

Electronic Supplementary Information for

**Two Dimensional Janus RuXY (X, Y = I, Br, Cl, F, X ≠ Y) Monolayers:
Ferromagnetic Semiconductors with Spontaneous Valley Polarization and
Tunable Magnetic Anisotropy**

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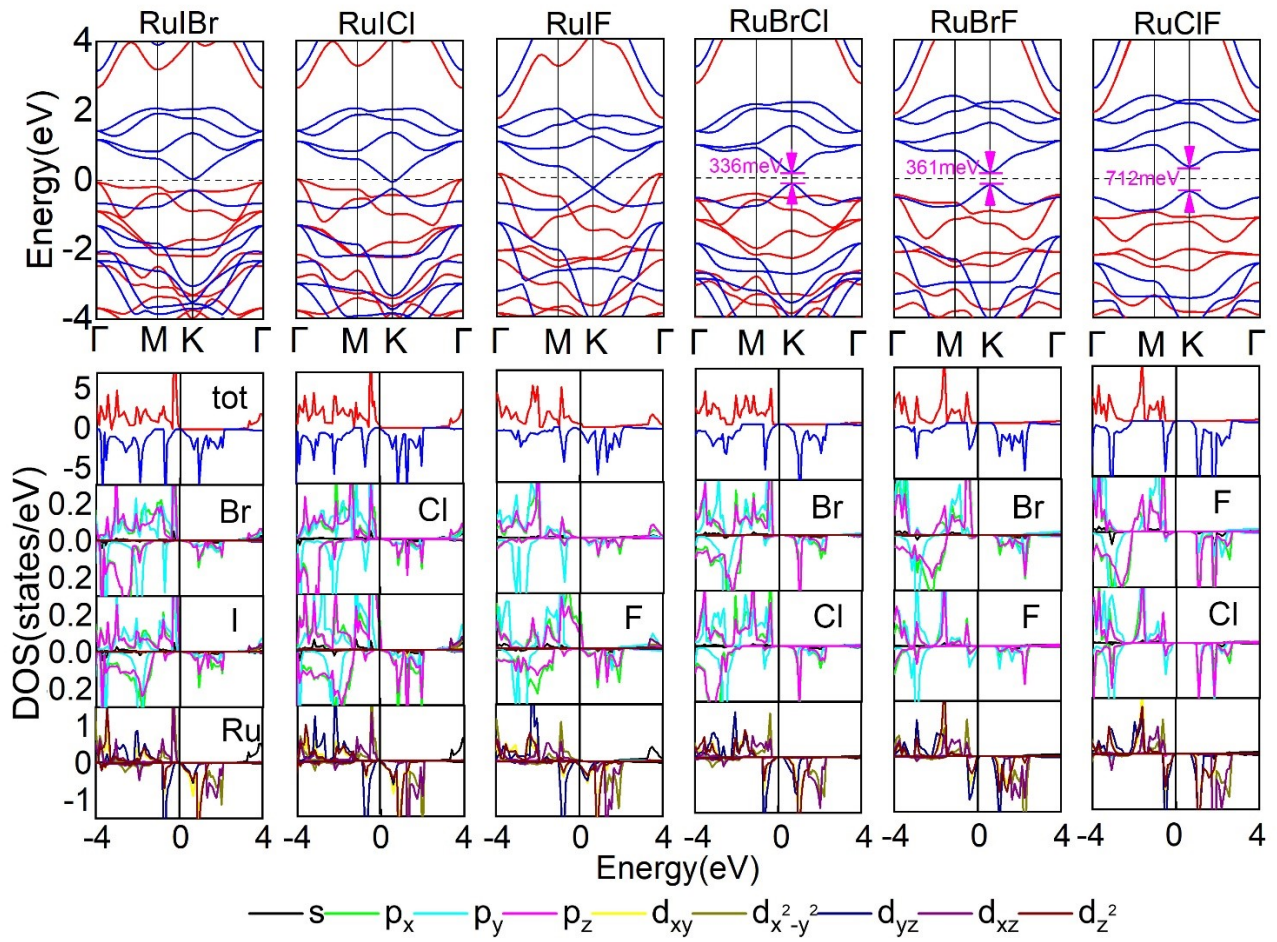


Fig. S1 The band structures and density of states of Janus RuXY monolayers (X, Y = Br, I, Cl, F, X ≠ Y).

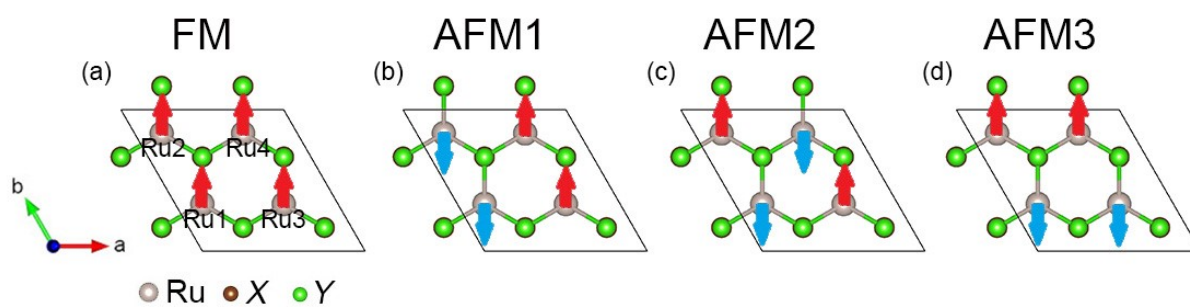


Fig. S2 The structures of Janus RuXY monolayers in (a) FM, (b) AFM1, (c) AFM2 and (d) AFM3 states. Two colored arrows indicate different spin directions.

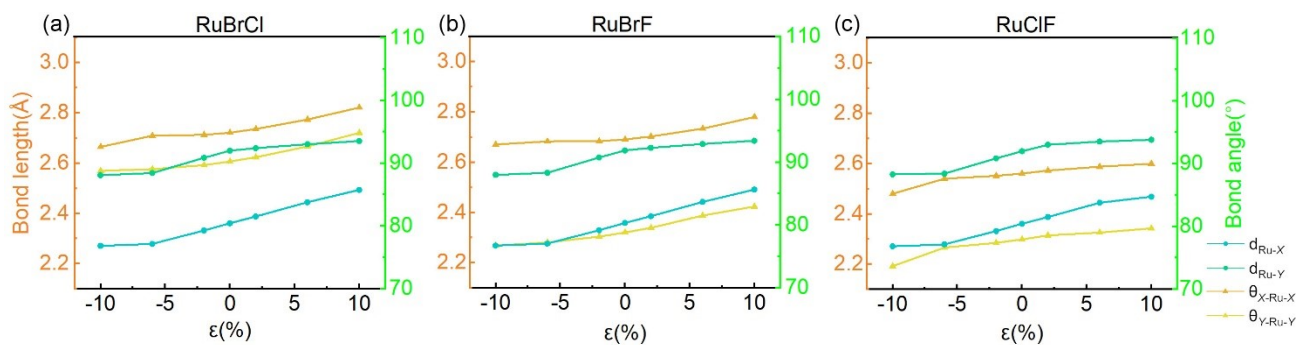


Fig. S3 Changes in bond length and bond angle of (a) RuBrCl, (b) RuBrF, (c) RuClF monolayers at different biaxial strains.

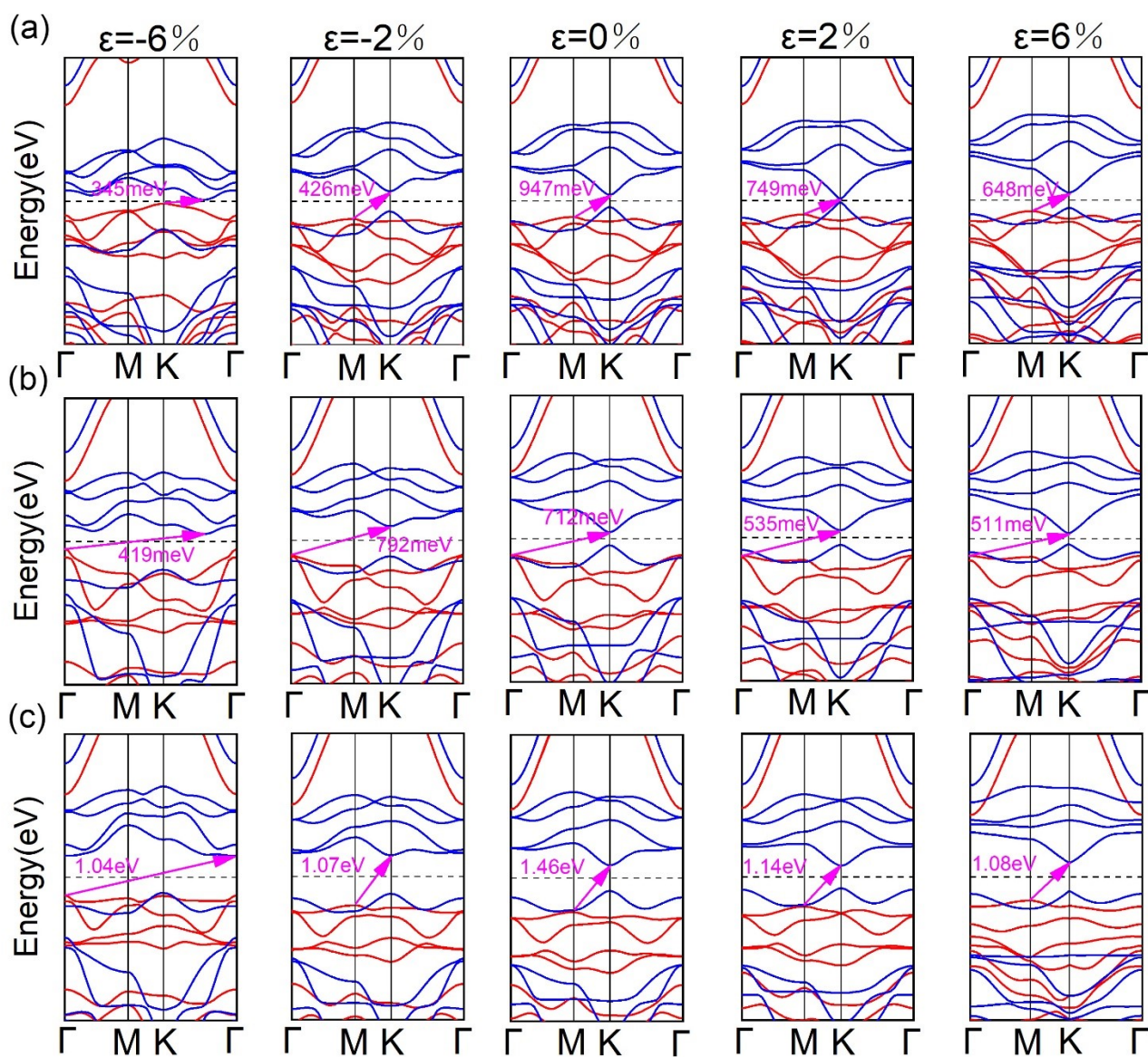


Fig. S4 The band structures without SOC of (a) RuBrF, (b) RuBrCl and (c) RuClF monolayers at different biaxial strains.

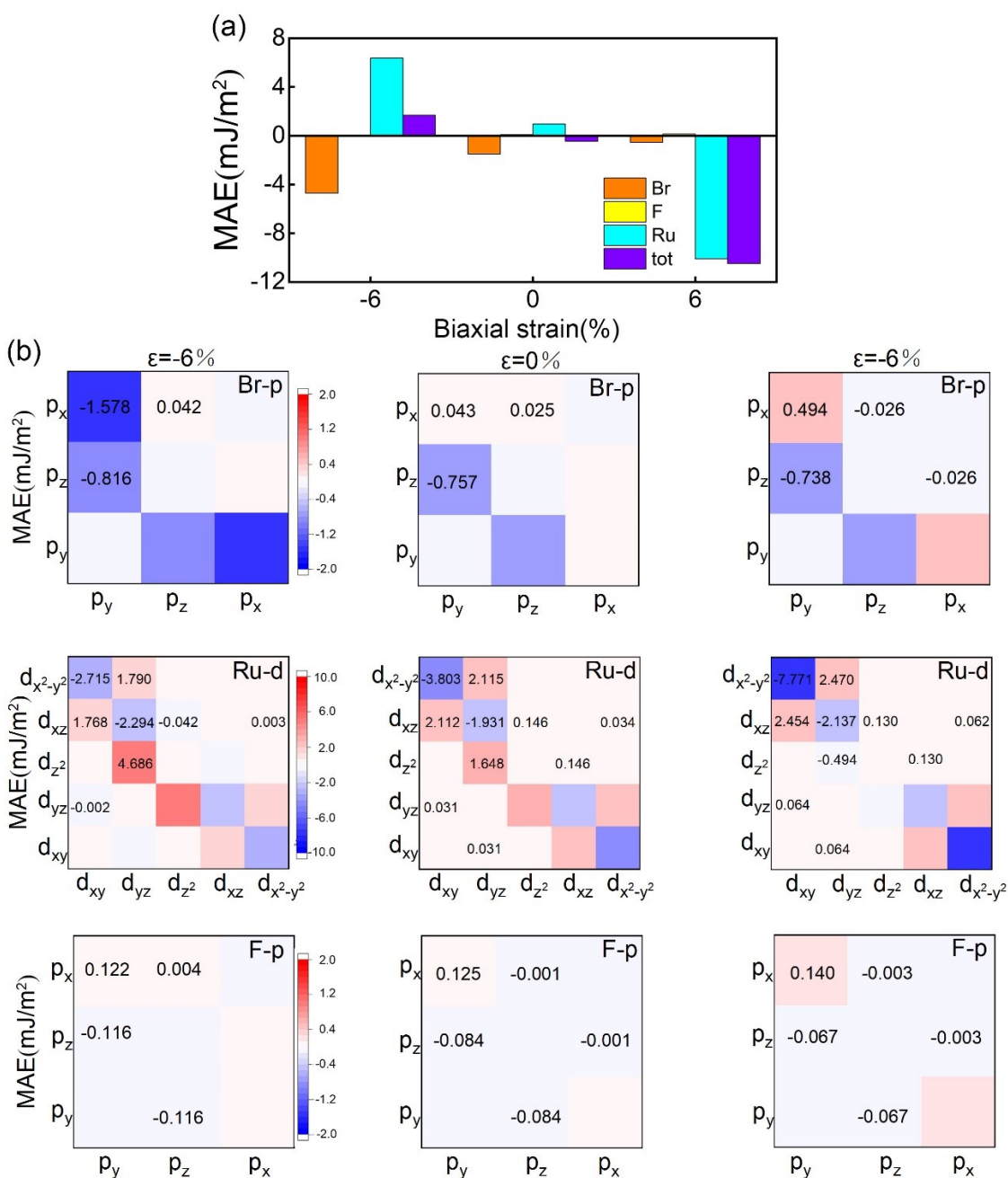


Fig. S5 (a) Total MAE and (b) the orbital-resolved MAE in RuBrF monolayer at different biaxial strains. The positive and negative values indicate PMA and IMA, respectively.

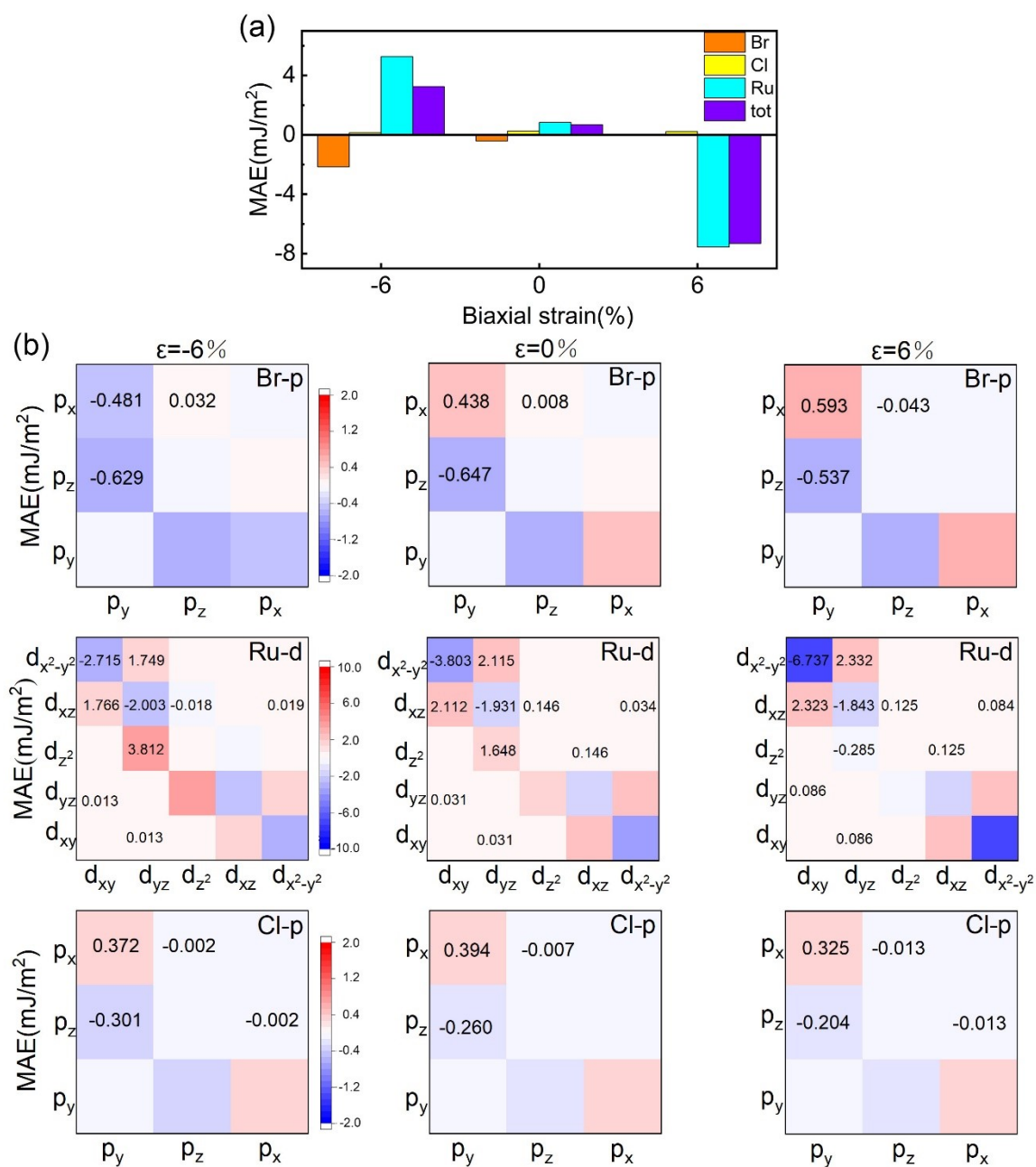


Fig. S6 (a) Total MAE and (b) the orbital-resolved MAE in RuBrCl monolayer at different biaxial strains. The positive and negative values indicate PMA and IMA, respectively.

Table S1 The total energy(eV) of the RuXY monolayers with the different magnetic configuration.

| | E_{AFM1} (eV) | E_{AFM2} (eV) | E_{AFM3} (eV) | E_{FM} (eV) | Magnetic ground state |
|--------|-----------------|-----------------|-----------------|---------------|-----------------------|
| RuIBr | -37.324 | -37.325 | -37.325 | -37.562 | FM |
| RuICl | / | / | / | / | / |
| RuIF | / | / | / | / | / |
| RuBrCl | -41.427 | -41.427 | -41.427 | -41.873 | FM |
| RuBrF | -45.916 | -45.916 | -45.916 | -46.695 | FM |
| RuClF | -48.582 | -48.582 | -48.582 | -49.247 | FM |