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Topological Insulator Behavior of WS_2 Monolayer with Square-octagon Ring Structure

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Abstract. We report electronic behavior of an allotrope of monolayer WS_2 with a square octagon ring structure, refereed to as (so-WS_2) within state-of-the-art density functional theory (DFT) calculations. TheWS_2 monolayer shows semi-metallic characteristics with Dirac-cone like features around Γ. Unlike p-orbital's Dirac-cone in graphene, the Dirac-cone in the so-WS_2 monolayer originates from the d-electrons of the W atom in the lattice. Most interestingly, the spin-orbit interaction associated with d-electrons induce a finite band-gap that results into the metal-semiconductor transition and topological insulator-like behavior in the so-WS_2 monolayer. These characteristics suggest the so-WS_2 monolayer to be a promising candidate for the next-generation electronic and spintronics devices.

Keywords: Monolayer, TMDs, Electronic Structure, DFT , Topological Insulator
PACS: 71.15.-m, 71.20.-b, 73.22.-f, 64.60.-i

INTRODUCTION

Transition metal dichalcogenides (TMDs) monolayers such as MoS_2[1-2] have emerged as most interesting two dimensional (2D) materials due to their unique mechanical, electronic and optical properties that show tunability with external electric field and mechanical strain [3-6]. 2D TMDs generally posses exotic properties in hexagonal (H) and trigonal (T) phase [7-8], however, it has been recently shown that monolayer TMDs can become 2D topological insulators (TIs) when they transform into 1T' structure [9].

Recently, energetically and thermodynamically stable allotrope of monolayer MoS_2 namely *so-MoS_2* has been found to possess graphene-like Dirac cone structure that opens up the possibilities for developing high performance electronic and spintronic devices [10]. Distinct from graphene, monolayer so-MoS_2 possess d-electron Dirac fermions which has Fermi velocity comparable with graphene.

Inspired by the above study, in this paper, we present electronic behavior of so-WS_2 monolayer with and without spin-orbit coupling (SOC) effect, within the state-of-art density functional theory (DFT) based calculations.

COMPUTATIONAL DETAILS

DFT calculations are performed using Projector-Augmented Wave (PAW) pseudopotential implementation of Vienna Ab-initio Simulation Package (VASP)[11]. The electrons exchange and correlation effects are described by generalized gradient approximation (GGA) functional of Perdew-Burke-Ernzerhof (PBE). Kohn-Sham wave functions are expanded in a plane-wave basis set with a kinetic energy cutoff of 400 eV on a (20 × 20 ×1) Monkhorst-Pack grid using Gaussian smearing of 100 meV. A 25 Å vacuum region perpendicular to monolayer is used to overcome the interaction between periodic images.

RESULTS AND DISCUSSIONS

The so-WS_2 monolayer consists of repeated square-octagon (so) rings in a square lattice as shown in

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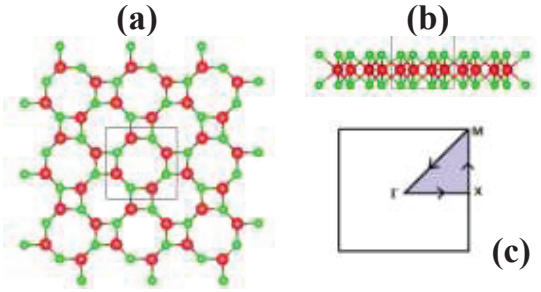

FIGURE 1. Crystal structure of the so-WS_2 monolayer : (a) top view (b) side view. Red circles represent W atoms and green circles represent S atoms. Unit cell is shown by solid lines. (c) The Brillouin zone with high symmetry paths.

Figure 1 (a and b). The primitive cell of so-WS_2 contains four W and eight S atoms in square bravais lattice with *p4* symmetry. Note that most stable phase of WS_2 is hexagonal (H) with *p6m* symmetry that contain one W and two S atoms per primitive cell [3].

Similar to the monolayer H-WS_2 which form six-member ring i.e. hexagons, so-WS_2 can be seen as triatomic layer where W atom is sandwiched between the two S planes to form eight-member ring (Figure 1). Note that eight-member and four-member ring in TMDs are found to posses at the grain boundaries of H-MX_2 monolayers [12].

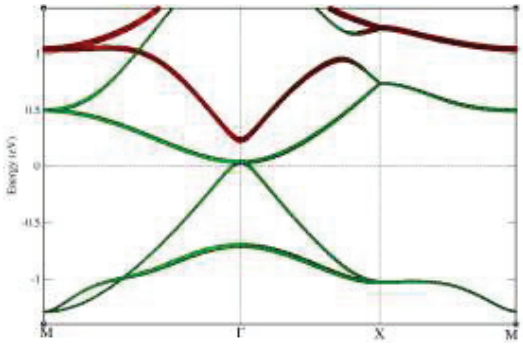

FIGURE 2.Orbitals-resolved electronic band structure of the so-WS_2 monolayer. Red color represents contributions from $d_{x^2-y^2}/d_{xy}$ orbitals and green color represents contributions from d_{z^2} orbitals of W atom. Fermi level is set at 0 eV.

Our calculated lattice constant of the so-WS_2 monolayer is 6.37 Å which is nearly same (6.36 Å) as reported for so-MoS_2 [10]. Despite nearly equal lattice constant, their electronic band structure show distinctly different features in terms of bands dispersion. Note that electronic band structure was calculated along M-Γ-X-M high symmetry directions of a square Brillouin zone [Figure 1(c)]. Valance band maximum (VBM), conduction band minimum (CBM) and CBM+1 are well separated from VBM and CBM

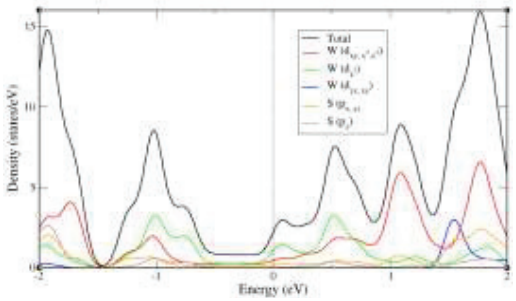

FIGURE 3. Total and partial density of states of the so-WS_2 monolayer. Fermi level is set at 0 eV.

(Figure 2) at Γ, whereas these points meet at a single Dirac point in so-MoS_2 monolayer [10]. However, in both the band structures, semi-metallic characteristics with Dirac-cone like features in VBM and CBM+1 at Γ (Figure 2) is observed.

In the so-WS_2 monolayer, $d_{x^2-y^2}/d_{xy}$ and d_{yz}/d_{xz} orbitals of W are doubly degenerated in energy while d_{z^2} is singly degenerated. VBM is mainly composed of d_{z^2} orbitals of W with small contributions from $d_{x^2-y^2}/d_{xy}$ orbitals, CBM is mainly contributed from d_{z^2} orbitals of W atoms. Similarly, CBM+1 at Γ has primary contributions from $d_{x^2-y^2}/d_{xy}$ orbitals of W atoms. It is found that S atoms and d_{yz}/d_{xz} orbitals of

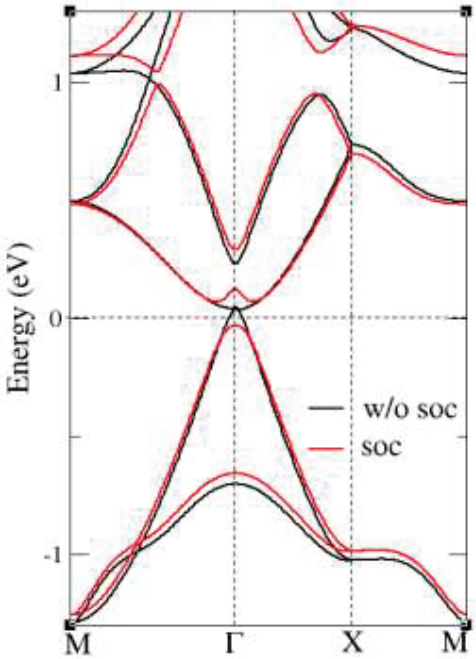

FIGURE 4. Electronic band structure of the so-WS_2 monlayer with and without the spin-orbit coupling (soc) effect.

W have negligible contributions at VBM, CBM and CBM+1 levels. These observations are in line with the so-MoS_2 monolayer [10]. The metallic character of so-WS_2 is also supported by the metallic density of states near Fermi energy (Figure 3). Significant hybridization of S states with d states of W has been found above 1 eV from Fermi level in both valence and conductions bands.

Most interestingly, by turning on the spin-orbit coupling (SOC) effect, VBM and CBM at Γ shifts downward and upward respectively inducing band-gap that results into the metal-semiconductor transition (Figure 4). The SOC-induced band-gap opening strongly suggests the so-WS_2 monolayer to be a two-dimensional topological insulator. The band-gap originates from the strong spin-orbit interactions of the d-electrons of W atoms around the Fermi energy.

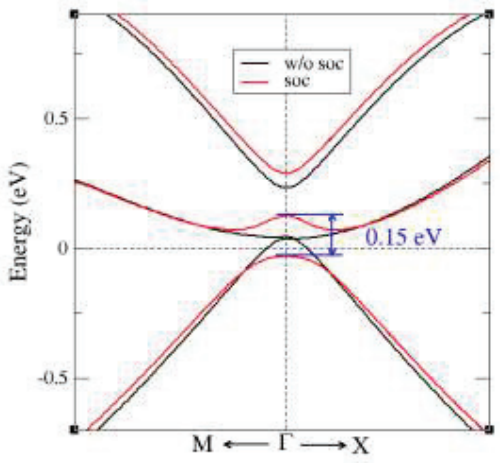

FIGURE 5. Electronic band dispersion and SOC induced band gap in the vicinity of Γ .

The SOC-induced splitting between degenerate bands at Γ results into 150 meV band-gap in the so-WS_2 monolayer (Figure 5). It is found that the SOC effect splits VBM and CBM as large as 65 and 85 meV, respectively at Γ. Similarly, CBM+1 and VBM-1 levels get shifted by 50 and 40 meV, respectively. Conical features at VBM and CBM+1 levels at Γ get flattened (as shown in Figure 5) when we turn on the SOC effects, indicating the existence of heavy fermions at Γ along with massless Dirac fermions in the direction of Γ-X and Γ-M due to linear band dispersions in the Brillouin zone.

CONCLUSIONS

In conclusions, first principles calculations have been performed to investigate the electronic behavior of monolayer WS_2 with the square-octagon ring bravais lattice. The so-WS_2 monolayer is found to be semi-mettalic with Dirac-cone like features around Γ. The SOC effects induced ~ 150 meV band-gap, thereby, suggesting so-WS_2 to be 2D topological insulator. Our study suggests that engineering the lattice of WS_2 and other 2D TMDs may found promising applications in the area of spintronics, photonics and high performance electronics.

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