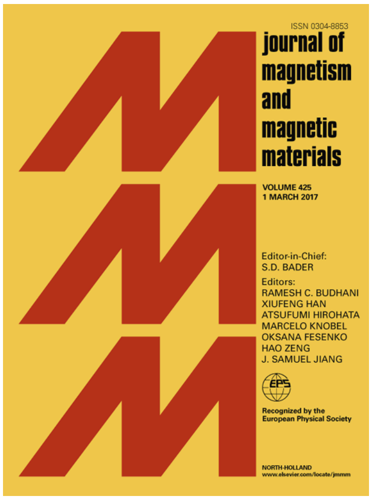

Single-atom vacancy in monolayer phosphorene: a comprehensive study of stability and magnetism under applied strain

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PII: S0304-8853(18)30849-7
DOI: https://doi.org/10.1016/j.jmmm.2018.06.016
Reference: MAGMA 64036

To appear in: *Journal of Magnetism and Magnetic Materials*

Please cite this article as: J.M. Morbec, G. Rahman, P. Kratzer, Single-atom vacancy in monolayer phosphorene: a comprehensive study of stability and magnetism under applied strain, *Journal of Magnetism and Magnetic Materials* (2018), doi: https://doi.org/10.1016/j.jmmm.2018.06.016

Single-atom vacancy in monolayer phosphorene: a comprehensive study of stability and magnetism under applied strain

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Using first-principles calculations based on density-functional theory we systematically investigate the effect of applied strain on the stability and on the electronic and magnetic properties of monolayer phosphorene with single-atom vacancy. We consider two types of single vacancies: the symmetric SV-55|66, which has a metallic and non-magnetic ground state, and the asymmetric SV-5|9, which is energetically more favorable and exhibits a semiconducting and magnetic character. Our results show that compressive strain up to 10%, both biaxial and uniaxial along the zigzag direction, reduces the formation energy of both single-atom vacancies with respect to the pristine configuration and can stabilize these defects in phosphorene. We found that the magnetic moment of the SV-5|9 system is robust under uniaxial strain in the range of −10 to +10%, and it is only destroyed under biaxial compressive strain larger than 8%, when the system also suffers a semiconductor-to-metal transition. Additionally, we found that magnetism can be induced in the SV-55|66 system under uniaxial compressive strain larger than 4% along the zigzag direction and under biaxial tensile strain larger than 6%. Our findings of small formation energies and non-zero magnetic moments for both SV-5|9 and SV-55|66 systems under zigzag uniaxial compressive strain larger than 4% strongly suggest that a magnetic configuration in monolayer phosphorene can be easily realized by single-vacancy formation under uniaxial compressive strain.

I. INTRODUCTION

Two-dimensional (2D) materials have been attracting increasing interest and new materials have been explored—silicene, germanene, hexagonal boron nitride, transition metal dichalcogenides, to cite a few [1–4]—since the discovery of graphene in 2004 [5]. Moreover, 2D materials continue to be one of the most interesting topics in condensed-matter physics and materials science due to their distinctive properties and promising applications in nanoelectronics and spintronics.

In 2014, a few-layer phosphorene (the 2D counterpart of layered black phosphorus) was successfully fabricated via mechanical exfoliation of bulk black phosphorus [6, 7] and immediately attracted considerable attention [8–15]. Phosphorene has a characteristic puckered structure [see Fig. 1], which leads to a substantial anisotropy of its mechanical behavior [16], electric conductance [6, 9] and optical responses [11], distinguishing it from many other isotropic 2D materials. It has been considered to be an attractive material for nanoelectronic applications due to its high hole mobility: values as high as 984 $\mathrm{cm^2V^{-1}s^{-1}}$ were obtained in few-layer phosphorene field-effect transistor with thickness of ∼10 nm [7], and a theoretical study has estimated that hole mobility along the zigzag direction may reach values in the range of 10,000–26,000 $\mathrm{cm^2V^{-1}s^{-1}}$ for monolayer and 3,000–4,600 $\mathrm{cm^2V^{-1}s^{-1}}$ for five-layer system [9]. Additionally, phosphorene has been observed to exhibit a direct band gap, with optical gaps varying from 1.73 eV for monolayer to 0.83 eV for the trilayer system [17], which makes it interesting for optoelectronic applications since a large portion of the electromagnetic spectra can be covered by varying the number of layers.

Monolayer phosphorene has been theoretically predicted to sustain tensile strain up to 30% along the armchair direction and up to 27% along the zigzag direction [18]; this superior flexibility is attributed to the phosphorene puckered structure and opens an avenue for exploring strain-engineering in this system. For example, first-principles studies have found that the band gap of monolayer phosphorene can be tuned from direct to indirect with compressive strain up to 12% [19, 20] and the prefered mobility direction rotates by 90° under biaxial tensile strain between 3 and 6% [21]. We would like to mention that controllable strain can be applied to 2D materials by (i) bending a flexible substrate: after a 2D material has been deposited and adheres to the planar substrate, it is exposed to uniaxial tensile/compressive strain on the convex/concave side of the bent substrate, and by (ii) piezoelectric stretching: piezoelectric materials can be used to apply biaxial strain to 2D materials [22].

Moreover, strain-engineering in defective phosphorene has also attracted significant interest [23–25] since theoretical studies reported that single- and double-atom vacancies have lower formation energies in monolayer phosphorene when compared with graphene and silicene [26], and the asymmetric single-atom vacancy (SV-5|9), which is the most stable single-vacancy configuration in phosphorene [26, 27], may exhibit non-zero magnetic moment whereas the symmetric single-vacancy (SV-55|66) and the double-atom vacancies have non-magnetic ground state [26–29]. In this paper, we present a comprehensive investigation of the stability and the electronic and mag-

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