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Semi-metallic bilayer MS_2 (M = W, Mo) induced by Boron, Carbon, and Nitrogen impurities

Mohammed H. Mohammed[a,b,*], Ahmed S. Al-Asadi[a,c], Falah H. Hanoon[b]

[a] Department of Physics, Southern Illinois University Carbondale, Carbondale, IL 62901, United States
[b] Department of Physics, College of Science, Thi Qar University, Nassiriya 64000, Iraq
[c] Department of Physics, College of Education for Pure Science, Basrah University, Basrah 61001, Iraq

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ABSTRACT

We performed the first-principle density functional theory (DFT) calculation to investigate the structural and electronic properties of the bilayer (BL) MS_2 (M = W and Mo) with and without Boron (B), Carbon (C), and Nitrogen (N) impurities (added in the center between the slabs). We used the DFT method, which implemented in the Quantum espresso package, to calculate the electronic band structure, band gap, density of states (DOS), total energy, and chemical potential. In the pristine case, the BL structure of both WS_2 (Tungsten disulfide) and MoS_2 (Molybdenum disulfide) showed indirect electronic bandgap of 1.37 eV and 1.26 eV, respectively. A semimetal behavior with a zero-band gap was detected with (B, C, and N)-doped MoS_2 and (B and N)-doped WS_2 while a direct band gap of ~ 0.1 eV was revealed in the case of C-doped WS_2. The electronic DOS for the BL WS_2 and MoS_2 were also calculated in the present of B, C, and N impurities. These impurities changed the shape and reduced the value of the DOS, which confirmed all the obtained results in this report. The aforementioned outcomes show the possibility of manipulating the structural properties of the MS_2 materials for countless applications related to photo-and gas-sensing devices as well as energy storage related applications.

1. Introduction

Recently, low-dimensional (LD) nanostructures have taken significant attentions of the focus of many researchers owing to their high-performance, tailored geometries as well as high surface-area-to-volume ratios comparing to the bulk counterparts [1–3]. Among many LD nanostructures, scientists are focusing on the two-dimensional (2-D) nanomaterials/nanostructures to fabricate a high performance nano-devices due to their potential in fundamental science researches and applications of engineering [4–7]. Beyond graphene, transition metal dichalcogenides (TMDCs) of MX_2 (M = Mo, W, Pt etc., X = S, Se, Te) have taken a substantial amount of curiosity due to their strongly bonded layer along with a week interlayer what allow to isolate single and/or a few layers of these materials using different experimental methods [8,9]. These single and/or a few layers are different from their bulk counterparts owing to their remarkable structures, mechanical and optical properties along with the ability to engineer the optical band gap. Several of TMDCs (e.g. MoS_2, WSe_2, PtS_2, $PtSe_2$ and WS_2) were studied theoretically and experimentally [10–14] and these studies found out that their electronic band structures depend mostly on the number of X-M-X layers. Layered materials of TMDCs, such as MoS_2, is collected of stacks of sandwiches S-Mo-S layers, which are held together by van der Waals interactions [15–18]. Due to its unique electronic, optical and catalytic properties, single and/or a few layer of MoS_2 were previously used for many potential applications such as SL MoS_2 based-transistor [9], and BL MoS_2 based-photovoltaics catalyst [19,20]. Another rising star of the TMDCs family is WS_2 (stacks of sandwiches S-W-S layers), which is a nonmagnetic semiconductor and also used in various applications, such as a toxic gas sensing, a protein and pH sensing, biochemical devices [5–7] and also to fabricate high performance optoelectronic devices, such as light emitting diodes (LEDs), lasers, optical cavities, and photodetectors [21–26].

The crossover of MX_2 band gap from indirect-to-direct outcomes from local move of valence band hills and conduction band valleys in the Brillouin zone. In particular, it is possible to control the electronic band gap from indirect-to-direct by manipulation the number of the MS_2layers [27].

In addition to the controlling the electronic structure of these materials through the number of layer, many methods such as chemical doping have been successfully utilized to manipulate and improve the electronic properties of the TMDCs in order to overcome the limitations of using these materials in applications related to quantum information

* Corresponding author. Department of Physics, Southern Illinois University, Carbondale, IL 62901, USA.
E-mail address: mohammed1@siu.edu (M.H. Mohammed).

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