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Strain-modulated magnetic behavior in Li-doped WS_2 monolayer

M. Luo[a,*], H.H. Yin[b]

[a] Department of Physics, Shanghai Polytechnic University, Shanghai, 201209, PR China
[b] School of Electronics and Information, Nantong University, Nantong, 226019, PR China

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ABSTRACT

Magnetic properties of Li-doped WS_2 monolayer under strain are investigated by ab initio methods. Without strain, the Li-doped WS_2 monolayer is a magnetic nano material and the total magnetic moment is about 0.99 μ_B. We applied strain to Li-doped WS_2 monolayer from −10% to 10%. The magnetic properties are modified under different strain, the doped system gets a maximum value of 1.89 μ_B at 10% compressive strain and a minimum value of 0 μ_B at −5%. The coupling between 3p states of S and 5d states of W is responsible for the strong strain effect on the magnetic properties. Our studies predict Li-doped WS_2 monolayer under strain to be candidates for application in spintronics.

1. Introduction

Graphene is known as the most studied two-dimensional (2D) materials due to their special properties and potential applications in nanoelectronics and spintronics [1–4]. The impressive progress in graphene research has motivated scientists to explore other 2D materials [5]. Recently, 2D transition-metal dichalcogenides (TMD) have become a hotspot [6–8]. Among the TMD materials, WS_2 and MoS_2 monolayer with a direct band gap configuration have been extensively investigated because of many intriguing physical and chemical properties [9–14].

As is known to all, by doping at a low concentration, transition metal (TM) atoms could verify the magnetic properties of 2D materials and modulate the electronic properties obviously [15]. Monolayer MoS_2 has potential applications in spintronics and nano devices, and the Mn, Fe, Co or Zn doped MoS_2 monolayer are promising material to become 2D dilute magnetic semiconductors (DMS) [16,17]. The structure of WS_2 monolayer is similar to MoS_2 monolayer and previous studies verified that WS_2 monolayer also has superior electronic properties than that of MoS_2 [10,18]. It is possible to change the carrier type in WS_2 by replacing of W by other metal atoms [19]. However, to our knowledge, there is not so much research on the magnetic properties of nonmagnetic metal elements doped WS_2. In addition, strain engineering is another effective and promising method to modify the electronic and magnetic properties of materials [20–23], such as induce and controlling the magnetism in 2D TMD [24–27]. Therefore, these findings motivate us to study the unrevealed magnetic properties of nonmagnetic metal, Li doped WS_2 by applying a strain.

In this paper, we employ ab initio methods and study magnetic properties of Li-doped monolayer WS_2 by low doping concentration (2.08%). It is found that one Li dopant could induce a magnetic moment (0.99 μ_B) without strain. Next, strain

* Corresponding author.
E-mail address: luomin@sspu.edu.cn (M. Luo).

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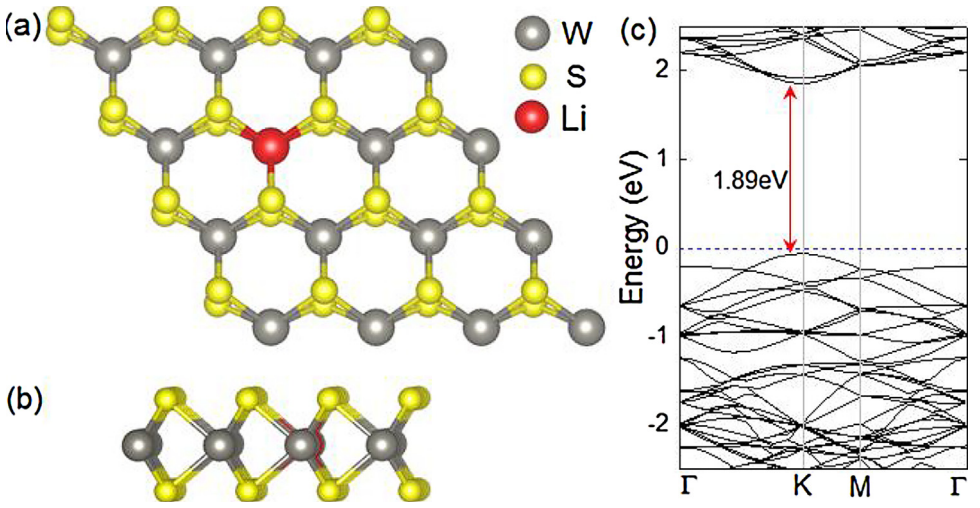

Fig. 1. Schematic structure showing (a) top and (b) side view of $4 \times 4 \times 1$ Li-doped WS_2 monolayer; (c) The band structure of pure $4 \times 4 \times 1$ WS_2 monolayer.

Table 1
The calculated Li—S and W—S bond length, d_{Li-S}, d_{W-S}, magnetic moment $M_{tot}(\mu_B)$, and total energy of doped system E_{tot}, and the formation energy in different experimental conditions E_{form} in Li-doped WS_2.

Strain (%)	d_{Li-S} (Å)	d_{W-S} (Å)	M_{tot} (μ_B)	E_{tot} (eV)	E_{form} (eV)	
					W-rich	S-rich
−10	2.342	2.364	0.0	−341.287	15.674	12.556
−7	2.353	2.376	0.0	−351.876	11.093	10.529
−5	2.384	2.385	0.0	−356.904	7.511	6.106
−3	2.426	2.396	0.88	−360.401	3.718	2.472
0	2.484	2.415	0.99	−363.173	2.641	1.303
3	2.561	2.436	1.06	−363.250	2.977	1.898
5	2.621	2.451	1.07	−362.035	5.995	5.373
7	2.686	2.466	1.24	−359.958	7.604	6.235
10	2.794	2.491	1.89	−355.540	11.042	9.350

effect on the magnetic properties has been studied, ranging from −10% to 10%, and the magnetic moment changes from 0 μ_B to 1.89 μ_B gradually. The magnetic moment gets a maximum of 1.89 μ_B at 10% tensile strain and disappears at the −5% compressive strain. While the strain is applied, the system turns into a narrow-gap (0.13 eV) semiconductor. Our finding might have some motivations in designing new spintronic devices. In this work, we just can give theoretical calculation results and discuss the effect on the magnetism and electronic properties with strain. The larger strain could be achieved in experiments in the future.

2. Method

All calculations are performed with density functional theory (DFT) [28] which are embedded in the soft of the Vienna ab initio simulation package (VASP 5.4). We employed GGA-PBE [29] functional and PAW [30] method, an energy cut off of 450 eV, and $6 \times 6 \times 1$ k-points for geometry optimization are used. The lattice parameter of monolayer WS_2 is about 3.16 Å. The vacuum is 20 Å between adjacent supercells. The convergence of force optimization is set at 0.02 eV/Å.

3. Results and discussions

Firstly, we study the magnetic properties of one Li doped $4 \times 4 \times 1$ WS_2 monolayer and the doping concentration is about 2.08%, as shown in Fig. 1. From our calculations, a magnetic moment of 0.99 μ_B was observed for one-Li-doped system. Then the band structures of pure WS_2 monolayer is given in Fig. 1c. From Fig. 1c, for pure WS_2, the spin-up and spin-down band structures are symmetric, so that there are no magnetism. With the one Li-doped WS_2 monolayer, as shown in Fig. 4c, the impurity states around the Femi level (E_F) in the spin-up and spin-down parts are asymmetric. Hence, the system is magnetic.

Next, we study magnetic properties of Li-WS_2 monolayer by applying strain, ranging from −10% to 10% . Geometric parameters, total magnetic moment (M_{tot}), total energy (E_{tot}) and formation energy (E_{form}), which are listed in Table 1. The formation energy is estimated as $E_{form} = E_{(doped)} - E_{(pure)} + n(\mu_W - \mu_{Li})$, and $E_{(doped)}$ is the energy of Li-doped WS_2 monolayer. $E_{(pure)}$ is the energy of pure WS_2. μ_W and μ_{Li} are the chemical potential of one W atom and one Li dopant, respectively, here