Supplementary Information (SI)

Tunable electronic and optical properties of Janus Al_2M_2ClBr (M=O, S) monolayers as UV photodetectors applications

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Table S1 Calculated effective masses for Janus Al_2M_2ClBr (M=O, S) monolayers by PBE+SOC and HSE06+SOC.

Material	Method	Direction	m_e^*/m_0	m_h^*/m_0
Al_2O_2ClBr	PBE+SOC	x	0.52	0.23
		y	0.34	8.08
	HSE06+SOC	x	0.58	0.23
		y	0.37	7.95
Al_2S_2ClBr	PBE+SOC	x	1.00	0.81
		y	0.19	0.26
	HSE06+SOC	x	0.97	0.81
		y	0.19	0.26

Table S2 Mulliken charges and overlap populations of Janus Al_2M_2ClBr (M=O, S) monolayers after geometry optimization by PBE and PW91 methods.

method	materials	species	charge	bonds	population
PBE	Al_2O_2ClBr	Al_1	1.35	O_1- Al_1	0.56
		Al_2	1.50	O_2- Al_2	0.55
		O_1	-1.08	O_2- Al_1	0.59
		O_2	-1.08	O_1- Al_2	0.59
		Cl_1	-0.41	Al_2- Cl_1	0.71
		Br_1	-0.28	Al_1- Br_1	0.73
	Al_2S_2ClBr	Al_1	0.84	S_1- Al_1	0.54
		Al_2	1.01	S_2- Al_2	0.54
		S_1	-0.61	S_2- Al_1	0.97
		S_2	-0.60	S_1- Al_2	0.97
		Cl_1	-0.40	Al_2- Cl_1	0.63
		Br_1	-0.24	Al_1- Br_1	0.66
PW91	Al_2O_2ClBr	Al_1	1.35	O_1- Al_1	0.56
		Al_2	1.51	O_2- Al_2	0.55
		O_1	-1.09	O_2- Al_1	0.59
		O_2	-1.09	O_1- Al_2	0.59
		Cl_1	-0.41	Al_2- Cl_1	0.71
		Br_1	-0.28	Al_1- Br_1	0.73
	Al_2S_2ClBr	Al_1	0.84	S_1- Al_1	0.54
		Al_2	1.01	S_2- Al_2	0.54
		S_1	-0.61	S_2- Al_1	0.97
		S_2	-0.60	S_1- Al_2	0.97
		Cl_1	-0.40	Al_2- Cl_1	0.63
		Br_1	-0.24	Al_1- Br_1	0.66

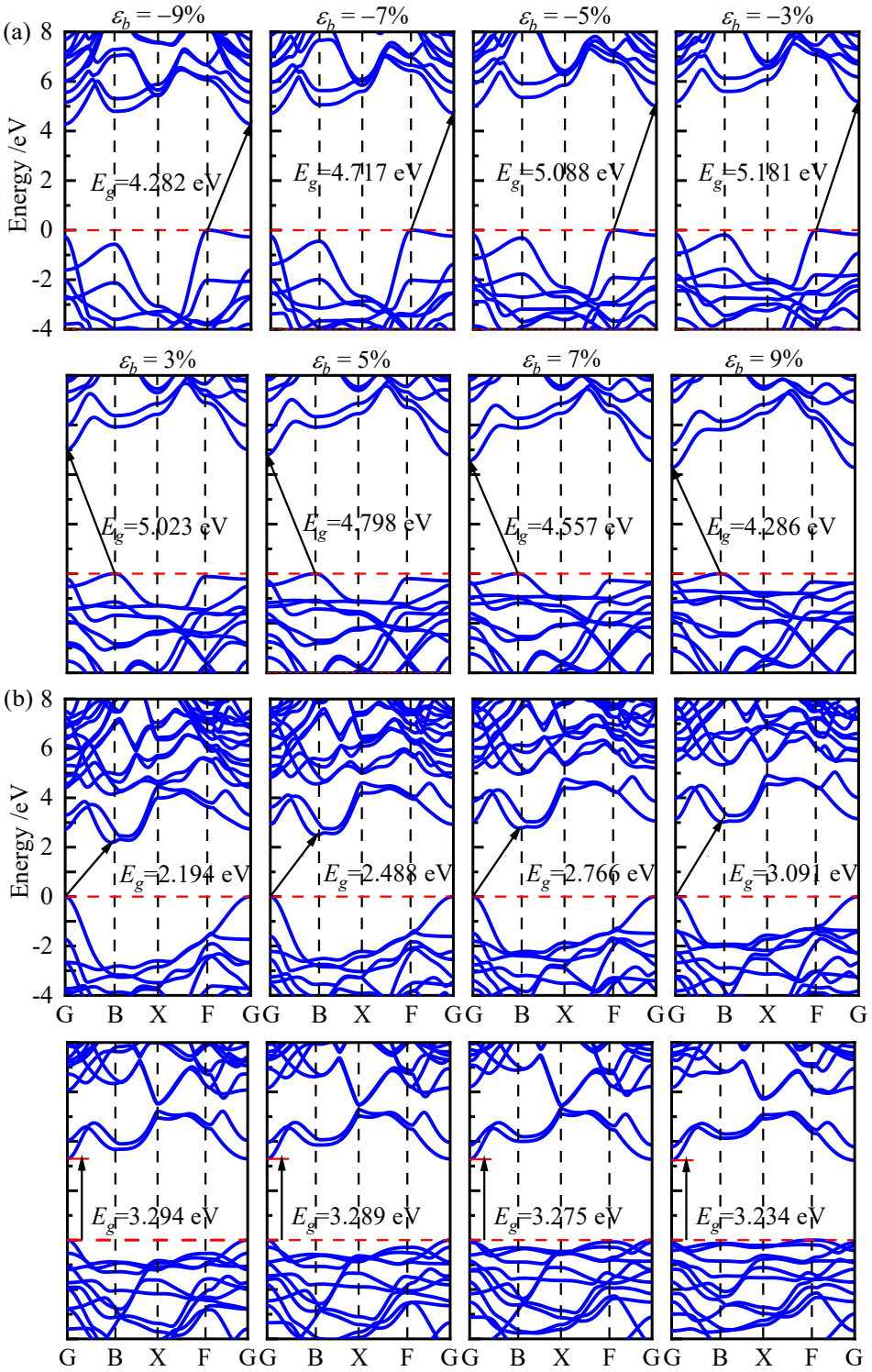

Fig. S1. Band structures of Janus (a) Al_2O_2ClBr and (b) Al_2S_2ClBr monolayers under different strain ε_b.

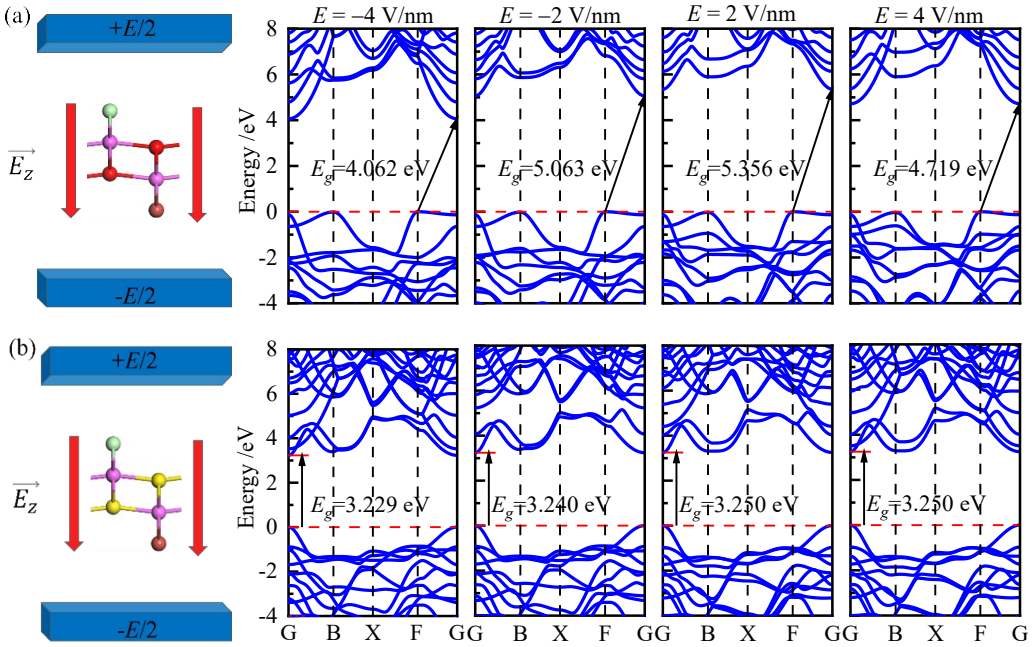

Fig. S2. Band structures of Janus (a) Al_2O_2ClBr and (b) Al_2S_2ClBr monolayers under different electric field *E*.

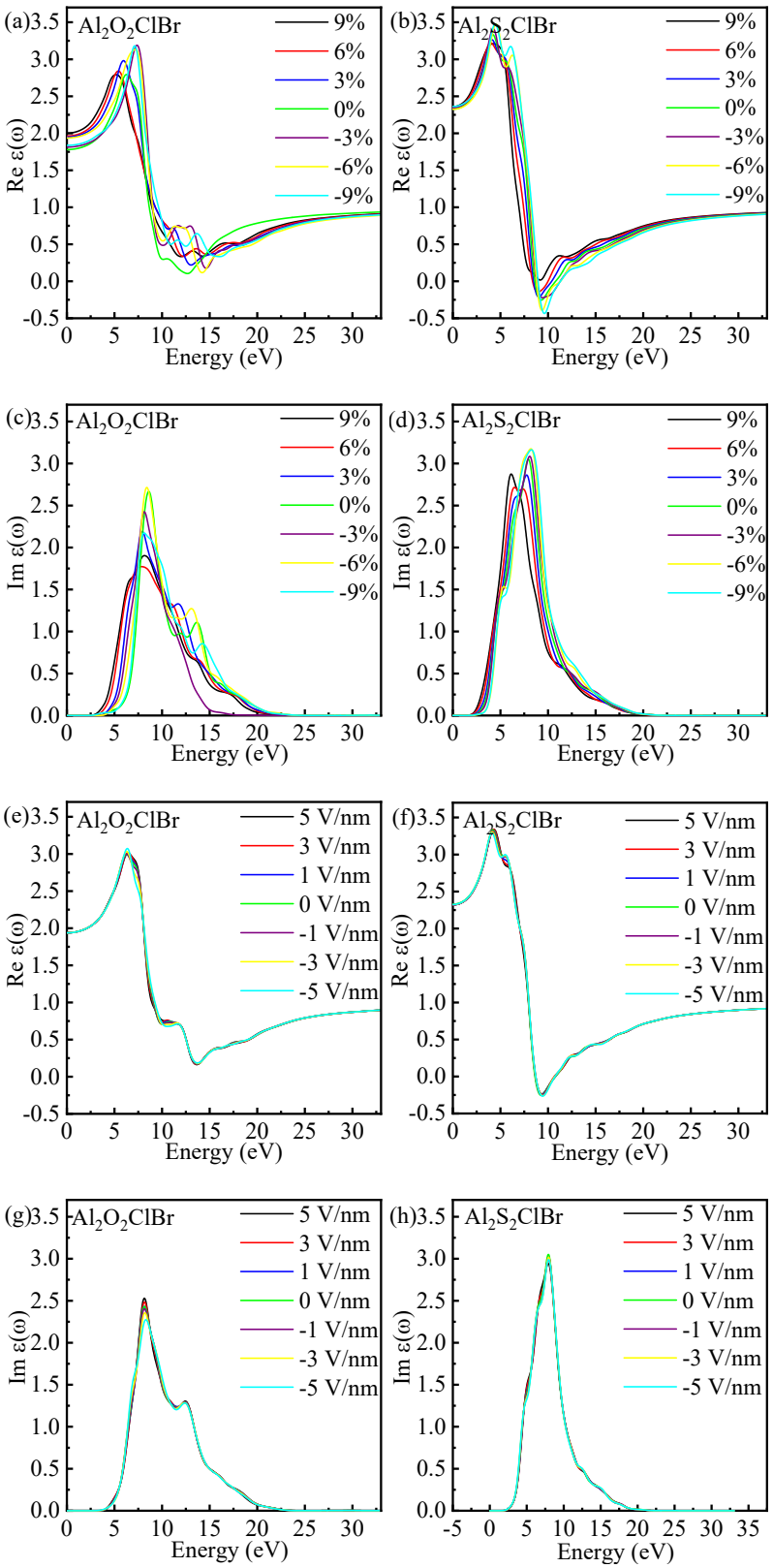

Fig. S3. The changes of the real part of the dielectric and the imaginary part of the dielectric of Janus Al_2O_2ClBr and Al_2S_2ClBr monolayers under different biaxial strain ε_b (a-d) electric field E (e-h).