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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, referred to as (so-WS$_2$) within state-of-the-art density functional theory (DFT) calculations. The WS$_2$ monolayer shows semi-metallic characteristics with Dirac-cone like features around $\Gamma$. 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

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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 possess 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-the-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
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 $d_{z^2}/d_{xz}$ orbitals of W are doubly degenerated in energy while $d_{z^2}$ is singly degenerated. VBM is mainly composed of $d_{x^2}$ 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 $d_{y^2}/d_{xz}$ orbitals of...
W have negligible contributions at VBM, CBM and CBM+1 levels. These observations are in line with the so-MoS2 monolayer [10]. The metallic character of so-WS2 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 conduction 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-WS2 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](image.png)

**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-WS2 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 WS2 with the square-octagon ring bravais lattice. The so-WS2 monolayer is found to be semi-metallic with Dirac-cone like features around Γ. The SOC effects induced ~ 150 meV band-gap, thereby, suggesting so-WS2 to be 2D topological insulator. Our study suggests that engineering the lattice of WS2 and other 2D TMDs may find promising applications in the area of spintronics, photonics and high performance electronics.

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**REFERENCES**