Pis'ma v ZhETF, vol. 106, iss. 10, pp. 644 – 645

Magnetic properties of Na-doped WS_2 monolayer in the presence of isotropic strain

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Submitted 10 October 2017
Resubmitted 18 October 2017

DOI: 10.7868/S0370274X17220106

Since successful preparation of graphene, the study of two-dimensional (2D) crystals has become one of the most rapidly developing areas due to their extraordinary physical and chemical properties with a wide range of promising applications. Recently, 2D transition-metal dichalcogenides (TMD) have aroused enormous research attention. Among the TMD materials, WS_2 monolayer has been extensively investigated because of its novel physical and chemical properties [1–31]. It has been verified that by doping transition metal (TM) atoms into 2D materials at a low concentration could tune the electronic properties obviously. 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 an effective way to modify the electronic and magnetic properties of materials, such as inducing and controlling the magnetism in 2D TMD. Therefore, as shown in Fig. 1a, we study magnetic properties of Na-doped monolayer WS_2 by the first-principles method. As shown in Fig. 1b, it is found that one Na dopant could induce a magnetic moment ($1.07\,\mu_B$) without strain. Next, strain effect on the magnetic properties has been studied, ranging from $-10\,\%$ to $10\,\%$, and the magnetic moment changes from $0\,\mu_B$ to $2.01\,\mu_B$ gradually. The magnetic moment gets a maximum of $2.01\,\mu_B$ at $10\,\%$ tensile strain and disappears at $-10\,\%$ compressive strain. While the strain is applied, the system transforms from indirect semiconductor to a direct narrow-gap (0.13 eV) semiconductor, as shown in Fig. 1c. Our finding might have some motivations in designing new spintronic devices.

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364017220039

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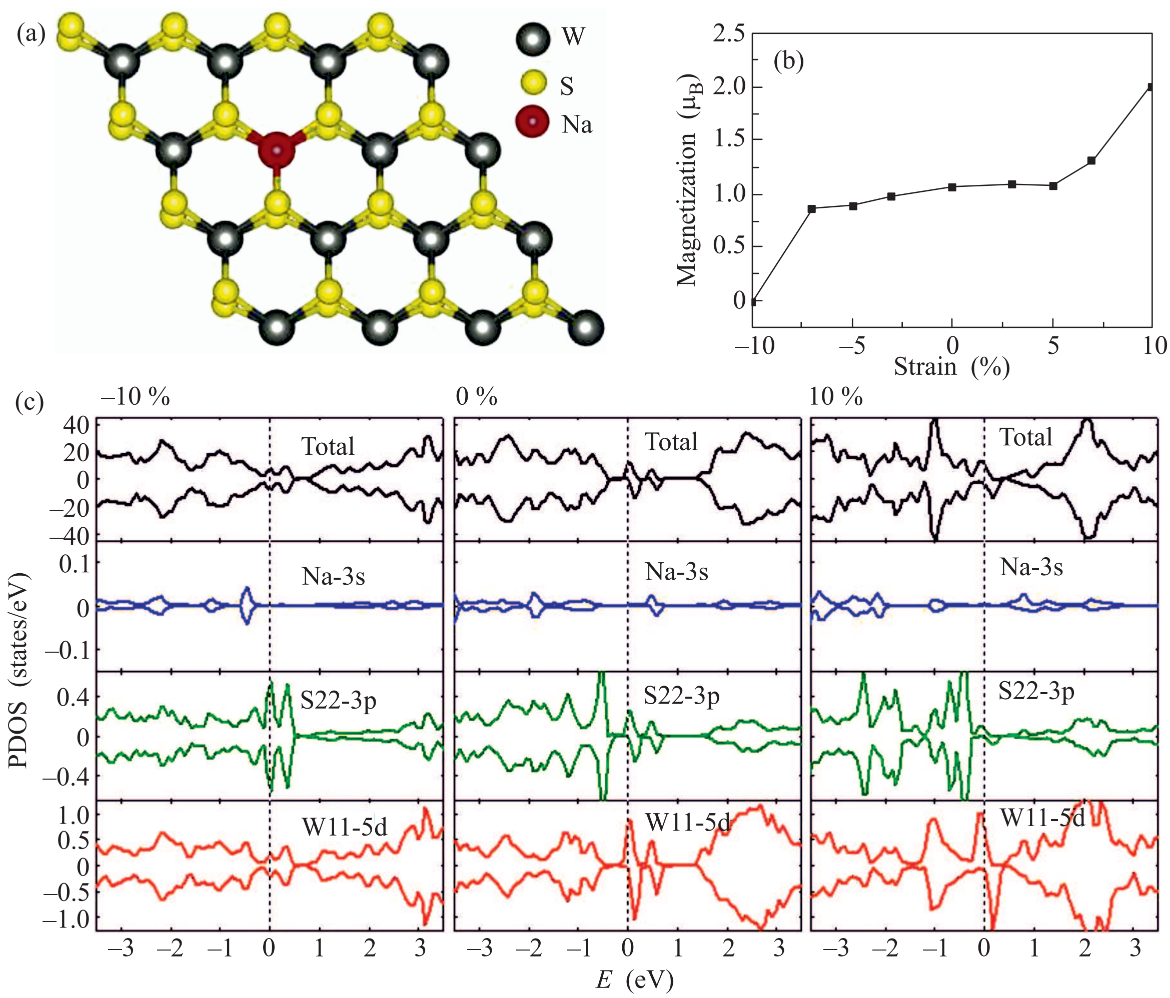

Fig. 1. (Color online) (a) – Top view of Na-doped $4 \times 4 \times 1$ WS_2 monolayer. (b) – Magnetic moment of Na-doped WS_2 monolayer versus strain. (c) – Band structures of Na-doped monolayer WS_2 with isotropic strain –10 %, 0 %, and 10 %, respectively

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