

Supplementary material
Sliding ferroelectricity and ferroelectric-valley coupling in Janus RuXY (X,
Y = Cl, Br, I) bilayers

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Table S1 The lattice constants a for AB stacking and sliding energy barriers ΔE of Janus RuXY ($X, Y = \text{Cl, Br and I}, X < Y$) different interfaces configurations.

	RuBrI		RuClBr		RuClI	
	I-I	Br-Br	Cl-Cl	Br-Br	I-I	Cl-Cl
$a(\text{\AA})$	3.762	3.769	3.537	3.532	3.69	3.702
$\Delta E(\text{meV})$	31.3	22.6	12.3	18.3	29.9	15.8

Table S2 The energy valley splitting at the K and K' points in the valence and conduction ($\Delta E_{\text{K}}^V, \Delta E_{\text{K}'}^V, \Delta E_{\text{K}}^C, \Delta E_{\text{K}'}^C$) for the Janus RuXY ($X, Y = \text{Cl, Br and I}, X < Y$) bilayers with X-X, Y-Y configurations under BA and AB stacking.

			ΔE_{K}^C (eV)	$\Delta E_{\text{K}'}^C$ (eV)	ΔE_{K}^V (eV)	$\Delta E_{\text{K}'}^V$ (eV)
			RuBrI	I-I	BA	0.191
		AB	0.179	0.191	0.089	0.104
	Br-Br	BA	0.225	0.21	0.065	0.005
		AB	0.21	0.225	0.05	0.065
RuClBr	Cl-Cl	BA	0.01	0.025	0.26	0.245
		AB	0.025	0.01	0.245	0.26
	Br-Br	BA	0.02	0.02	0.27	0.236
		AB	0.02	0.02	0.236	0.27
RuClI	Cl-Cl	BA	0.128	0.129	0.135	0.134
		AB	0.129	0.128	0.134	0.135
	I-I	BA	0.083	0.075	0.198	0.185
		AB	0.075	0.083	0.185	0.198

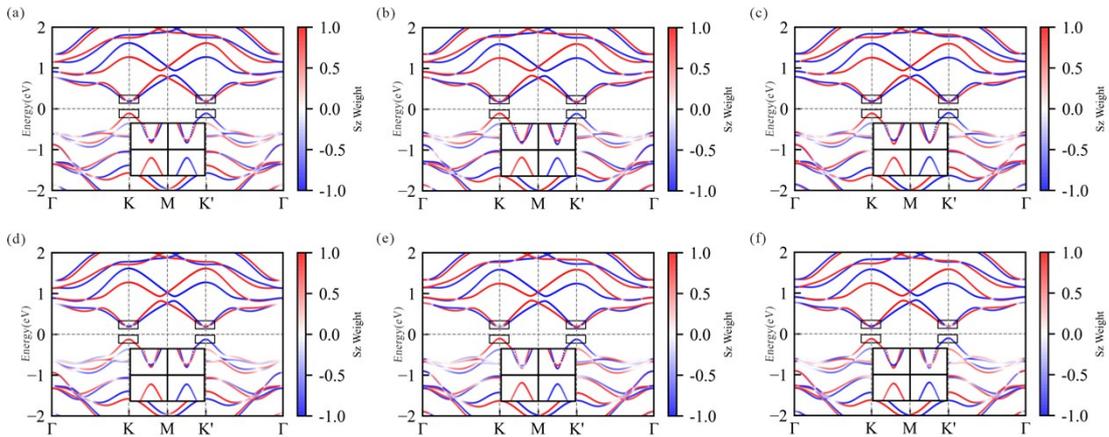


Fig. S1 The spin projection bands for the AA, BA and AB stackings of the Janus RuClBr bilayer: (a)-(c) Cl-Cl configuration; (d)-(f) Br-Br configuration. Red and blue bands represent the spin-up and spin-down channels, respectively.

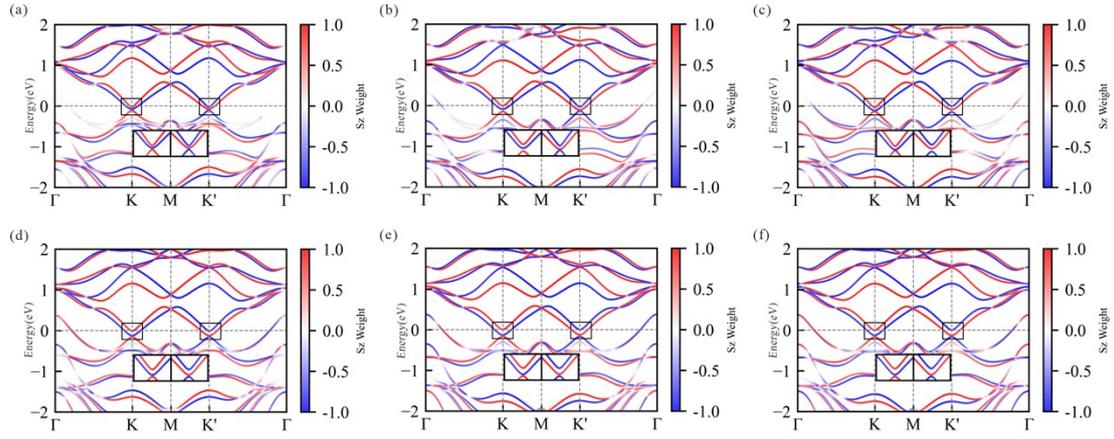


Fig. S2 The spin projection bands for the AA, BA and AB stackings of the Janus RuCl₂ bilayer: (a)-(c) I-I configuration; (d)-(f) Cl-Cl configuration. Red and blue bands represent the spin-up and spin-down channels, respectively.

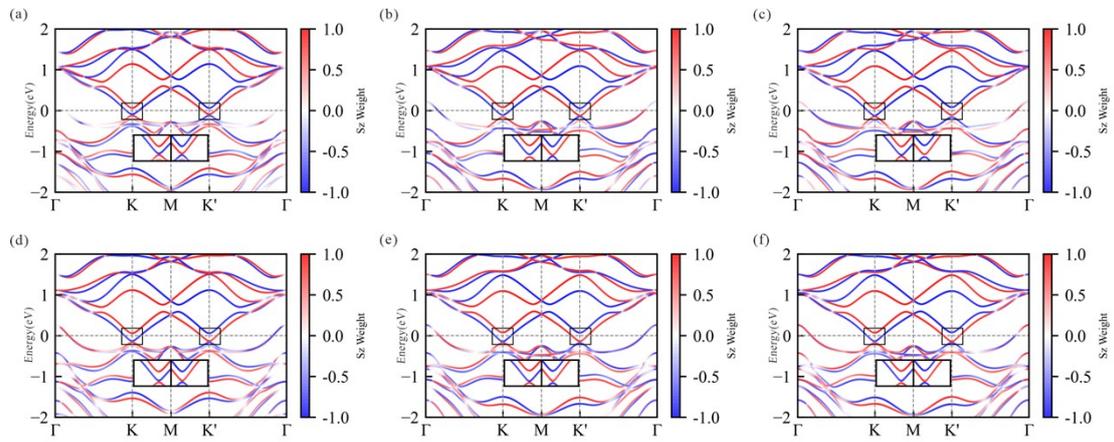


Fig. S3 The spin projection bands for the AA, BA and AB stackings of the Janus RuBr₂ bilayer: (a)-(c) I-I configuration; (d)-(f) Br-Br configuration. Red and blue bands represent the spin-up and spin-down channels, respectively.

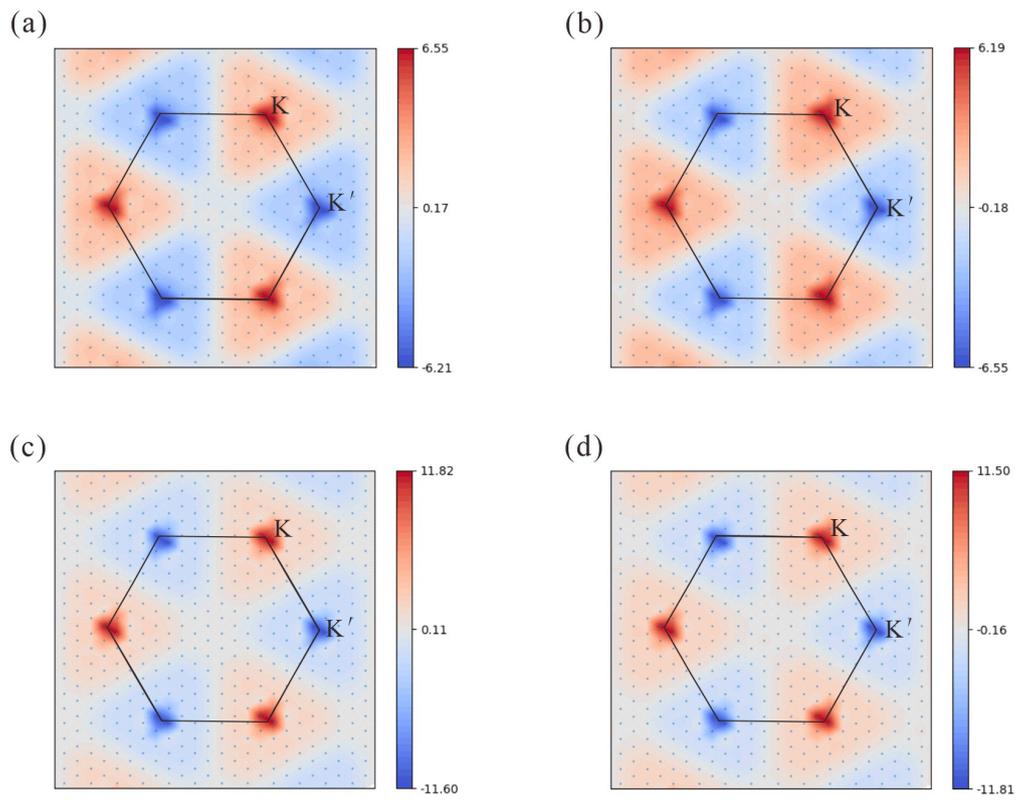


Fig. S4 The Berry Curvature for the BA and AB stackings of the Janus RuBrI bilayer: (a)-(b) I-I configuration; (c)-(d) Br-Br configuration.

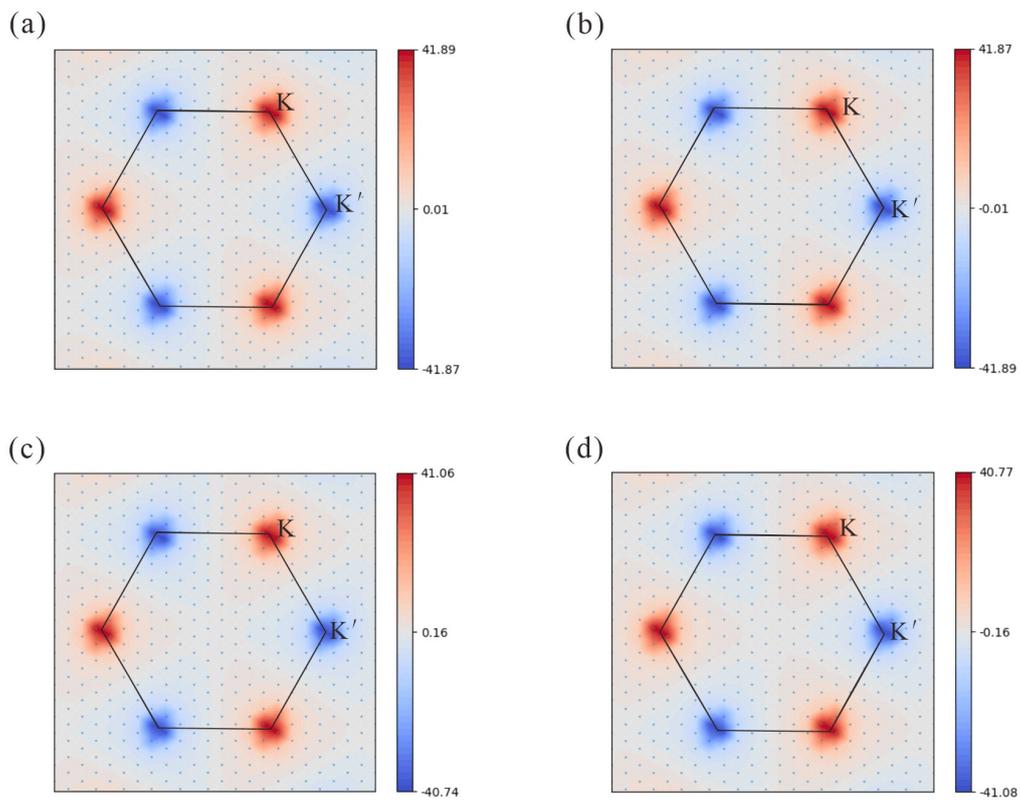


Fig. S5 The Berry Curvature for the BA and AB stackings of the Janus RuClBr bilayer: (a)-(b) Cl-Cl configuration; (c)-(d) Br-Br configuration.

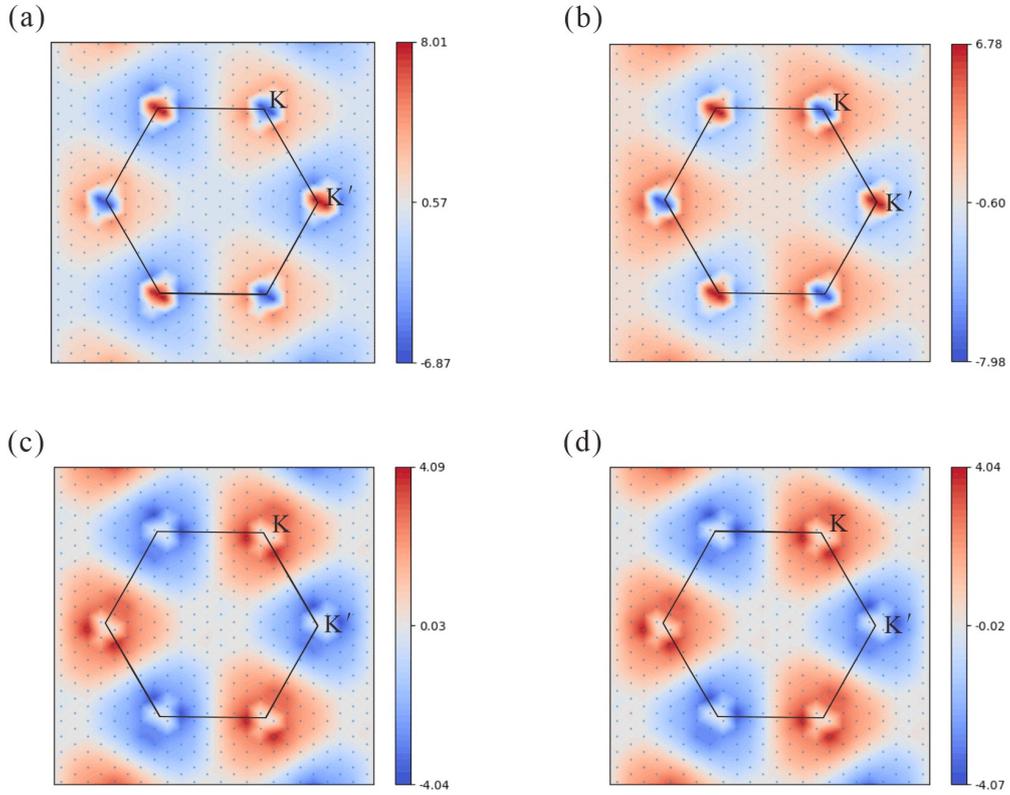


Fig. S6 The Berry Curvature for the BA and AB stackings of the Janus RuClI bilayer: (a)-(b) I-I configuration; (c)-(d) Cl-Cl configuration.

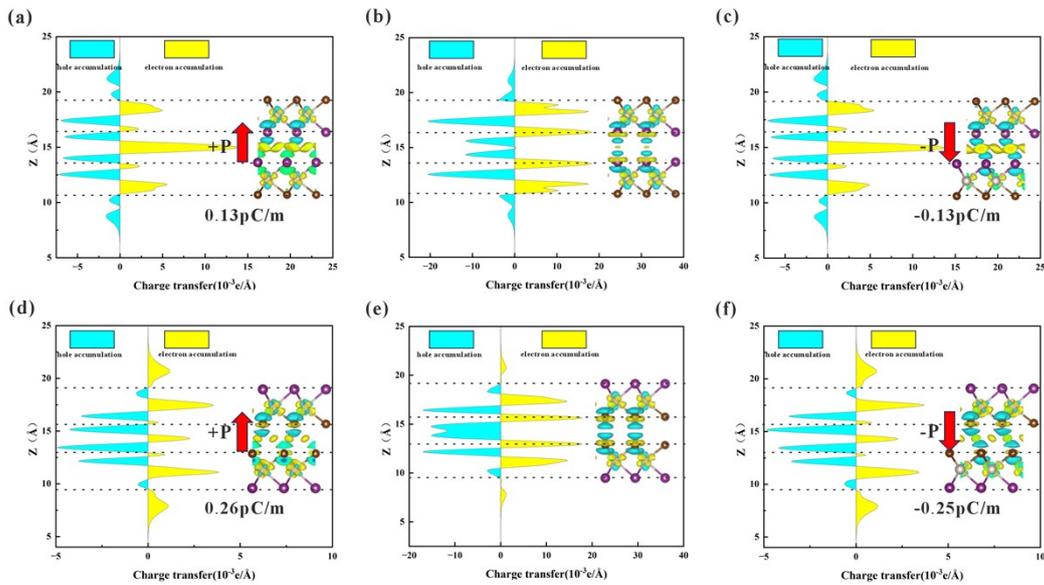


Fig. S7 Interlayer charge density and planar-averaged differential charge density

along the z-axis for the BA, AA and AB stackings of the Janus RuBrI bilayer. (a)-(c) I-I configuration; (d)-(f) Br-Br configuration. Yellow and blue-green isosurfaces represent electron accumulation and depletion, respectively.

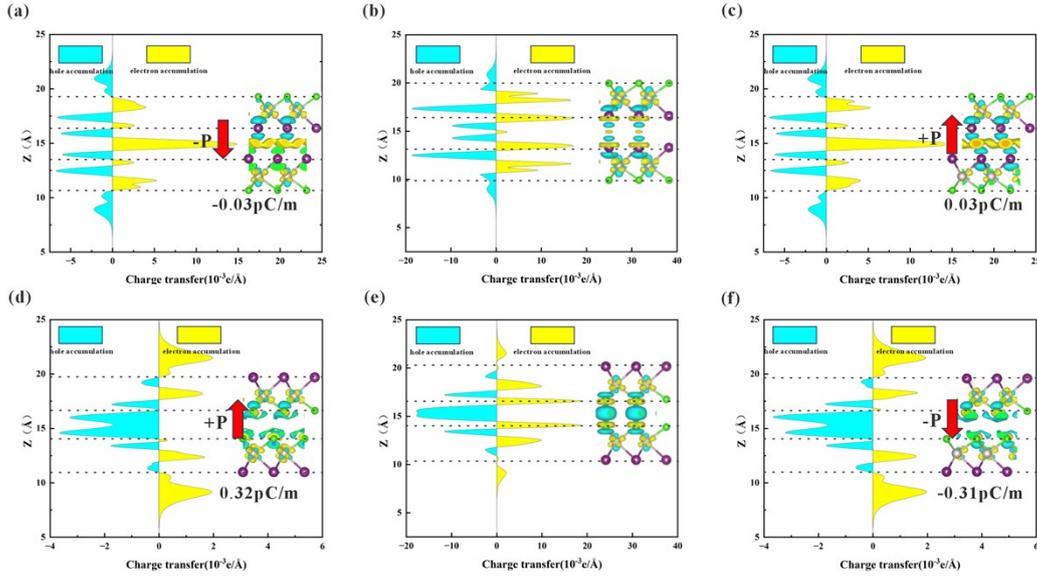


Fig. S8 Interlayer charge density and planar-averaged differential charge density along the z-axis for the BA, AA and AB stackings of the Janus RuClI bilayer. (a)-(c) I-I configuration; (d)-(f) Cl-Cl configuration. Yellow and blue-green isosurfaces represent electron accumulation and depletion, respectively.

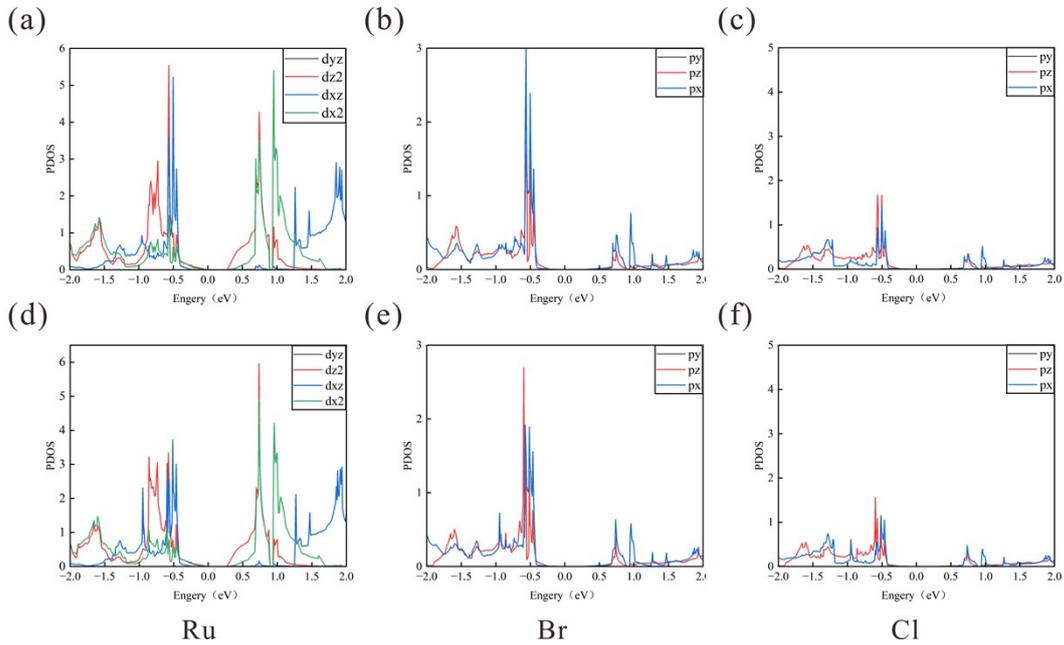


Fig. S9 The projected density of states (PDOS) of Ru, Br, and Cl in the Janus RuClBr bilayer under AA (non-polarized) and BA (ferroelectric) stacking configurations. (a)-(c) AA stacking; (d)-(f) BA stacking.