Electronic Supplementary Information for

Band Inversion and Switchable Magnetic Properties of two-dimensional RuClF/WSe_2 van der Waals Heterostructures

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Table S1 Calculated Lattice Constant: a_0 (Å), Lattice mismatch rate: δ (%), interlayer distance: d_0 (Å), local Magnetic Moments: M (μ_B), Binding energy: E_b (eV).

Stacking models	Stacking patterns	a_0	δ	d_0	M	E_b
Model-1	W-Ru-1	3.310	0.61	3.543	3.432	-0.224
Model-2	W-F.top	3.309	0.61	3.539	3.429	-0.264
Model-3	Se-Ru-1	3.310	0.61	3.544	3.428	-0.273
Model-4	W-Ru'-1	3.310	0.61	3.551	3.428	-0.262
Model-5	Se-Ru'-1	3.309	0.61	3.546	3.430	-0.264
Model-6	W-Ru-2	3.323	0.61	3.748	3.336	-0.239
Model-7	W-Cl.top	3.323	0.61	3.744	3.336	-0.190
Model-8	Se-Ru-2	3.324	0.61	3.736	3.334	-0.223
Model-9	W-Ru'-2	3.325	0.61	3.732	3.337	-0.237
Model-10	Se-Ru'-2	3.324	0.61	3.741	3.336	-0.227

Table. S2 The lattice constants and atomic coordinates of RuClF/WSe_2-model-3 heterostructure.

a[Å]	3.3101057765282484	0.0000000000000000	0.0000000000000000
b[Å]	-1.6550528882641240	2.8666356917070352	0.0000000000000000
c[Å]	0.0000000000000000	0.0000000000000000	29.8030552301675442
Cl	0.0000000000000000	0.0000000000000000	0.3910231726384690
F	0.0000000000000000	0.0000000000000000	0.4918357503687479
Ru	0.6666666870000029	0.3333333429999996	0.4481663407255119
Se	0.6666666870000029	0.3333333429999996	0.7078638572085396
Se	0.6666666870000029	0.3333333429999996	0.5950981142939543
W	0.3333333429999996	0.6666666870000029	0.6514827447647733

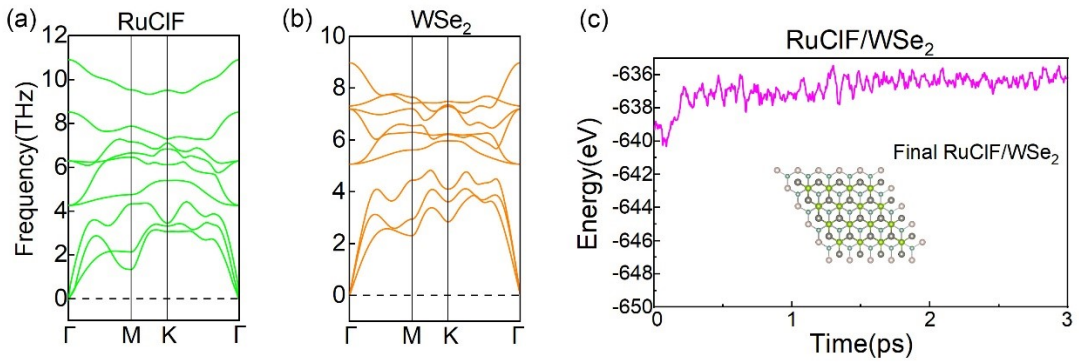

Fig. S1 Phonon spectrum of (a) RuClF, (b) WSe_2 monolayers. (c) Simulation of potential energy fluctuations in RuClF/WSe_2 heterostructure after 3ps.

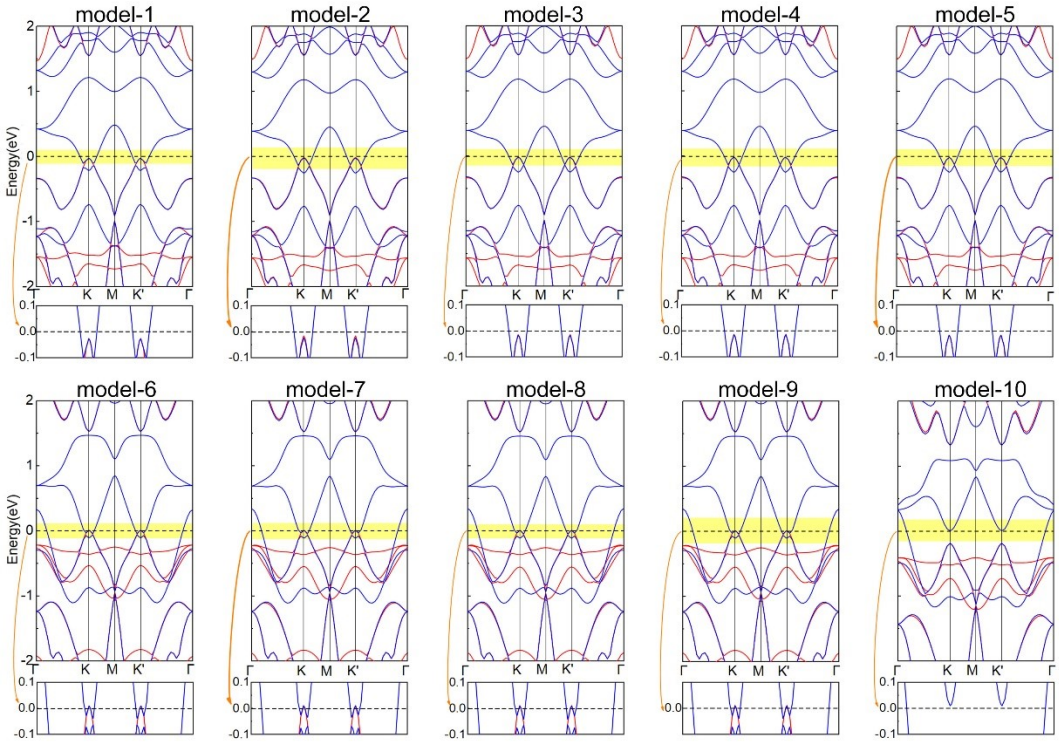

Fig. S2 Band structures of $RuClF/WSe_2$ heterostructures without SOC with different stacking models.

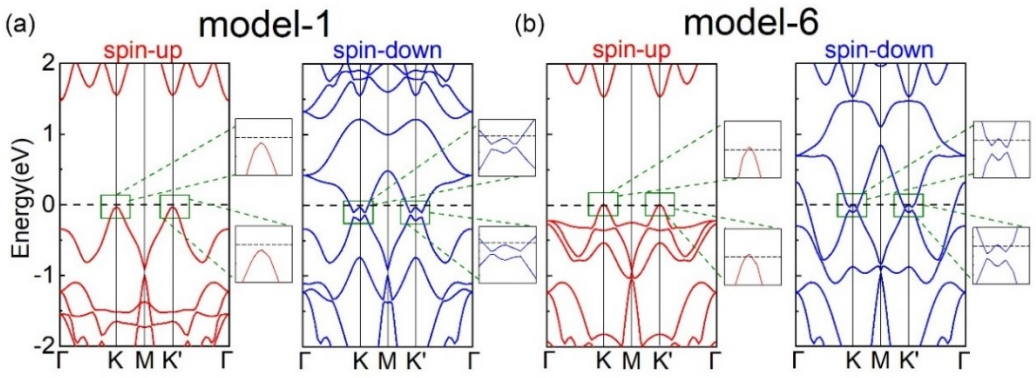

Fig. S3 Band structures of spin-up and spin-down channels of (a) RuClF/WSe_2-model-1 and (b) RuClF/WSe_2-model-6 heterostructures.

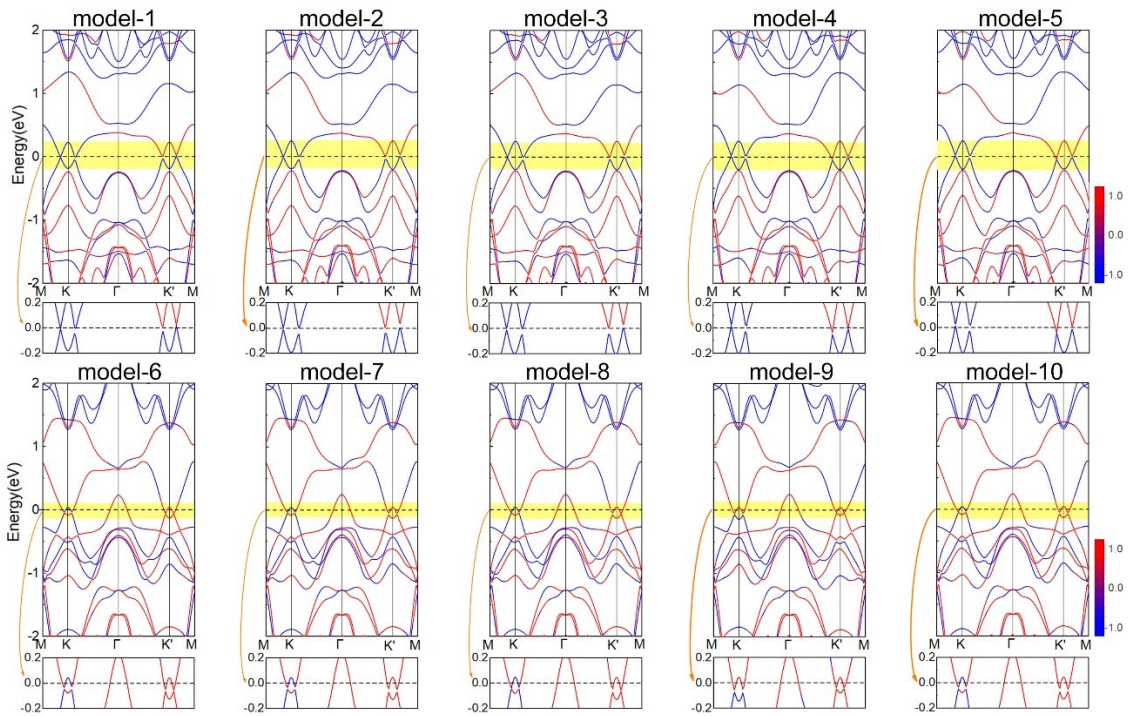

Fig. S4 Band structures of $RuClF/WSe_2$ heterostructures with SOC with different stacking models.

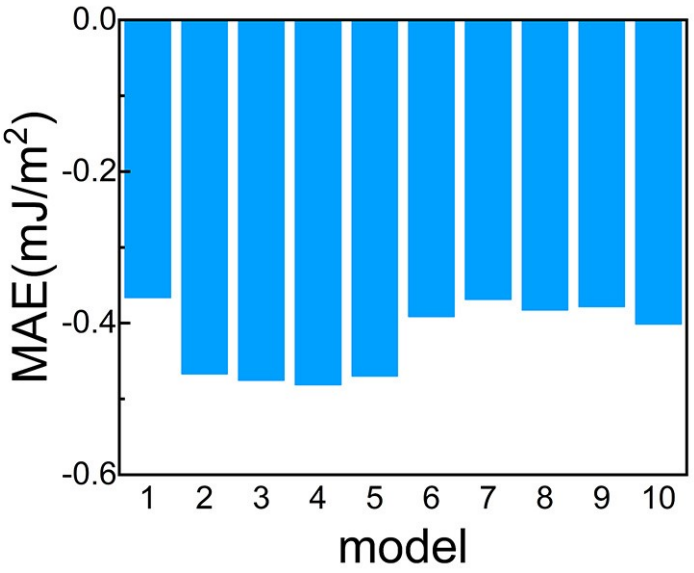

Fig. S5 Total magnetic anisotropy of RuClF/WSe_2 heterostructures with different stacking models.

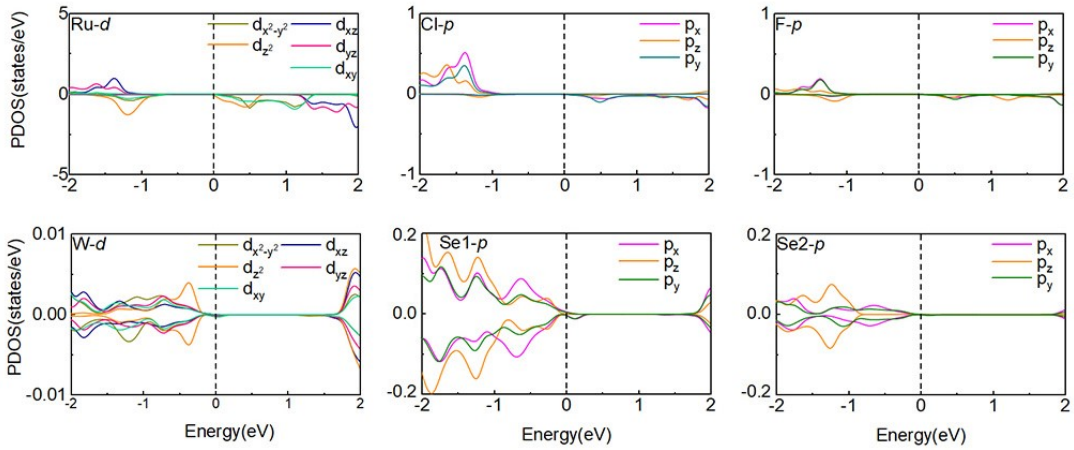

Fig. S6 PDOS of each element of RuClF/WSe_2 heterostructure. The Fermi level is set as 0eV.