Comprehensive analysis of 3D & 2D model of MoS_2

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Abstract

Analysing MoS_2 using DFT calculations provides a good approximation to experimental data [Reference to experimental data here!!!]. Looking at both bulk and thinlayer MoS_2, it was discovered that the bandstructures for these two structures differed quite a lot. Where the bulk MoS_2 gave a indirect band gap and the thinlayer MoS_2, showed a direct bandgap. BLABLABLA

Checklist

1 Work on either MoS_2- Molybdenum disulfide or WS_2 tungsten disulfide. Both of which have the same crystal structure so-called isotypic and is classified as transition metal dichalcogenide. The primitive unit cell of WS2 consists of one tungsten atom and two sulphur atoms, arranged in a trigonal prismatic configuration. Valleytronics (from valley and electronics) is an experimental area in semiconductors that exploits local minima ("valleys") in the electronic band structure.

* **Properties of MoS_2**

  bulk properties of MoS_2. MoS2 occurs naturally as the mineral 'molybdenite'. In its bulk form, it appears as a dark, shiny solid. The weak interlayer interactions allow sheets to easily slide over one another, so it is often used as a lubricant. It can also be used as an alternative to graphite in high-vacuum applications, but it does have a lower maximum operating temperature than graphite. Bulk MoS2 is a semiconductor with an **indirect bandgap** of 1.2eV, and is therefore of limited interest to the optoelectronics industry.
  In the case of MoS2, the spin splitting in conduction band is in the meV range, it is expected to be more pronounced in other material like WS2.

  Thinlayer properties of MoS_2
  Individual layers of MoS2 have radically different properties compared to the bulk. Removing interlayer interactions and confining electrons into a single plane results in the formation of a **direct bandgap**

* **Properties of WS_2**

  The monolayer film possesses a direct bandgap of 2.1 eV.

2 Relax the crystal structure, submit job and find total energy as lattice parameter a is altered. Use birch_murnaghan.py to fit these points into a E(a) plot, where minimum energy corresponds to the favored lattice constant for a system at equallibrium. Another interesting thing one may do, is to check when total energy is converged, as well as k-points.

3

4 tail -n 20 OUTCAR- Last 20 lines in OUTCAR, Total CPU-time is displayed here.

I. Introduction

Molybdenum sulfides has a so-called isotypic crystal structure and is classified as transition metal dichalcogenide. In this paper, one will investigate both bulk and monolayer structures of MoS_2 2H. This kind of arrangement of molybdenum sulfide is trigonal prismatic, which means that the sulfides is arranged in a symmetric order above and underneath the molybdenum atom.

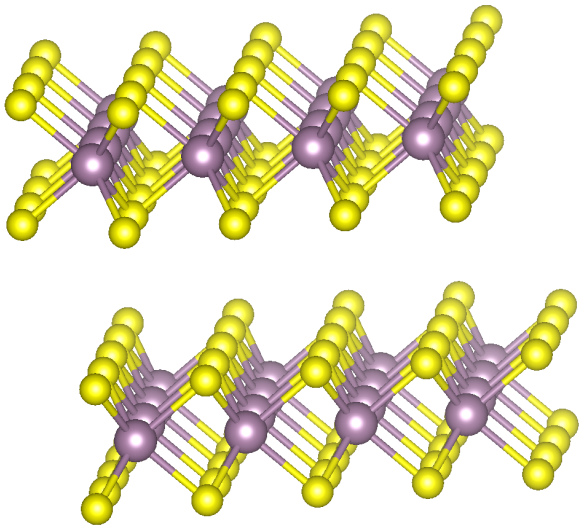

Figure 1: Illustration of the bulk MoS_2 2H. Where the yellow illustrates the sulfides and purple molybdenum atoms

MoS_2 occurs naturally in nature as molybdenite. in its bulk form, as we will investigate, it appears as a dark, shiny solid. The bulk layer sheets is held up by weak Van der Waals forces. These forces is the holding stone of the bulk solid. In bulk form it is often used as a lubricant, due to its weak interlayer forces. As for the thinlayer MoS_2, we extrapolate the layer of the bulk MoS_2. We will investigate which properties that change as we go from bulk to thinlayer film. By looking at density of states for both systems and investigating the bandstructures. Further more when analysing MoS_2, we will use standardize self-consistent calculation method in which the Hartree Fock method is applied. We will After that investigate the increase in accuracy when doing vasp calculations with HSE06 hybrid functional.

II. Method

III. Implementation

IV. Numerical results

V. Discussion

VI. Conclusion