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Strain tuning of magnetism in transition-metal atom doped phosphorene

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ABSTRACT

Using first-principles calculations, we studied the magnetic properties of 3d transition-metal (TM) atoms doped phosphorene. The magnetic moments are 1.02, 2.00, 3.00, 4.04, 1.01 and 0.93 μ_B for Ti, V, Cr, Mn, Fe and Ni doped phosphorene, respectively. However, there is no spin polarized state in the Sc and Co doped systems. TM atoms doped phosphorene system becomes a magnetic half-metal or a magnetic semiconductor, which depends on the species of impurity atoms. The strain is a promising way to tune the magnetic moment of TM atoms doped phosphorene systems. A small biaxial strain could induce a magnetic transition from a state with magnetic moment to another state in phosphorene doped by Fe or Mn atom. For Mn doped system, the magnetic moment changes from 2 μ_B to 4 μ_B. For Fe doped system, the magnetic moment changes from 1 μ_B to 3 μ_B. The results establish the potential for black phosphorus utilization in innovative spintronic devices.

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1. Introduction

Two-dimensional (2D) materials are expected to replace traditional semiconductor silicon material, due to their remarkable properties and potential applications in nanoelectronics and spintronics. Although graphene is a fascinating 2D material, the absence of a band gap limits its applications of large-off current and high on–off ratio for graphene-based electronic devices [1–4]. Other 2D materials, such as h-BN, and MoS_2, have been widely studied in various contexts. While h-BN with large bandgap makes it difficult to tune the source drain current using the gate voltage [5–7], and the relatively low mobility in MoS_2 (around 200 $cm^2\ V^{-1}\ s^{-1}$) limits its device applications [8]. Development of the field requires more 2D materials that exhibit properties that may lead to specific improved performance, which are semiconducting preferably with a direct gap, has high carrier mobility and the potential to form excellent contacts with known electrode materials. More recently, black phosphorus as a 2D p-type material has been performed [9]. Black phosphorus is a promising candidate due to its presence of a direct and finite band gap (0.31–0.35ev) [10–13], high carrier mobility, which is the highest values up to 1000 $cm^2\ V^{-1}\ s^{-1}$ [9,14], and other intriguing electronic properties distinctive [15–18].

In all forms of phosphorus allotropes, orthorhombic black phosphorus is the most stable form under normal conditions. Black phosphorus, the space group of the crystal belongs to CMCA (No. 64), with eight P atoms in a unit cell. In a single layer,

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each P atom is joined with three neighbors P atoms by covalent bonds, while the layers are bound together by weak interlayer van der Waals force, similarly to graphite [19–24]. Black phosphorus is composed of single element, different from graphene, the atoms in a single layer black phosphorus are not sitting in a flatland. Instead, the phosphorus atoms are evenly distributed between two half layers, forming a puckered honeycomb structure due to the sp^3 hybridization [10,12,13,25,26]. The puckered honeycomb structure leads to different properties compared with graphene, h-BN, MoS_2, WSe_2, etc [7,27–30].

Recently, the electronic and structural properties of monolayer and few-layer phosphorene have been investigated [11,31,32], which have shown that the band gap of phosphorene depends on the number of stacked layers (N) [17,32]. Besides, the unique anisotropic structure of phosphorene leads to a highly anisotropic optical, electronic behavior and strain response, etc [10,33–35]. Although many properties of phosphorene have been pointed out, more attractive properties have not been found. Our work focused on magnetic properties of 3d transition-metal atom doped phosphorene. It is well known that if magnetic moment can be introduced into phosphorene, the applications of phosphorene will be extended more widely in nanoelectronics and spintronics [25,26,36–38,39–41]. Various methods for introducing spin polarization have been developed [18,42]. In particular, substitution doping is well known and widely used method of manipulating the magnetic properties of phosphorene. For example, transition-metal atoms including Sc, Ti, V, Cr, Mn, Fe, Co, Ni can substitute one phosphorus atom in monolayer black phosphorus, respectively, which modulates the electronic and magnetic properties dramatically.

2. Computational method

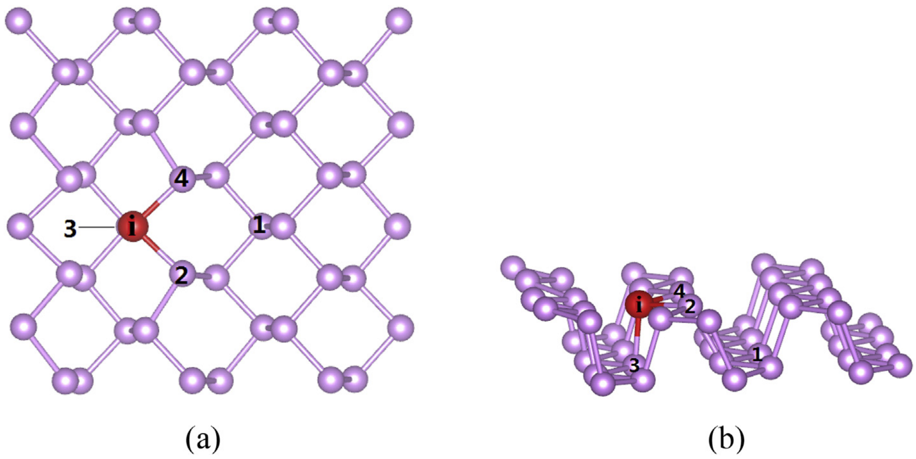
All calculations are performed based on the density functional theory (DFT) as implemented in the Vienna ab initio simulation package (VASP) [43]. Ultra soft pseudopotentials [44] as well as the electron–ion interaction is described by a projector augmented wave (PAW) method [45] using Perdew–Burke–Ernzerhof (PBE) pseudopotentials [46]. All simulations are carried out for a 3 × 4 supercell with 47 Phosphorus atoms and a transition metal atom substitutes a P atom. By replacing a P atom with a transition metal atom, the impurity concentration is 2.08%. A 20 Å vacuum layer is adopted in our slab calculations to avoid interaction between the successive layers. The electronic wave functions were expanded in a plane-wave basis set using a kinetic energy cutoff of 500 eV and a 5 × 5 × 1 k-point sampling grid are used. The structural optimization is continued until the residual forces have converged to less than 0.01 eV/Å and all calculations are chosen to converge the total energy to less than 1×10^{-4}eV per unit cell. The amount of charge transfer between the doped atom and phosphorene is estimated from the grid based Bader charge analysis [47].

3. Results and discussion

3.1. The magnetic properties of TM doped phosphorene

Fig. 1(a) and (b) show the schematic illustration of the top and side views of a transition metal atom doped 3 × 4 supercell of a phosphorene monolayer. The lavender and red spheres i represent phosphorus atoms and impurity (Sc, Ti, V, Cr, Mn, Fe, Co, Ni), respectively.

To check the stability of different dopants, the binding energies (E_b) are calculated by using the formula:



(a)

(b)

Fig. 1. Schematic illustration of an impurity doped phosphorene: (a) Top view after the relaxation of the structure. (b) Side view after the relaxation of the structure. The red sphere i represents transition metal atom (Sc, Ti, V, Cr, Mn, Fe, Co, Ni). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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