Supporting Information

Janus VXY monolayers with tunable large Berry curvature

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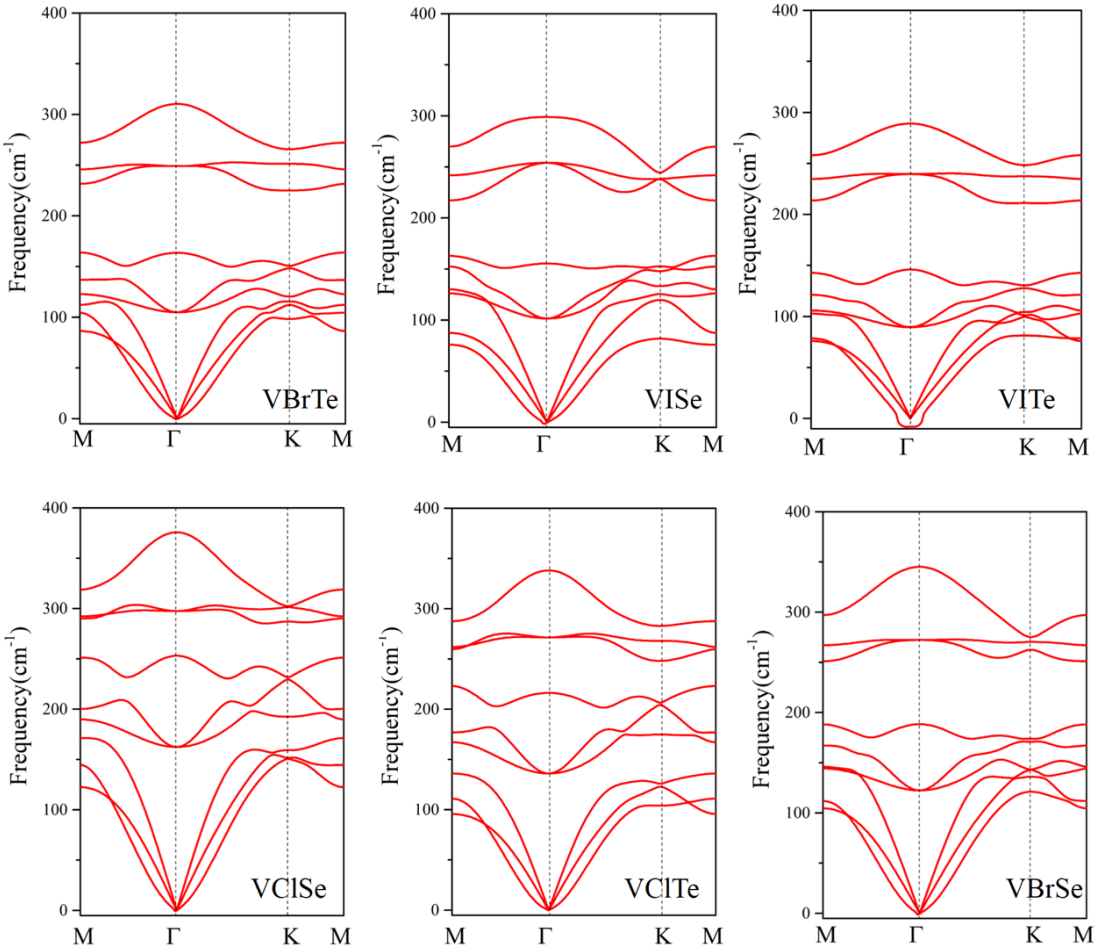

Fig. S1. The phonon band dispersion of VXY.

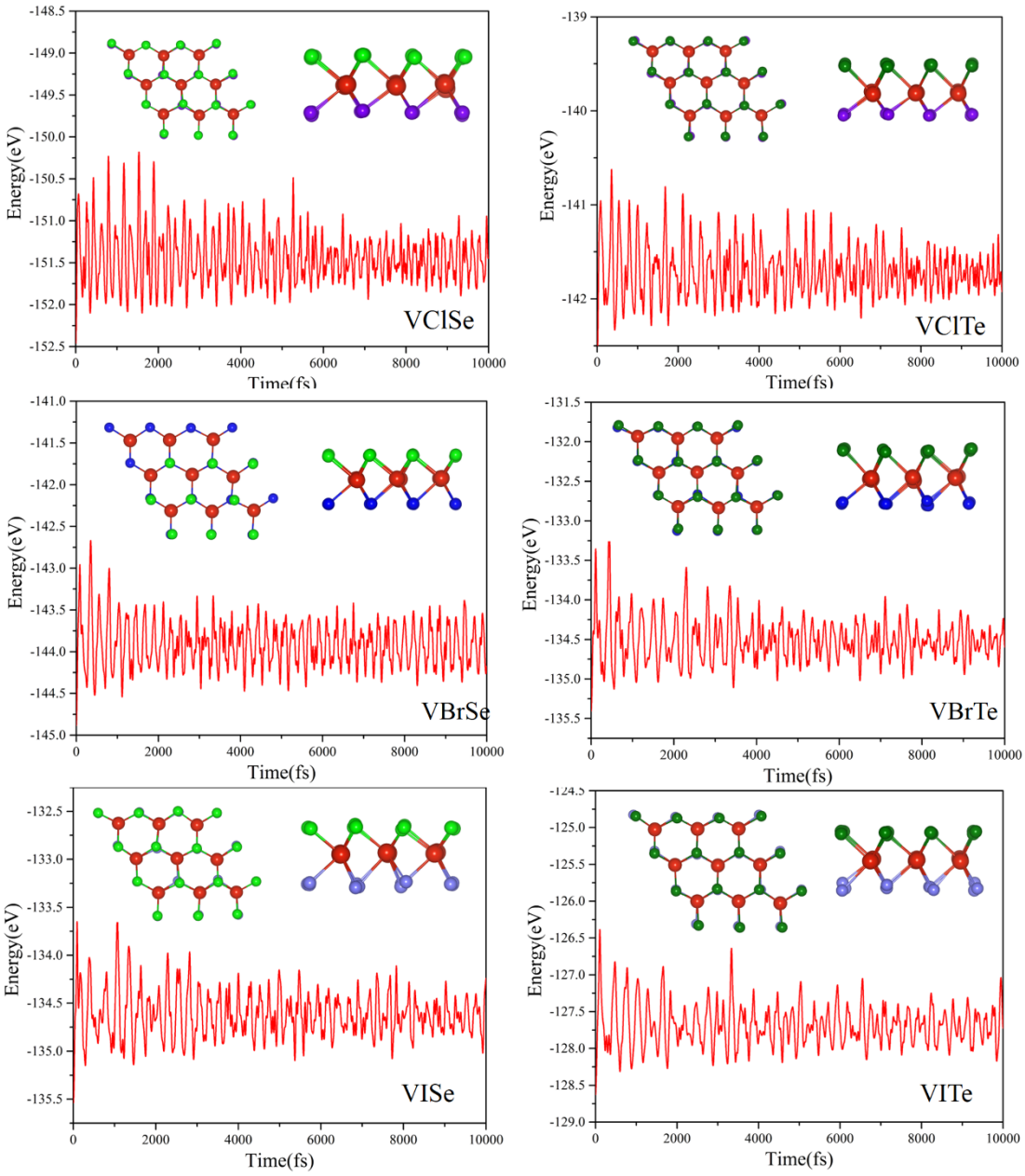

Fig. S2. Variations of the total energy and structure for VXY at 300 K during AIMD simulations.

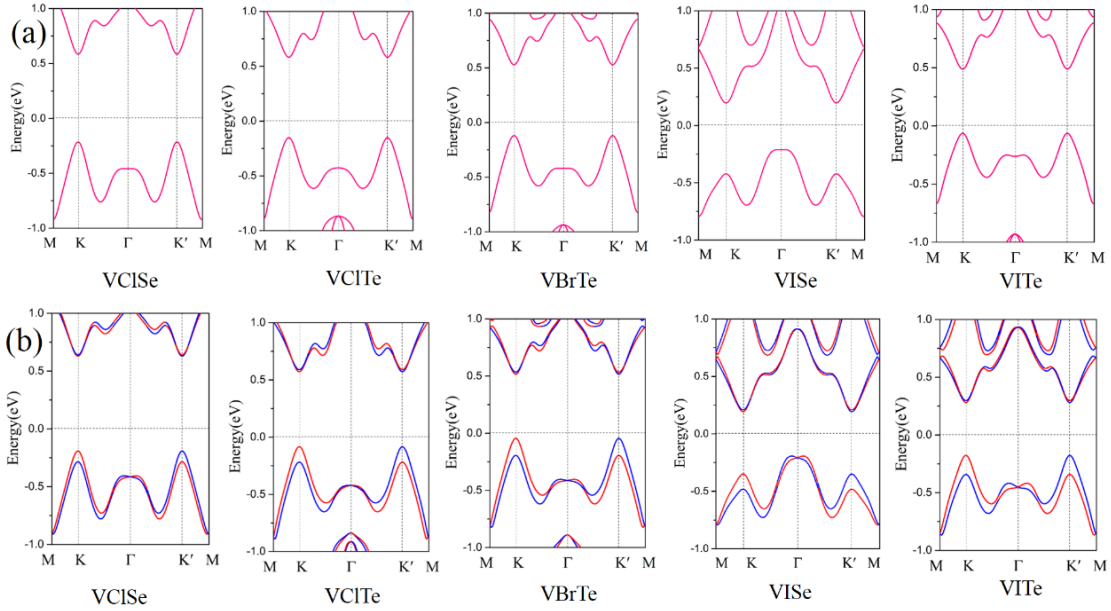

Fig. S3. The band of monolayer VXY without (a)and with(b) SOC, red and blue represent spin-up and spin-down.

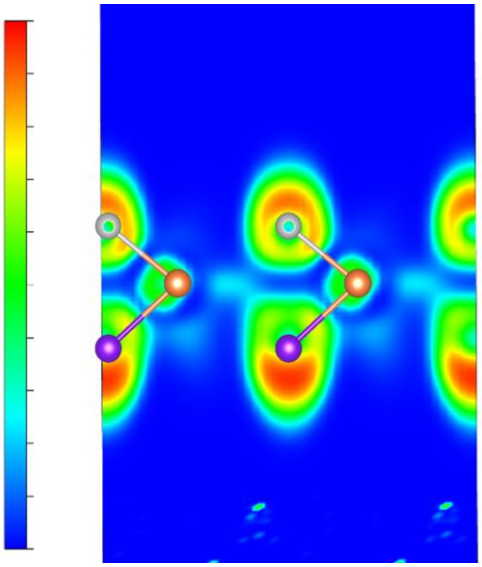

Fig. S4. Electron localization function (ELF) of Janus VBrSe in (110) plane.

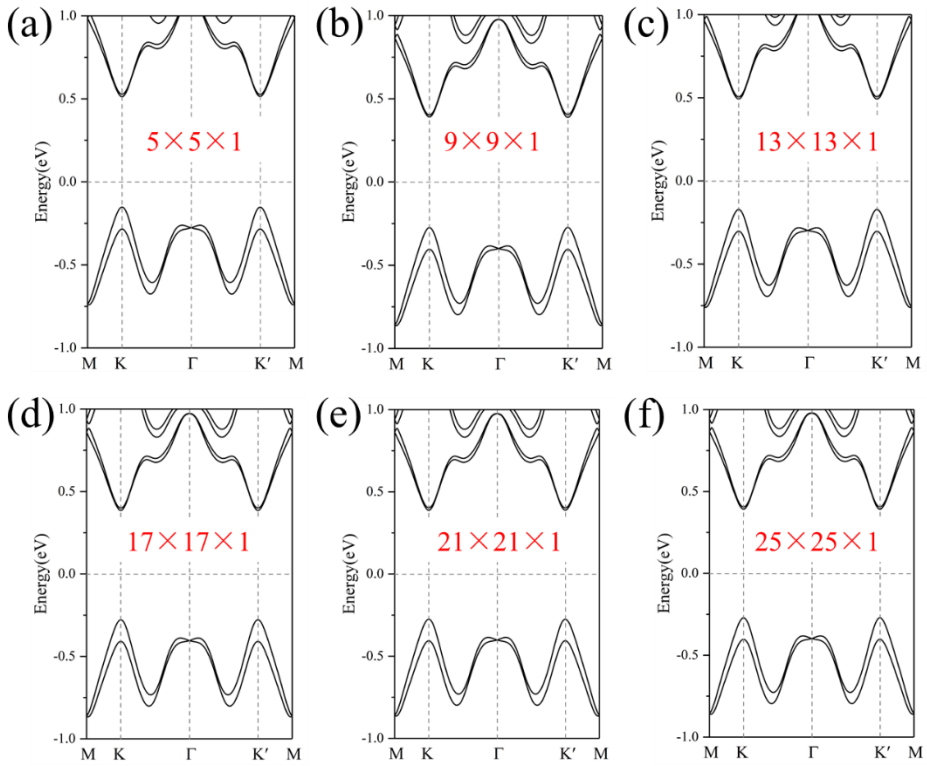

Fig. S5. Variation of Janus VBrSe energy band structures with k-points.

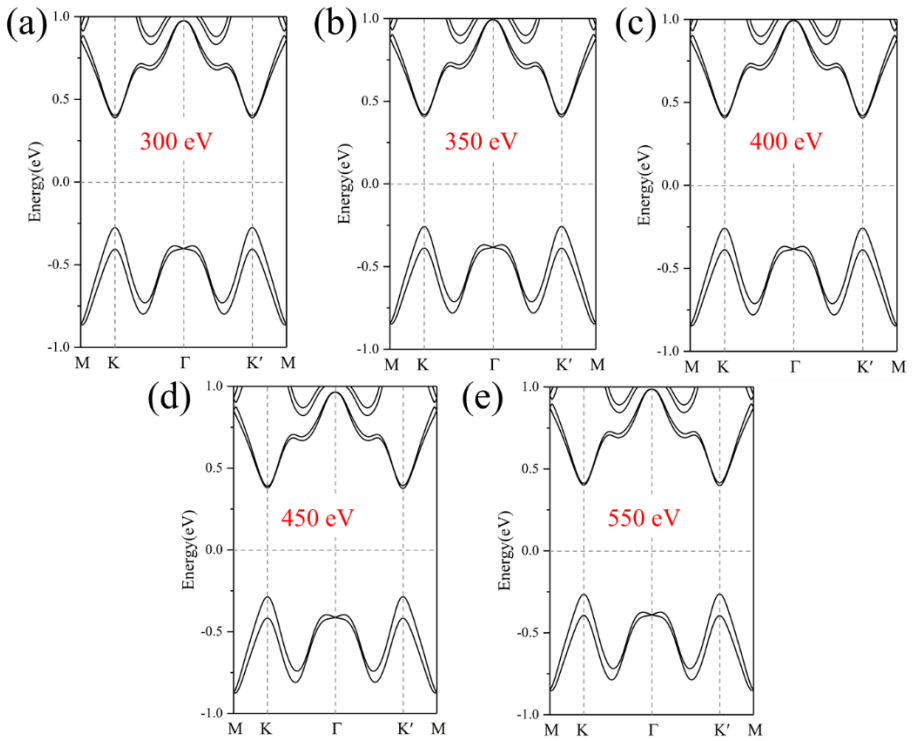

Fig. S6. Variation of Janus VBrSe energy band structures with energy cutoff.

Table S1. Band structure analysis of Janus VBrSe with different k-points and energy cutoff. E_g is the band gap at K point. E_r and K_r are the splitting of the energy and wave vector. α_r is Rashba parameter.

Type	E_g/SOC(eV)	E_r (meV)	K_r (Å^{-1})	α_r (meV Å)
5×5×1	0.665	15.1	0.170	177.65
7×7×1	0.664	14.4	0.170	169.41
9×9×1	0.665	14.6	0.170	171.76
11×11×1	0.665	14.7	0.170	172.94
13×13×1	0.664	15.3	0.170	180.00
17×17×1	0.663	15.5	0.170	182.35
19×19×1	0.663	15.5	0.170	182.35
21×21×1	0.663	15.2	0.170	178.82
23×23×1	0.665	14.7	0.170	172.94
25×25×1	0.664	15.4	0.170	181.18
300 eV	0.664	16.1	0.170	189.41
350 eV	0.663	15.5	0.170	182.35
400 eV	0.664	15.0	0.170	176.47
450 eV	0.665	14.4	0.170	169.41
550 eV	0.666	14.3	0.170	168.24

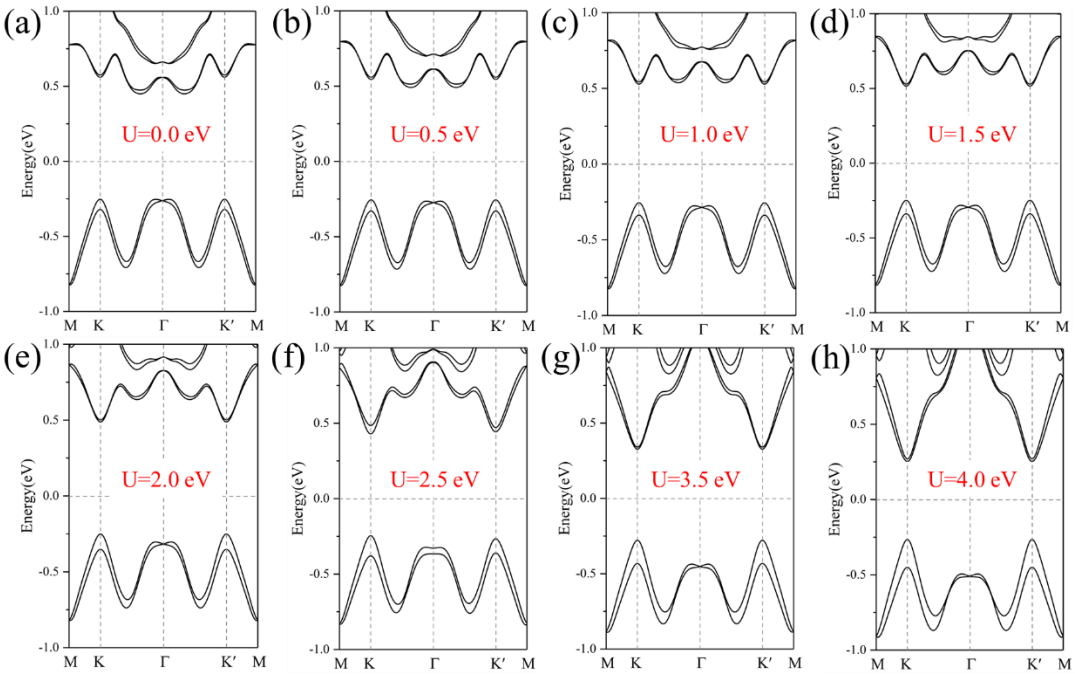

Fig. S7. Variation of Janus VBrSe energy band structures with Hubbard U values.

Table S2. Band structure analysis of Janus VBrSe with different Hubbard U values.

U (eV)	E_g/SOC (eV)	E_r (meV)	K_r (Å^{-1})	α_r (meV Å)
0.0	0.702(indirect)	8.59	0.186	92.37
0.5	0.746(indirect)	9.83	0.186	105.70
1.0	0.783	11.06	0.186	118.92
1.5	0.763	12.24	0.186	131.61
2.0	0.738	13.39	0.186	143.98
3.5	0.605	16.31	0.170	191.88
4.0	0.518	15.09	0.170	177.53

Table S3. Fitting results from first-principles band structure calculations around the K point.

Strain	a (Å)	t	$2\lambda_v$ (meV)	Ω_{PBE} (bohr^2)	$\Omega_{K.P}$ (bohr^2)
-4%	3.219	3.89	15.6	141.5	143.1
-3%	3.252	3.87	15.2	149.96	146.6
-2%	3.286	3.82	14.7	162.37	162.9
-1%	3.32	3.78	14.5	171.56	175.2
0%	3.353	3.76	14.1	182.73	180.4
1%	3.387	3.75	13.7	194.63	189.6
2%	3.42	3.69	13.2	209.78	207.3
3%	3.454	3.63	12.8	223.57	219.7
4%	3.487	3.61	12.1	231.69	230.8