Electronic supplementary information

Two-dimensional ferromagnetic semiconductor Cr_2XP: First-principles calculations and Monte Carlo simulations

Xiao-Ping Wei[a,b], Lan-Lan Du[a], Jiang-Liu Meng[a], Xiaoma Tao[c]

[a]*The School of Mathematics and Physics, Lanzhou Jiaotong University, Lanzhou 730070, P. R. China.*

[b]*Lanzhou Center for Theoretical Physics, Key Laboratory of Theoretical Physics of Gansu Province, Lanzhou University, Lanzhou, Gansu 730000, P. R. China*

[c]*College of Physical Science and Technology, Guangxi University, Nanning 530004, P. R. China.*

Email address: weixp2008@lzjtu.edu.cn (Xiao-Ping Wei[a,b])

Table S1: The optimized lattice constant (Å) and atomic position of Cr_2XP (X=P, As, Sb).

Materials	Space group	Lattice constant	Atomic position			
			Cr1	Cr2	P	X
Cr_2P_2	P4/nmm	4.17	(0,0,0.79)	(0.5,0.5,0.79)	(0,0,5,0.01)	(0.5,0,0.15
Cr_2AsP	P4/nmm	4.23	(0,0,0.08)	(0.5,0.5,0.82)	(0.5,0,0.15)	(0,0.5,0.10)
Cr_2SbP	P4/nmm	4.29	(0,0,0.09)	(0.5,0.5,0.09	(0.5,0,0.15)	(0,0.5,0.99)

The details of calculations for Curie temperature of Cr_2XP (X=P, As, Sb).

1. In order to obtain the exchange coupling parameters J for Cr_2XP magnetic system. Firstly, we perform a collinear calculations to optimized the structure and obtain the magnetic moment of Cr atoms. Subsequently, we calculate the total energies of different magnetic configurations and magnetization direction of Cr_2XP, we can obtain the magnetic anisotropy (MAE).

$$MAE = E_{\parallel} - E_{\perp} \tag{1}$$

According to the spin Hamiltonian of the magnetic system with magnetic anisotropy as follows:

$$H = -\sum_{i,j} J_1 S_i S_j - \sum_{i,k} J_2 S_i S_k - A S_i^z S_i^z \tag{2}$$

Further, the ferromagnetic states of Cr_2XP has the spin Hamiltonian:

$$E(FM) = E_0 - 16J_1S^2 - 16J_2S^2 - AS^2 \tag{3}$$

The anti-ferromagnetic1 states (AFM1) of Cr_2XP has the spin Hamiltonian:

$$E(AFM1) = E_0 + 16J_1S^2 - 16J_2S^2 - AS^2 \tag{4}$$

The anti-ferromagnetic3 states (AFM1) of Cr_2XP has the spin Hamiltonian:

$$E(AFM3) = E_0 + 16J_1S^2 - AS^2 \tag{5}$$

By the equs. 1~5, we can obtain the J_1=13.1meV, 17.7 meV and 83.0 meV; J_2=3.0 meV, 6.7 meV and 6.6 meV for Cr_2P_2, Cr_2AsP and Cr_2SbP. Finally, we adopt the Heisenberg model combined with the Metroplis algorithm in mcsolver code[1] to simulate the magnetization and specific heat capacity as a function of temperature, and find that their the Curie temperature are 278 K, 464 K and 1590 K for Cr_2P_2, Cr_2AsP and Cr_2SbP, which are evidently higher than room temperature.

[1] Liu L, Ren X., Xie J., et al, Magnetic switches via electric field in BN naoribbons, Appl. Surf. Sci. 480 (2019) 300.