Supplementary information

Strain-induced spin-gapless semiconductors and pure thermal spin-current in magnetic black arsenic-phosphorus monolayer

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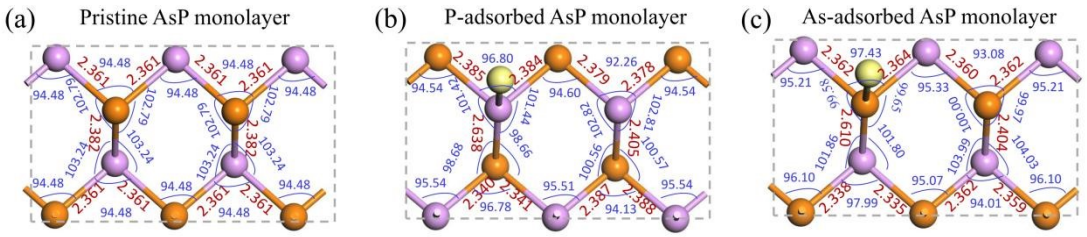

Fig. S1 (a)-(c) The optimized bond lengths and bond angles of the pristine AsP monolayer, P- and As-adsorbed AsP nanosheets, respectively.

Table S1: The optimized lattice constants (*a*, *b*, *c*), three angles (*α*, *ß*, *γ*) and the bond length (*l*) of P-Cl (As-Cl) for pristine AsP monolayer, P- and As-adsorbed AsP nanosheets, respectively.

	a (Å)	ł (Å)	⌊ (Å)	*α* (°C)	*ß* (°C)	γ (°C)	*l* (Å)
Pristine AsP	4.787	6.934	9.792	90	90	90	—
P-adsorbed AsP	4.593	6.996	9.997	89.957	90.885	89.980	2.194
As-adsorbed AsP	4.607	6.971	10.020	90.109	90.828	89.987	20285

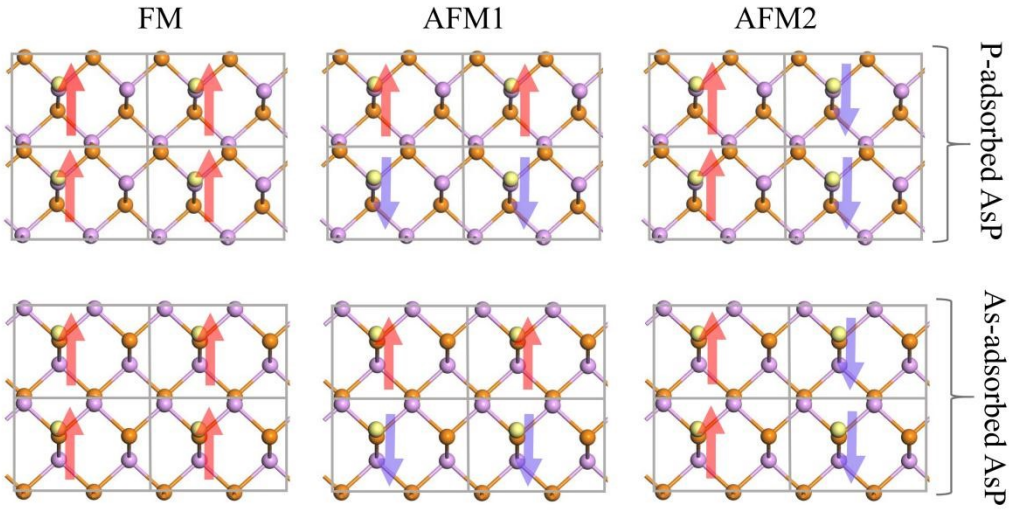

Fig. S2 Three different spin configurations of ferromagnetic (FM) and antiferromagnetic states (AFM1 or AFM2) for P- and As-adsorbed AsP monolayer, respectively.

Table S2: The energies (in meV) of antiferromagnetic states (AFM1 and AFM2) compared with the ferromagnetic (FM) state (set as 0).

	FM	AFM1	AFM2
P-adsorbed AsP	0	27.5	6.2
As-adsorbed AsP	0	22.4	5.8

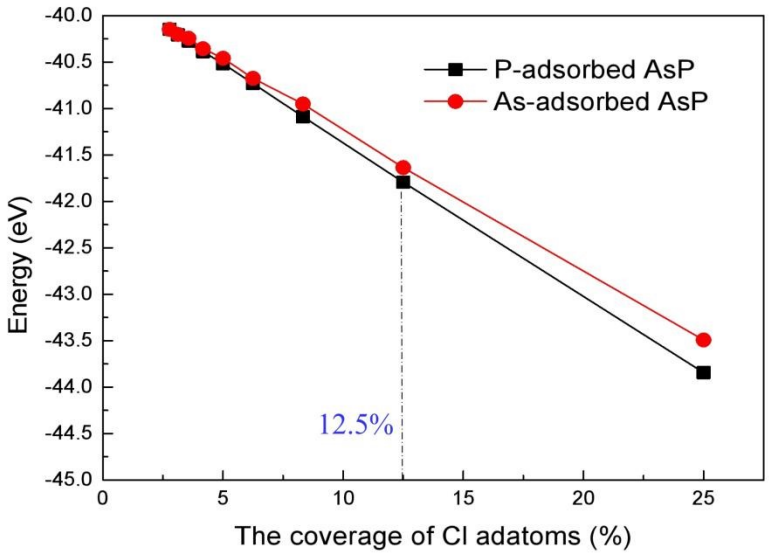

Fig. S3 The equivalent energies of the different coverages for Cl adatoms compared to P- and As-adsorbed monolayer with the 12.5% coverage, respectively.

Table S3: Binding energies of P- and As-adsorbed AsP monolayer, defined as E_b=Es-E_{AsP}-E_{Cl2}/2, where Es, E_{AsP} and E_{Cl2} stand for the energies of AsP monolayer with one Cl adatom, pristine AsP monolayer and Cl_2 molecule, respectively.

	E_b (eV)	E_S (eV)	E_{AsP} (eV)	E_{Cl2} (eV)
P-adsorbed AsP	-0.877	-41.793	-39.128	-3.575
As-adsorbed AsP	-0.720	-41.636	-39.128	-3.575

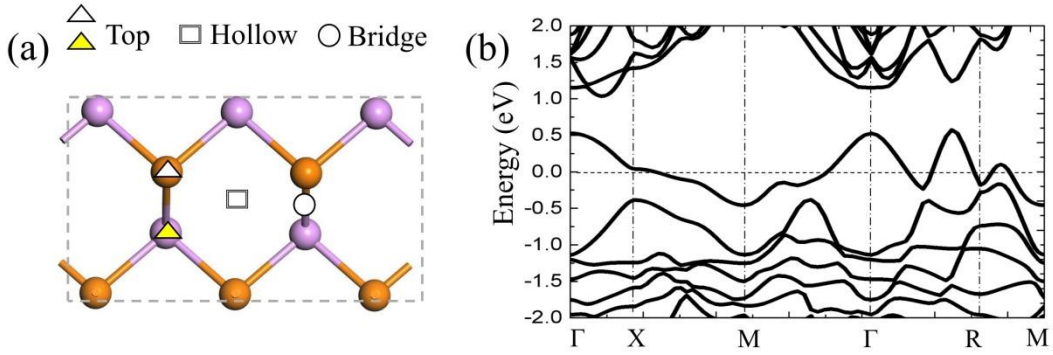

Fig. S4 (a) Three adsorption positions for AsP monolayer with the Cl adatom: top, hollow and bridge sites. (b) Band structures of AsP monolayer with the Cl adatom on bridge site.

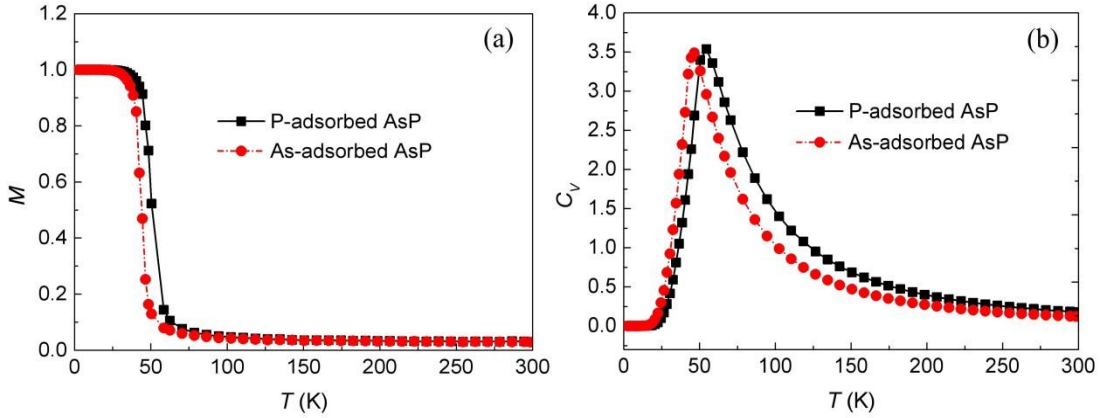

Fig. S5 Monte Carlo simulations for the P- and As-adsorbed AsP monolayer: (a) magnetism (M) and (b) heat capacity (C_V) versus temperature. We use the Heisenberg model to describe the spin interaction and the related lattice Hamitonian can be expressed as follows:

$$H = -J_1 \sum_{<i,j>} S_i S_j - J_2 \sum_{<k,l>} S_k S_l$$

where S_i, S_j and S_k, S_l refer to the spin operators on the nearest and next nearest-neighbour lattice points <i,j> and <k,l>, respectively. J_1 and J_2 stand for the nearest and next nearest-neighbour interaction energies, respectively, estimated by the energy difference between the ferromagnetic and anti-ferromagentic state shown in Table S2 and Fig. S2.

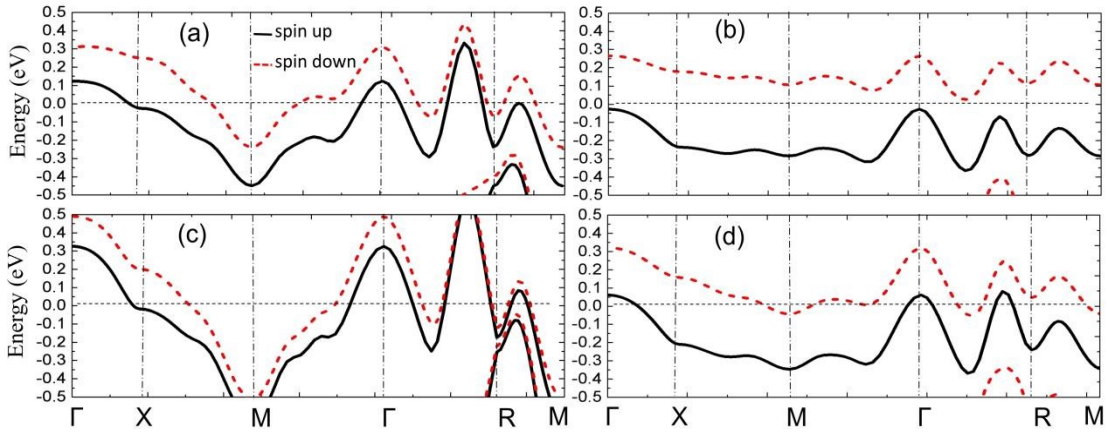

Fig. S6 (a) and (b) Band structures of the AsP monolayer with one P atom adsorbed by one fluorine (F) and one bromine (Br) atom, respectively. (c) and (d) Band structures of the AsP monolayer with one As atom adsorbed by one F and one Br atom, respectively.