Supplementary Material for:

The pure spin current and fully spin-polarized current induced by photogalvanic effect and spin-Seebeck effect in halogen-decorated phosphorene

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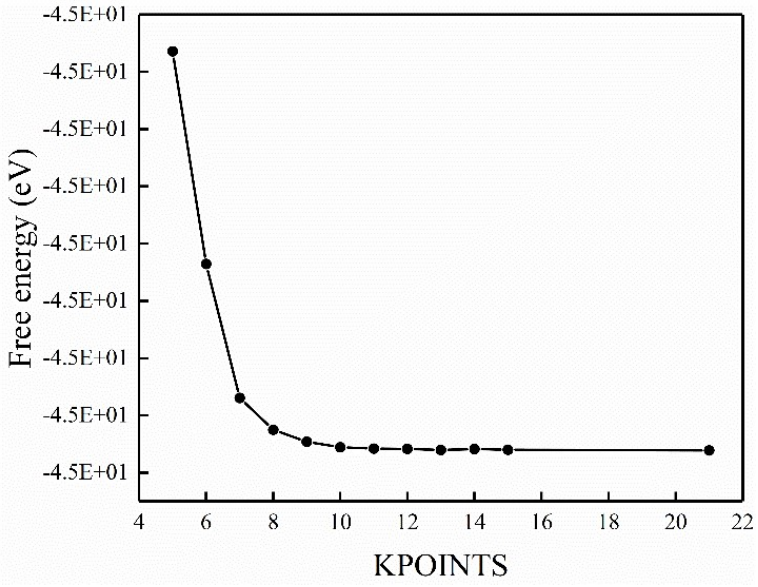

Fig. S1 The test of the number of k points.

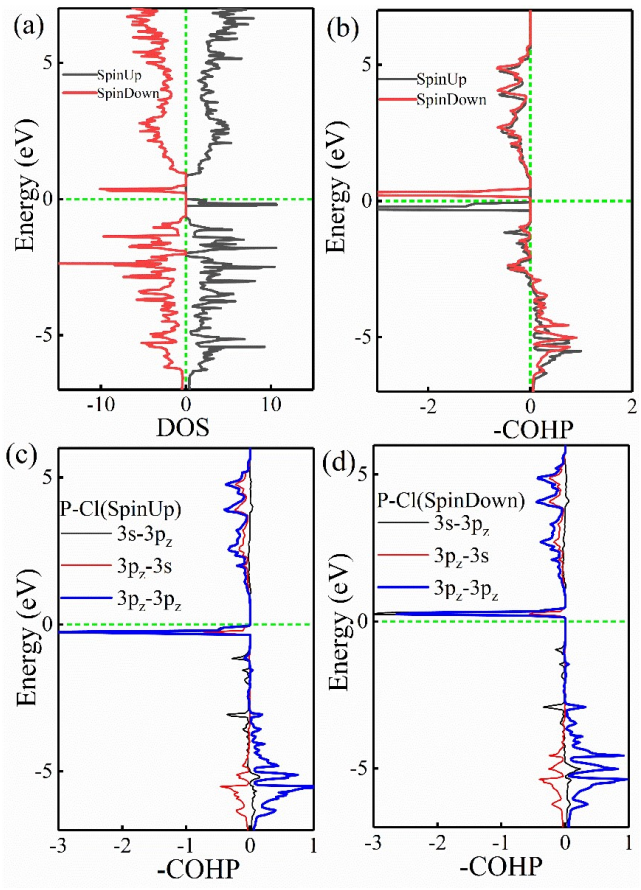

Fig. S2 (a) The density of states (DOS). (b) The crystal orbital Hamilton population (COHP) analysis. (c) and (d) Single orbital COHPs analysis.

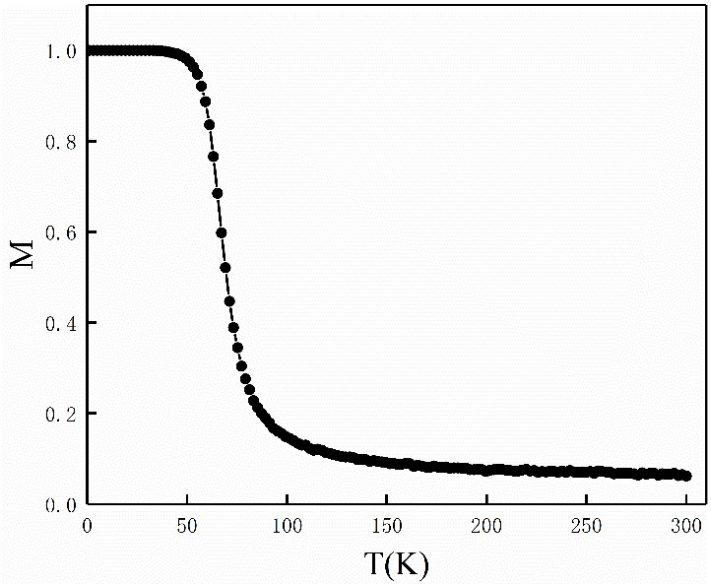

Fig. S3 Variation of magnetic susceptibility with temperature.

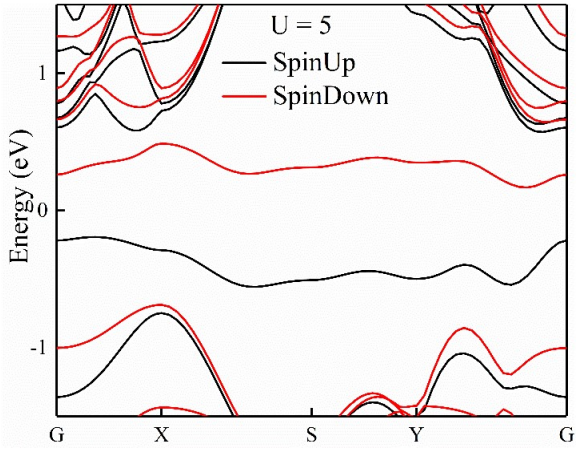

Fig. S4 The band structures for U value of 5 (U for 3p electrons of P atoms and Cl atoms).

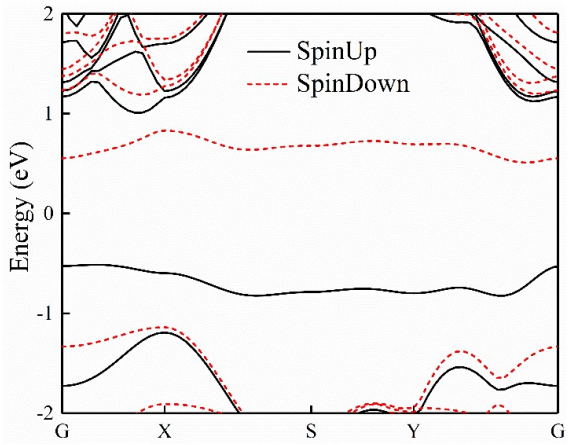

Fig. S5 The band structures calculated by HSE06.

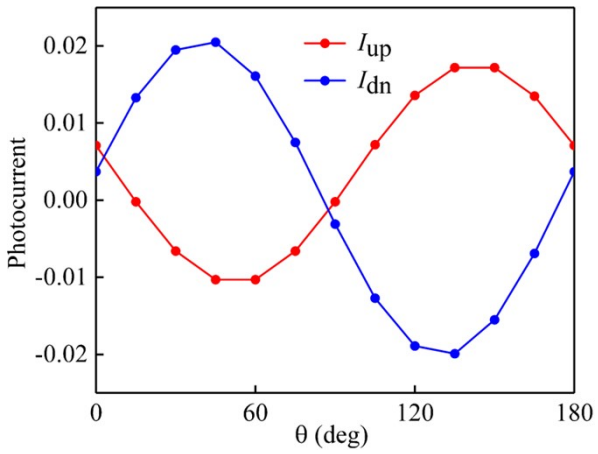

Fig. S6 The photocurrent at the photon energy of 1.2 eV.

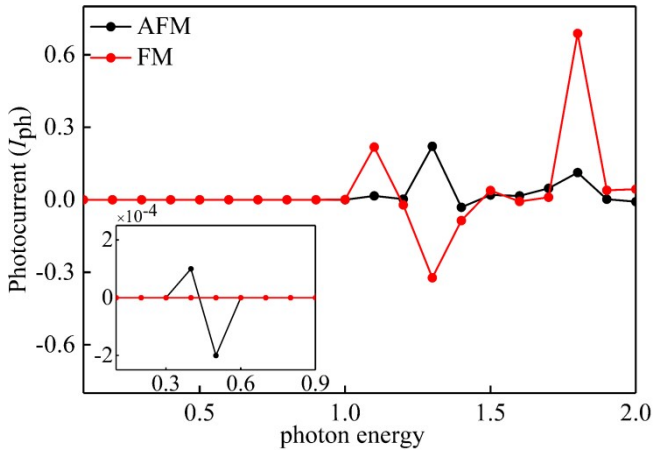

Fig. S7 I_{ph} of FM and AFM at the the polarization angle θ of 45°.

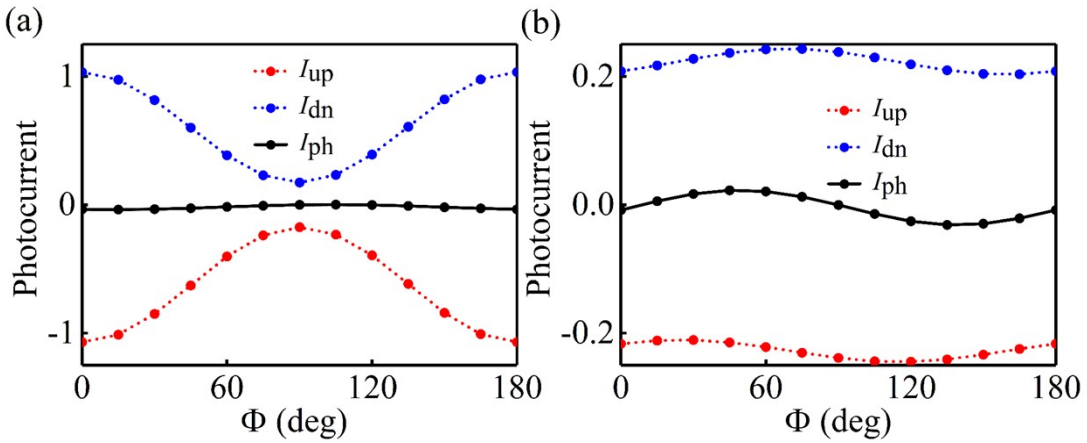

Fig. S8 The photocurrent under CPL at the photon energy of 1.3 eV (a) and 1.8 eV (b).

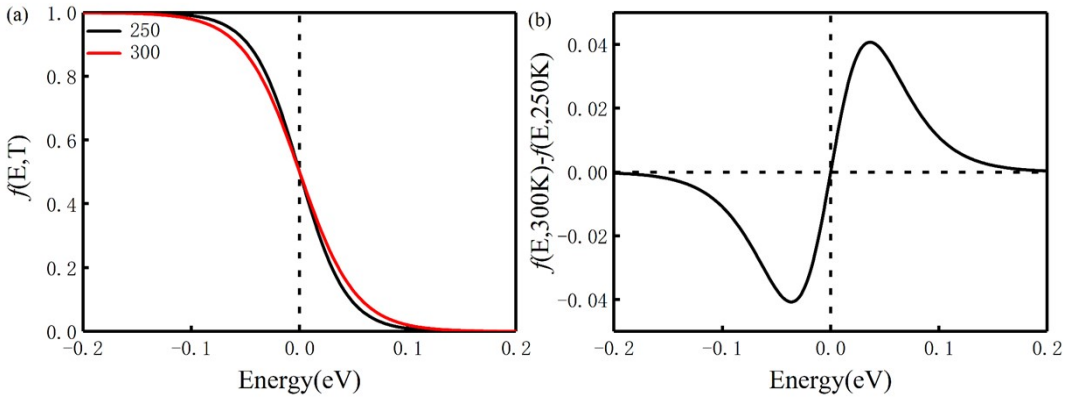

Fig. S9 (a) Fermi-Dirac distribution function at the temperature of 250 K and 300 K. (b) The Fermi distribution difference $f_L(E,300K) - f_R(E,250K)$.

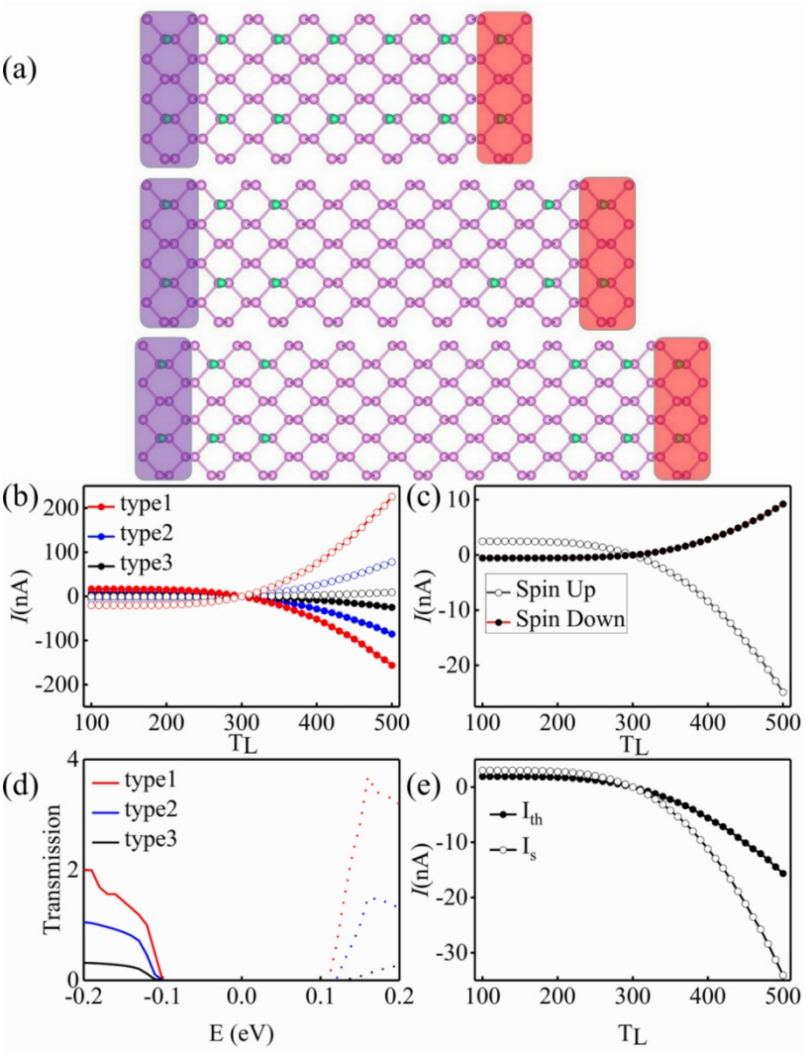

Fig. S10 (a) The device models of type1, type2 and type3. (b) The I_{up} and I_{dn} of the devices. (c) The I_{up} and I_{dn} of type3 device. Hollow and solid symbols represent spin up and spin down state respectively. (d) The transmission spectra of the devices. Solid lines and dotted lines represent spin up and spin down state, respectively. (e) The I_{th} and I_s of type3 device.

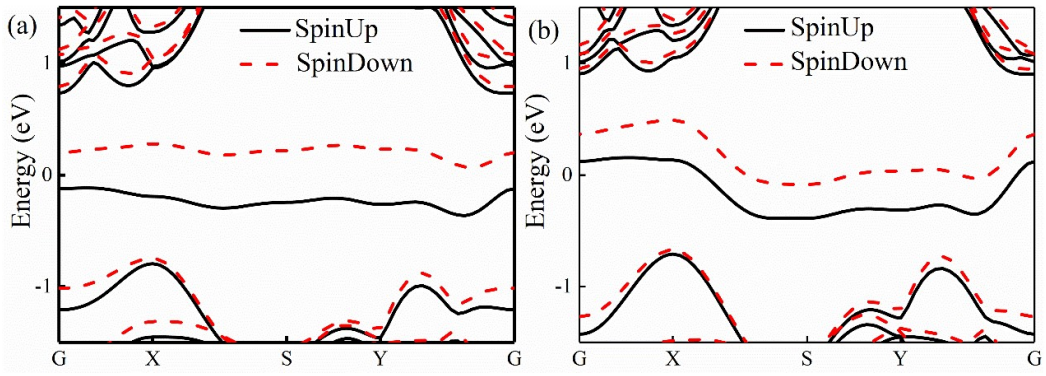

Fig. S11 The band structures of (a) Br-decorated phosphorene and (b) F-decorated phosphorene.

Table. S1 The bader charge analysis of system.

Atom	X(Å)	Y(Å)	Z(Å)	Charge(e)
P1	2.479	2.715	7.821	0.04646
P2	5.785	2.715	7.821	-0.03830
P3	2.479	1.899	9.932	-0.28076
P4	5.785	1.899	9.932	-0.05247
P5	0.826	0.401	9.932	-0.05161
P6	4.132	0.401	9.932	-0.05161
P7	0.826	4.206	7.821	0.00484
P8	4.132	4.206	7.821	0.00484
Cl	2.479	2.114	12.179	0.41861

Table. S2 The band gap for different U values(U for the 3p electrons of P atoms and Cl atoms).

U	1	2	3	4	5
Band Gap (eV)	0.2612	0.2893	0.3157	0.3392	0.3610