TWO-DIMENSIONAL MoS_2

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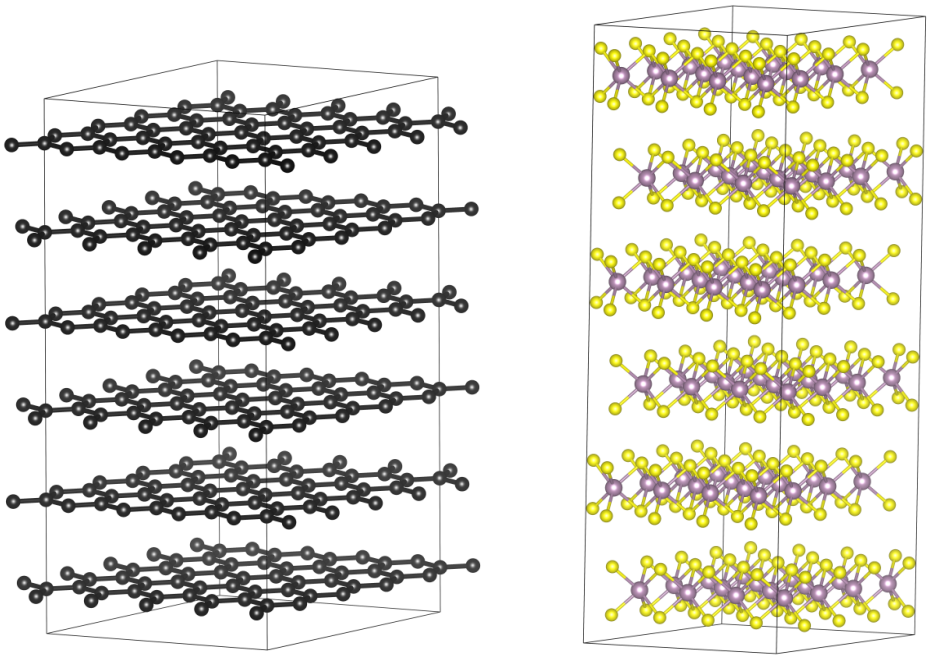
Contents

1 Introduction

Currently semiconductors are the basis of the technologies, within this wide group we can find novel materials as the bidemensional materials [1]. This types of crystal are composed of single or few atoms (very thin). A example is graphene, which is one atom thickness and a bandgap of 0 eV, graphene is widely study since it have wonderful properties. Other materials that belong to this wide family is the black phosporous and the Molybdenum disulfide (MoS_2).
In this work the material to study will be the bidimensional MoS_2. The crystal structure, electronic bands and electrical properties will be studied, as well as its synthesis and some applications.

2 MoS_2: Description

Similar to graphene, which is obtained from graphite. The monolayer MoS_2 is obtained from the bulk MoS_2 (Figure 1).



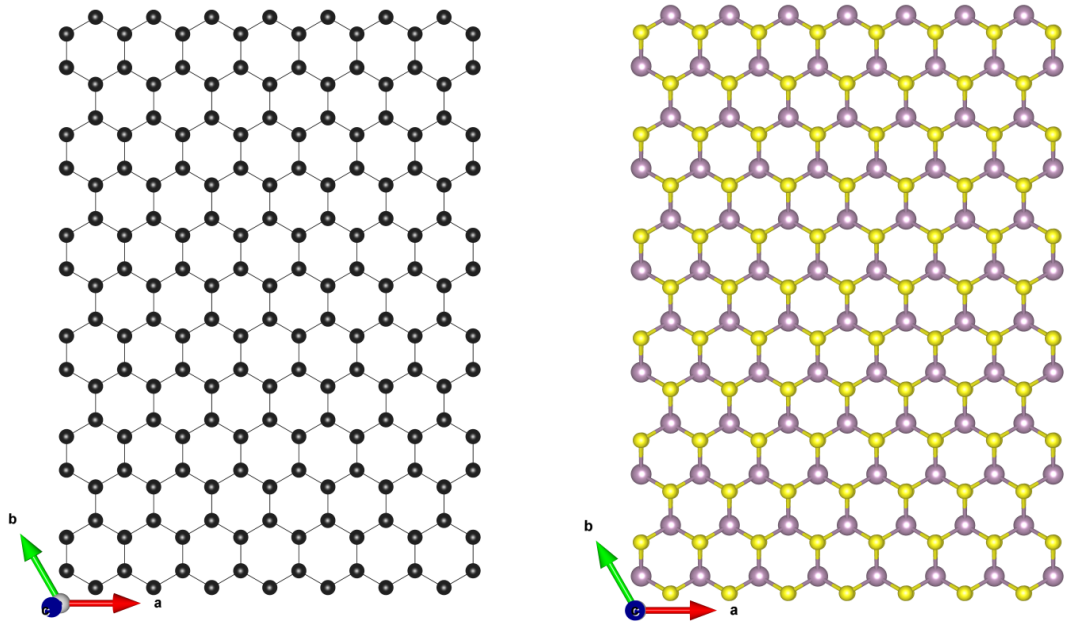
(a) Graphite (b) Bulk MoS_2

Figure 1: Both materials are composed of monolayers. The purple atoms are molybdenum and the yellow ones are sulfur.

2.1 Crystal estructure

This material is a transition-metal dichalcogenide and is composed by two types of atoms, molybdenum (Mo) and sulfur (S). Each atom have different electronic configuration, sulfur atoms have $1s^2 2s^2 2p^6 3s^2 3p^4$, while the molybdeum atoms have $[Ar]3d^5 4s^1$. Both atoms have 6 valence electrons.

At first glance it may seem that the crystal structure of MoS_2 is similar to the graphene, but that's not the case (Figure 2).



(a) Graphene (b) Monolayer MoS_2

Figure 2: Comparation.

The difference is in the thickness (Figure 3). Graphene only have one atom thickness, while monolayer MoS_2 consist of a sandwich structure (Figure 4).

(a) Graphene (b) Monolayer MoS_2

Figure 3: Thickness in both materials.

where each sublayer is a hexagonal lattice.

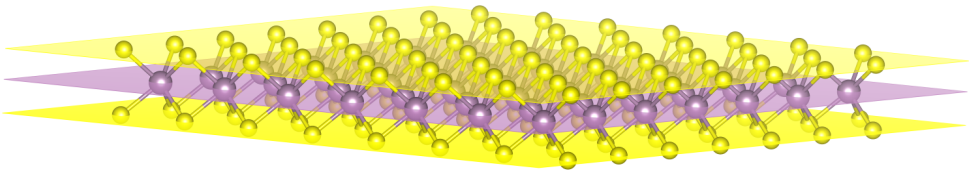


Figure 4: Sandwich structure.

2.2 Lattice parameters

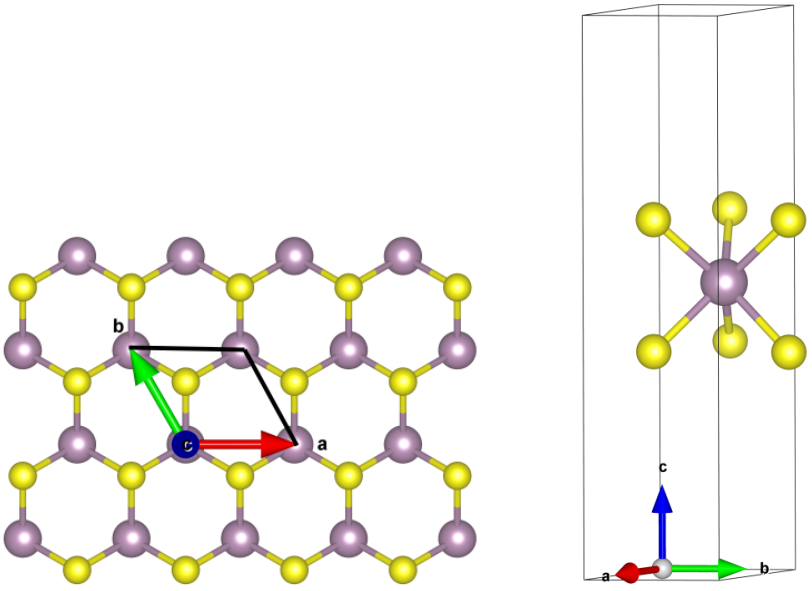
The primitive vectors (Figure 5) are given by:

$$\vec{a}_1 = a(1,0) \;\; , \;\; \vec{a}_2 = a\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \tag{1}$$

where the lattice parameters for the primitive cell is given by Table 1.

Table 1: Lattice parameters

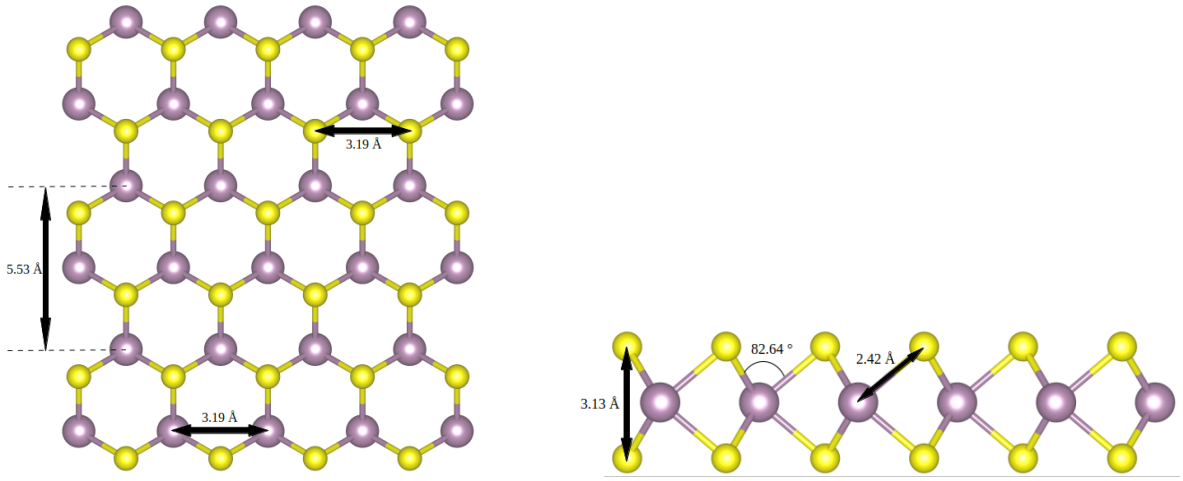
Constants (Å)	Angles	Volume (Å^3)
a = 3.19	$\alpha = 90°$	118.07
b = 3.19	$\beta = 90°$	
c = 13.37	$\gamma = 120°$	



(a) Primitive vectors (b) Primitive cell

Figure 5: Lattice in the real space.

It is also possible to obtained information about the lattice constants from different points of view (Figure 6).

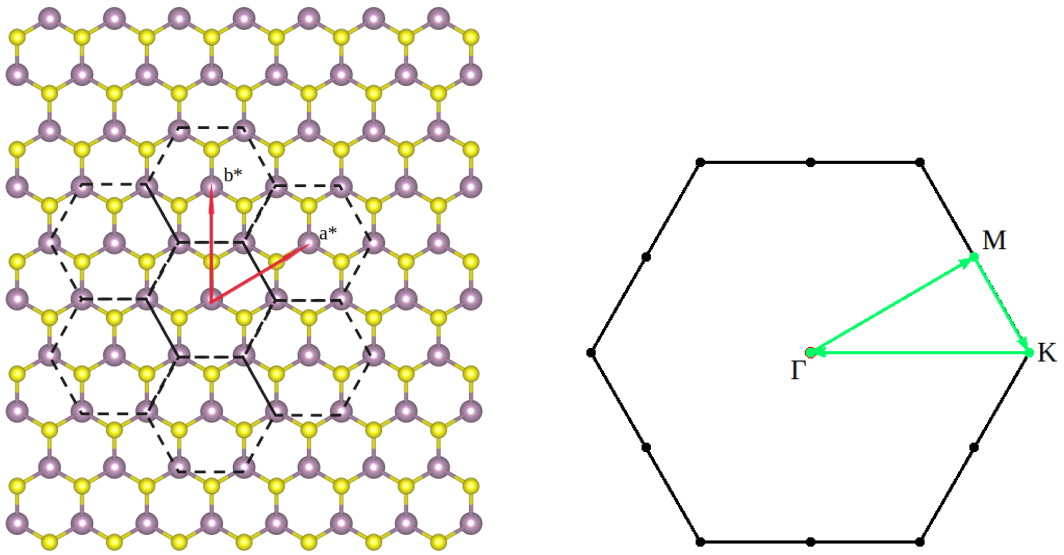


(a) Top view (b) Lateral view

Figure 6: Lattice constants.

For the reciprocal space (Figure 7), we can see that the primitive vectors are given by:

$$a^* = \vec{b}_1 = \frac{4\pi}{\sqrt{3}a}\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \quad , \quad b^* = \vec{b}_2 = \frac{4\pi}{\sqrt{3}a}(0,1) \tag{2}$$



(a) Primitive vectors for reciprocal lattice (b) Path in first Brillouin zone

Figure 7: Lattice in reciprocal space.

Paths for different structures have a standard definition [2].

3 Electronic properties

The structure was build using the bulk MoS_2 from The materials project [3]. For this section will be used the density functional theory (DFT), the calculations will be perform with VASP software.

You can find the steps for this calculations in the repository. Herein the calculations were performed with PBE pseudopotential.

3.1 Density of states (DOS)

In the DOS plot (Figure 8), the bandgap for MoS_2 is 1.86 eV.

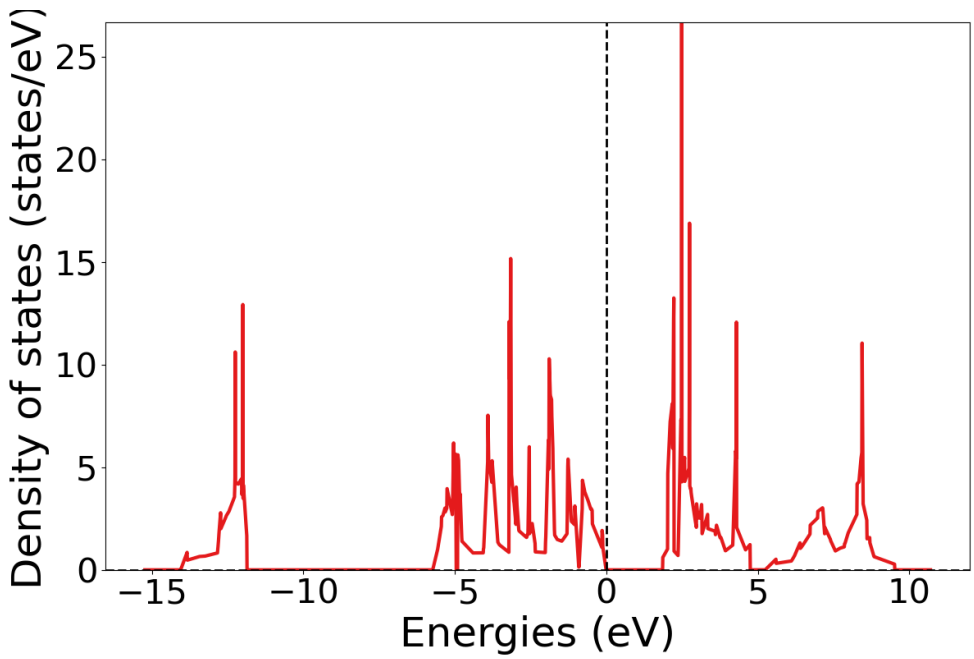


Figure 8: DOS for the monolayer MoS_2.

3.2 Band structure (spaghetti diagram)

Unlike bulk MoS_2, which have an indirect bandgap. The monolayer MoS_2 have a direct bandgap in K (Figure 9).

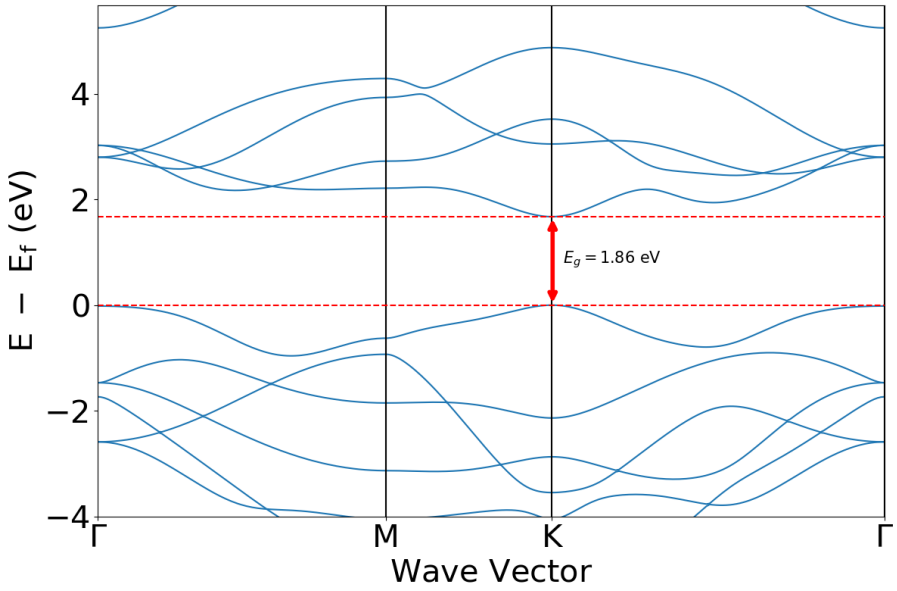


Figure 9: Band structure for the monolayer MoS_2.

From the Figure 9, it might appear that the maximum energy of the valence band occurs in Γ, but that's not the case. If we zoom the image, we can see that the maximum energy of the valence band occurs in K (Figure 10).

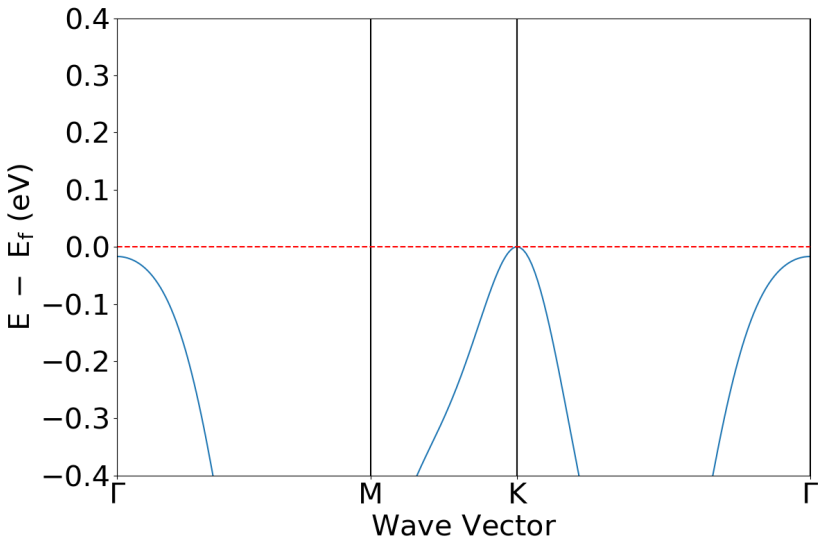


Figure 10: Zoom in the band structure.

This bandgap value is a good calculation compare with the literature [4], [5], [6] and [7]. Experimentally the bandgap reported is 1.90 eV from [8] and [9].

The figures of the structure crystal, the calculations and other details can be to find in Bidimen-

dional MoS2.

4 Electrical properties

The electrical properties usually are studied with the Hall effect in semiconductors. Hall effect help us to find information about the conductivity, mobility, resistivity and carrier concentration in the material.

Field-effect transistors (FETs) of monolayer MoS2 have demonstrated a high on/off current ratio exceeding 10^8 and the electron mobility of at least 200 cm^2/Vs at room temperature.

For this reason the FETs are important devices for study the properties in the material (Figure 11).

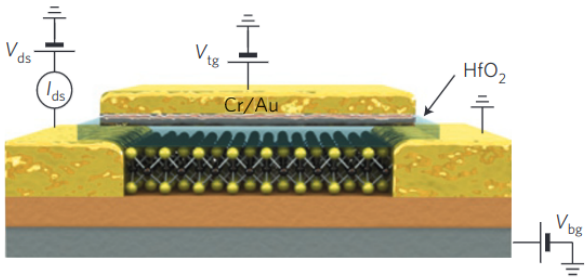
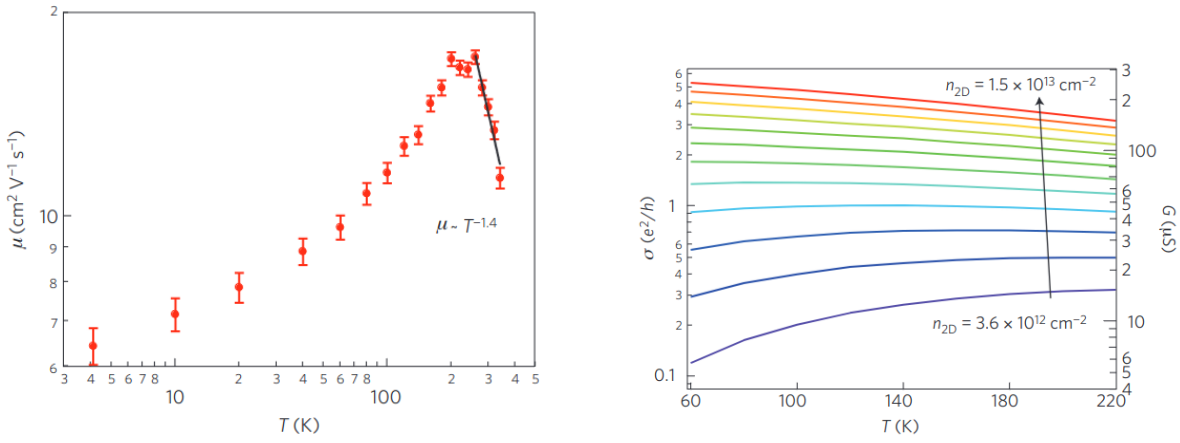


Figure 11: Measurement scheme in a FET. Taken from Radisavljevic and Kis, 2013 [10].

From this circuit is obtained results for the electron mobility and conductivity.



(a) Electron mobility

(b) Conductivity

Figure 12: Electrical properties as a function of temperature. Taken from Radisavljevic and Kis, 2013 [10].

The Figure 12 (a) shows us the importance of the charged impurities and how affect the electron transport. Here the mobility is obtained from the conductance. On the other hand, the Figure 12 (b) show the evolution of conductivity for different values of charge carrier density (n_{2D}).

5 Synthesis

Similarly to graphene, monolayer MoS_2 can be obtained from micromechanical exfoliation (using scotch-tape). This technique is possible due to the weak Van der Waals bonds between the layers in the bulk MoS_2.

Others more sophisticated techniques will be shown below with a brief description:

- **Liquid phase exfoliation:** For apply this technique, we must to start by using the bulk MoS_2. The exfoliation can perform shearing, stirring, grinding and bubbling using chemical compound. For example for generate bubbles we can use the electrolysis. The advantage of this technique is that it is cheap, but the quantities obtained are of low quality.
- **Solution chemical process:** For this technique is possible to used different methods, two common methods are the hydrothermal and solvothermal synthesis. Basically in both methods is mixed molybdate with sulfide or sulfur (chemical reaction) under high temperature and pressure for a very long time. The resulting compound is powder with different shapes. Under others conditions is possible to get powders or thin films, this depends of the precursor (chemical compound). For synthesize MoS_2, the MoO_x (precursor) reacts with H_2S under high temperature [11].
- **Chemical vapor deposition:** This technique is applied in thin and thick layers [5]. Precursors like H_2S or S are used in gas phase for pass over the Mo, which generate large areas of growth.
- **Metalorganic chemical vapor deposition:** This technique is a special case from Chemical vapor deposition. Herein it is put in a separate section because is of vital importance nowadays for production of single crystal expitaxial films. The main idea is similar to the Chemical vapor deposition with the difference that use organometallic precursors.
- **Atomic layer deposition:** This technique, similar to Chemical vapor deposition, is used for get thin and thick layers. The advantage is that monolayers can be obtained with very

few impurities. Most impurities are removed using an inert gas after using the precursors (H_2S or S) in gas phase.

6 Applications

Since is a semiconductor material, it can have applications in many areas like photodetectors, solar cells or field-effect transistors (FETs).

The most interesting application are the FETs. Its wide bandgap allow it to compete with the silicon in FETs applications since it have large ON/OFF current ratio exceeding 10^8. Usually this kind of devices are development for use in operational amplifiers in analogue circuits.

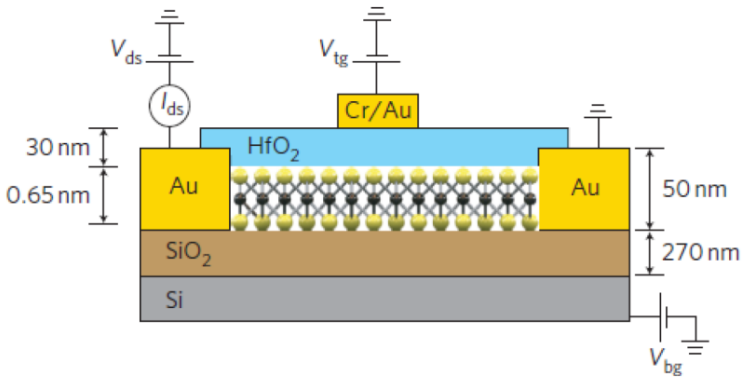


Figure 13: Scheme of a FET using monolayer MoS_2. Taken from Radisavljevic et al., 2011 [12].

From the Figure 13, we can see the monolayer on the substrates of SiO_2 and Si. It also used a gold source and drain. For this case the monolayer MoS_2 was obtained with atomic layer deposition technique.

The photodetectors also was development for use in x-ray imaging devices, since it had a fast response. Besides it consumes a low amount of energy. It also can be used in nonvolatile memory applications.

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