



Strain engineering of magnetic state in vacancy-doped phosphorene



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ABSTRACT

Inducing and manipulating the magnetism in two-dimensional materials play an important role for the development of the next-generation spintronics. In this letter, the effects of the biaxial strain on magnetic properties of vacancy-doped phosphorene are investigated using first-principles calculation. We find although only SV956 doping induces magnetism for unstrained phosphorene, the biaxial strain induces nonzero magnetic moment for SV5566 and DVA doped phosphorene. The biaxial strain also modulates the magnetic state for SV956, SV5566 and DVA doped phosphorene. The local magnetic moment derives from the spin polarization of the dangling bonds near the vacancy. The biaxial strain influences the local bonding configuration near the vacancy which determines the presence of dangling bonds, and then modulates the magnetic state. Our findings promise the synergistic effect of strain engineering and vacancy decoration is an effective method for the operation of phosphorene-based spintronic devices.

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1. Introduction

Since the discovery of graphene, the magnesium of two-dimensional (2D) nanomaterials has drawn public attention because of the promising applications in low-dimensional spintronics [1–4]. Nevertheless, graphene is a zero band-gap semiconductor. Its valance band couples with conduction band at the Dirac points, which hinders its application in low-dimensional spintronics [5,6]. Phosphorene [7,8], a monolayer of black phosphorus, was deposited by the mechanical exfoliation and turned out to be a kind of promising 2D material in the nanoelectronics because of its fascinating properties [9–13]. It is an appealing material that can be implemented into various electronic device applications including gas sensor, p–n junction, solar cell application [14–16]. Especially important aspects: phosphorene based field effect transistors (FETs) show a high charge-carrier mobility up to $10000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, much better than other typical 2D semiconductors, such as MoS_2 (around $200 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) [8]. Contrast to graphene, phosphorene is a direct band gap semiconductor with band gap of about 1.0 eV [17,18] which avoids the coupling between the valance and conduction bands, making phosphorene suitable for applications in spintronics.

Lattice defects, in particular vacancies, are usually unavoidable present in 2D nanomaterials as they are easily introduced during the fabrication or growth process [19–21]. At the same time, the lattice imperfections play an important role to enrich the properties of 2D nanomaterials [22–24]. For example, forming vacancies is an effective method to induce magnetic moment in 2D crystal. It has been shown that vacancies provide a source of magnetic moment to the graphene, h-BN, and MoS_2 [25–28]. The same as graphene, h-BN, and MoS_2 , phosphorene is also intrinsically nonmagnetic, but single vacancy induces a local magnetic moment [29,30].

It is crucial to understand the mechanisms underlying defect-induced functionalities and identify means to control them for the application of 2D crystal in spintronics. Previous researches have proved that the strain engineering is an effective approach to manipulate the magnetic moment of defective 2D semiconductors. Guinea et al. [31] showed that strain aligned with certain crystallographic directions can induce strong gauge field to open energy gaps and create uniform local magnetic field in graphene. Ouyang et al. [32] found that the strain can lead to switching between the magnetic states for h-BN monolayer with boron vacancy and divacancy. Zheng et al. [33] reported that the biaxial strain can induce magnetic moments in V_S , V_{S_2} , and V_{MoS_3} doped monolayer MoS_2 , and effectively manipulate the magnetization induced by V_{MoS_6} doping due to the change of Mo–Mo metallic bonds. As for the phosphorene, recent studies have declared that strain is an effective method to modify its anisotropic electronic mobility and band gap [34–36]. However, there are seldom studies about the function of strain on the magnetism of defect phosphorene.

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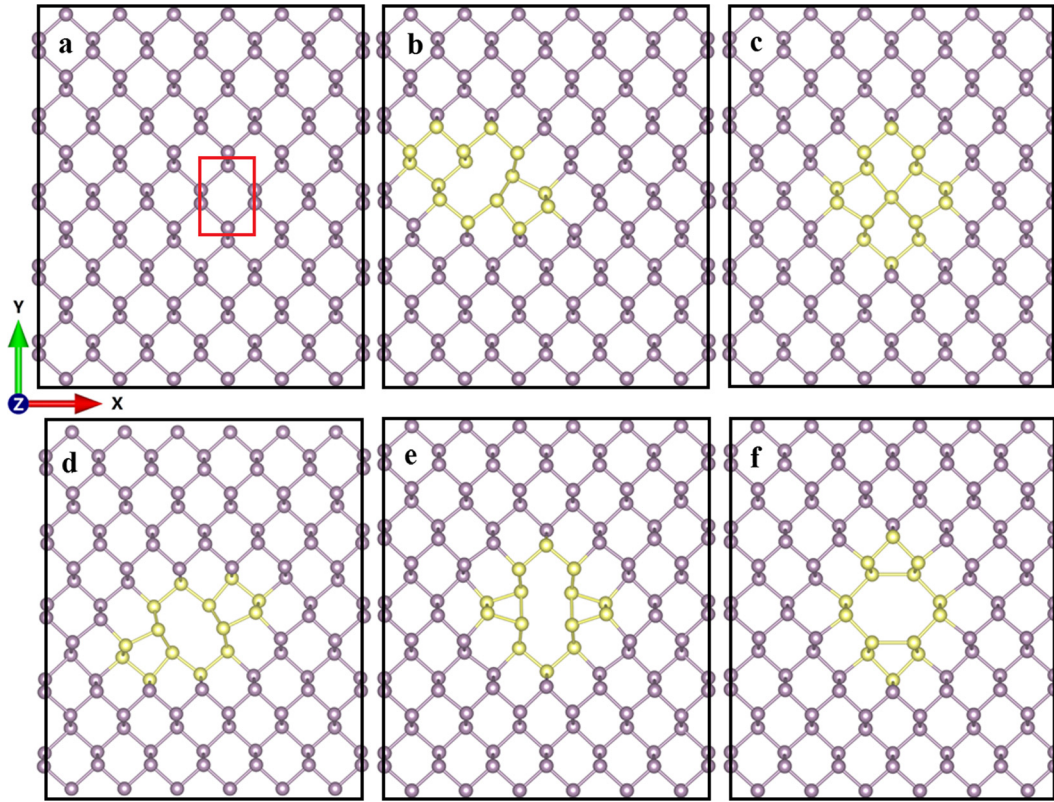


Fig. 1. Structure of intrinsic and vacancies doped phosphorene. (a) Intrinsic phosphorene, the red rectangle region indicates the primitive cell. (b)–(f) Show the defective phosphorene doped by SV956, SV5566, DVp, DV4104, and DVa, respectively. The yellow balls indicate the neighboring atoms at the vacancy. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

To this end, we examine the effects of the biaxial strain on magnetic properties of the vacancy doped phosphorene by first-principles calculations. We find that the biaxial strain can cause switching in the magnetic state and significant modifications of the doping levels for phosphorene with SV956, SV5566, and DVa doping. The strain-induced behaviors can be attributed to the changes of the bonding configuration localized at the vacancy. Our findings explicitly demonstrate that the synergistic effect between strain engineering and vacancy decoration can provide an effective approach to tailor electronic and magnetic state in phosphorene-based nanodevices.

2. Computational methods and models

Spin polarized density-functional theory (DFT) [37] calculations are performed using the Vienna ab-initio Simulation Package (VASP) [38] to study the structural, magnetic, and electronic properties of vacancy doped phosphorene. The projector-augmented wave (PAW) method [39] and the generalized gradient approximation modified by Perdew, Burke and Ernzerhof (GGA-PBE) [40] are employed to deal with the electronic exchange correlation functions. In this work, we mainly focus on the common defects: single vacancy (SV), and divacancy (DV). A 6×5 supercell of phosphorene is used and the vacancy concentration is no more than 1%. The vacuum space about 15 Å in the Z direction is chosen to eliminate the interactions between neighboring phosphorene sheets across the periodic boundary. All the unstrained structures are optimized without any symmetry constraints until the energy and forces are converged to 10^{-7} eV and 10^{-2} eV/Å, respectively. The Brillouin zone is sampled by $5 \times 5 \times 1$ and an energy cutoff of 400 eV is used.

An in-plane biaxial mechanical strain [$\varepsilon = (r - r_0)/r_0$] is applied to the defects doped phosphorene: ε is defined as function of

strain, r is the varying lattice constant after strain, r_0 is the lattice constant for a stress-free defect structure. We take 2% as strain interval, positive/negative on behalf of the tensile/compressive strain. Here, considered biaxial strain ranges from -8% to 10% and the properties of the system at each individual strain are investigated. Under each strain, all atoms are sufficiently relaxed with fixed lattice constant.

3. Results and discussions

3.1. Stability of defect phosphorene

The intrinsic properties of phosphorene is investigated at first. The primitive cell of phosphorene is shown in Fig. 1(a), with the lattice constants being $a = 3.30$ Å, and $b = 4.63$ Å. Our calculation also shows that the phosphorene is a direct band gap semiconductor with band gap of 0.91 eV at Gamma. Both the maximum of valance band and the minimum of conduction band is contributed by p state of phosphorus (P) atoms. Our above results agree with the previous reports [36]. On the basis of energy calculation, we find two kinds of single vacancy (named as SV956 and SV5566 shown in Fig. 1(b) and Fig. 1(c)) and three kinds of divacancy (named as DVp, DV4104, and DVa shown in Fig. 1(d), Fig. 1(e), and Fig. 1(f)). From Fig. 1(b), we find that because of the Jahn–Teller distortion, a construction bond is formed between two neighbor P atoms and another neighbor P atom with a dangling bond moves out of the plane in the SV956. For SV5566 as shown in Fig. 1(c), four construction bonds are formed in the vacancy, as a result, a local structure with two five-loop rings and two six-loop rings is formed. From Fig. 1(d) and Fig. 1(f), we find that both DVp and DVa have two five-loop rings and an eight-loop ring, named 585 ring, but an explicit difference between them is that the construction bond is formed between two P atoms in different layers

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