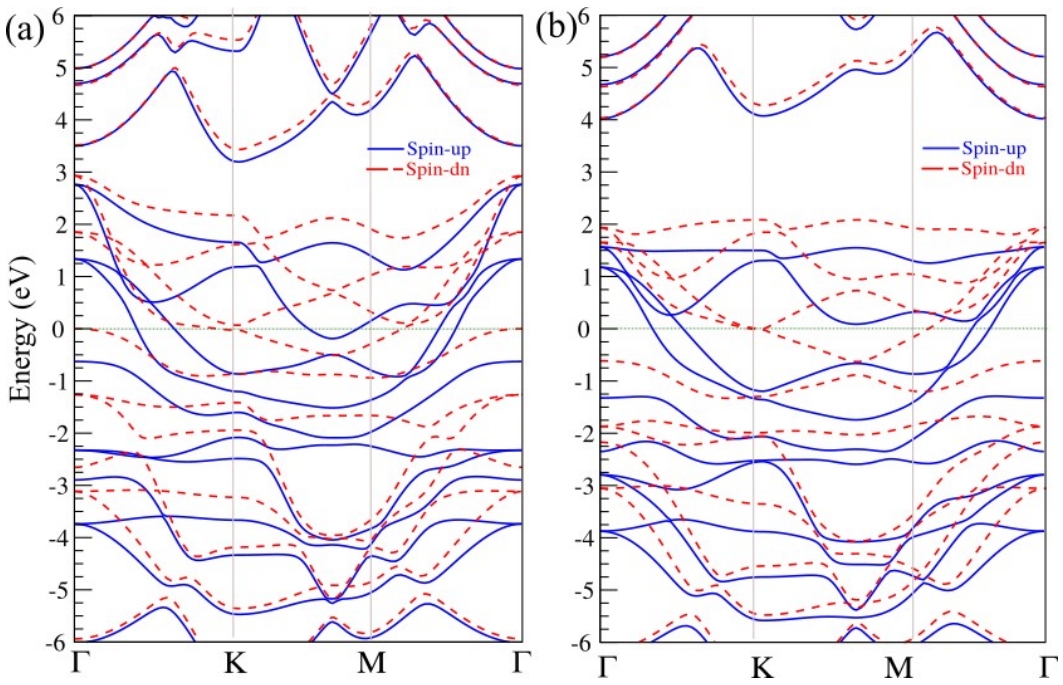

Figure S2: Band structures of (a) FeTeS and (b) FeSeS using the functional of GGA. The zero of energy is at Fermi level.

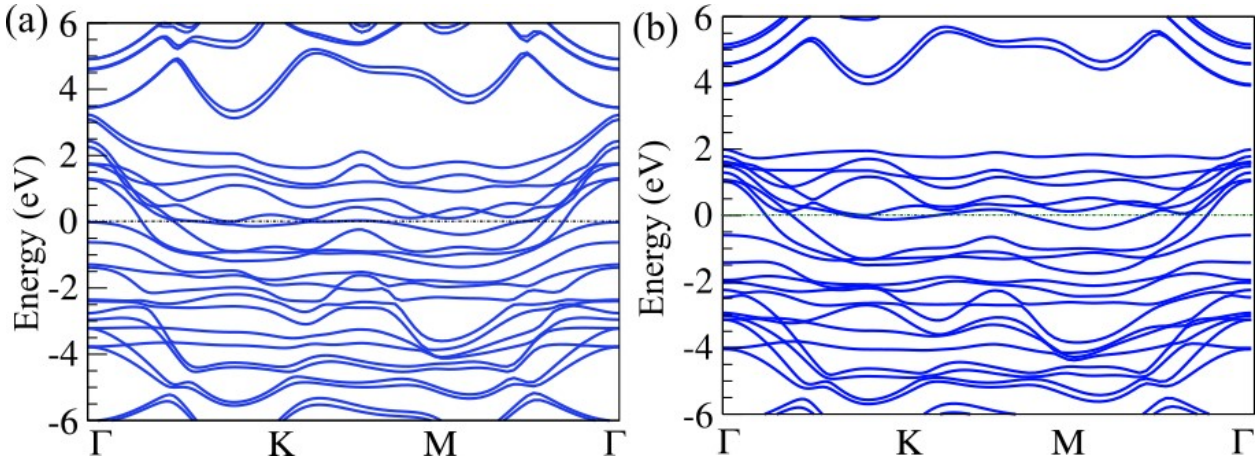

Figure S3: Band structures of (a) FeTeS and (b) FeSeS Janus monolayers. with considering SOC+U . The zero of energy is at Fermi level.

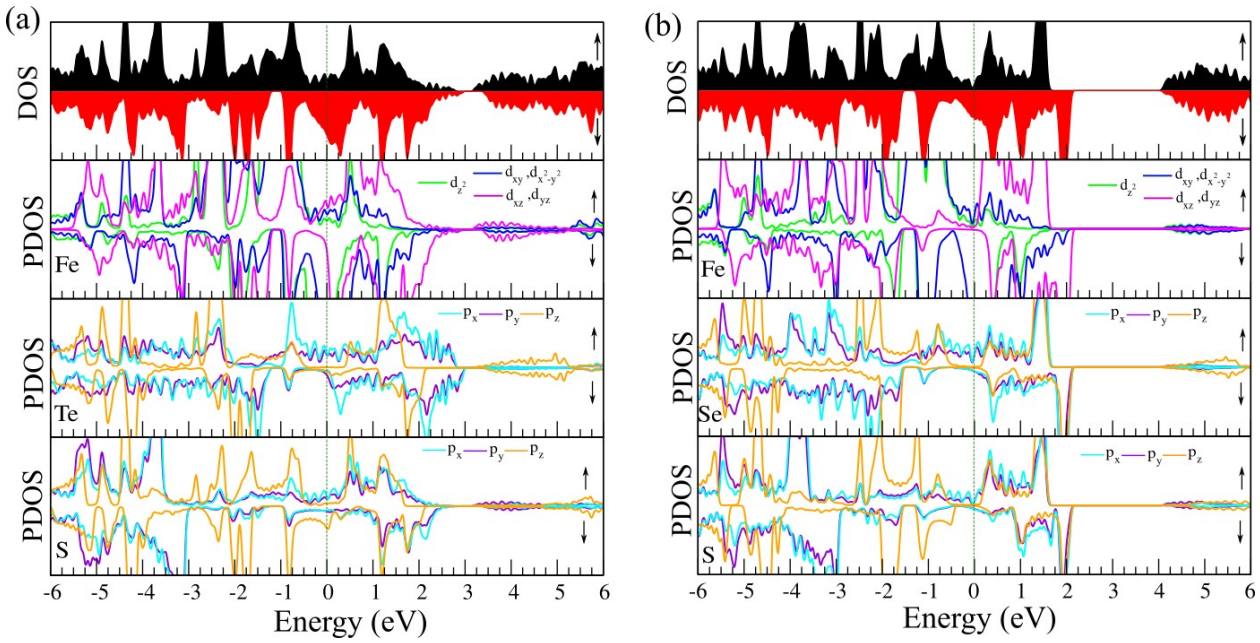

Figure S4: DOS and PDOS of (a) FeTeS and (b) FeSeS Janus monolayers. The contribution from each shell of the effective orbitals are shown separately and the zero of energy is set at Fermi level.

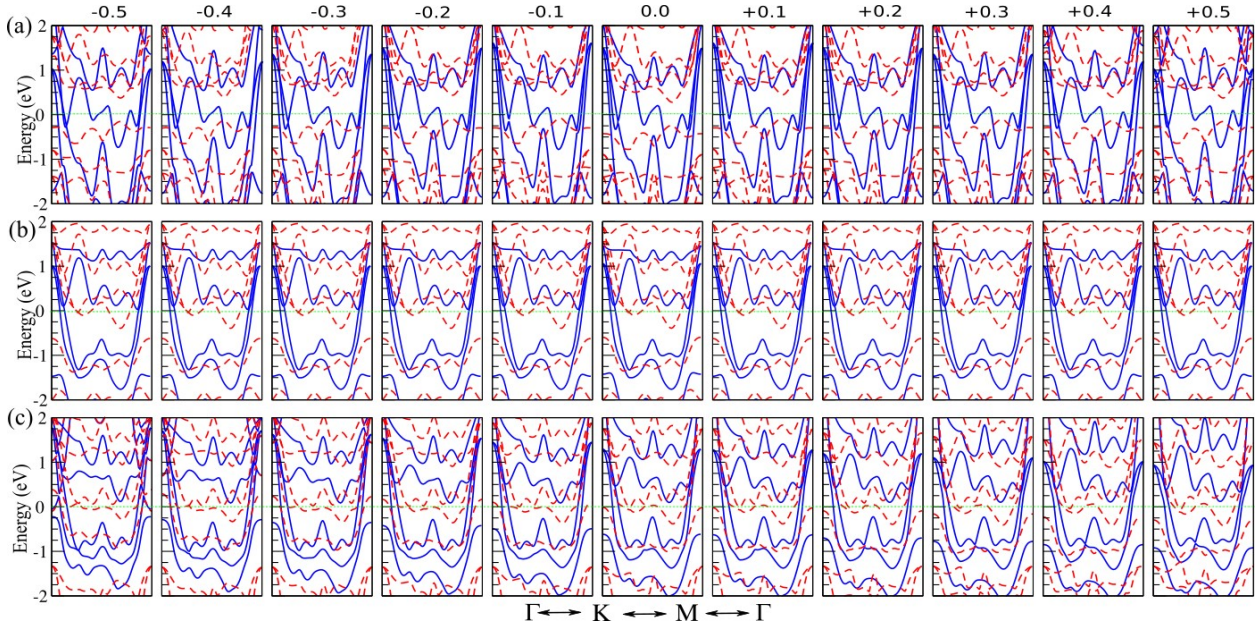

Figure S5: Band structures of (a) FeTe2, (b) FeSeS and (c) FeTeS janus monolayers when under the application of electric field.