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The Structure, Scope and Potential of the Layered Two Dimensional Transition Metal Dichalcogenide: MoS_2

Ashish Sharma[1] and Charu Madhu[2]

[1,2]University Institute of Engineering and Technology Panjab University, Chandigarh
E-mail: [1]ashishsharma.5790@gmail.com, [2]charu_uiet@pu.ac.in

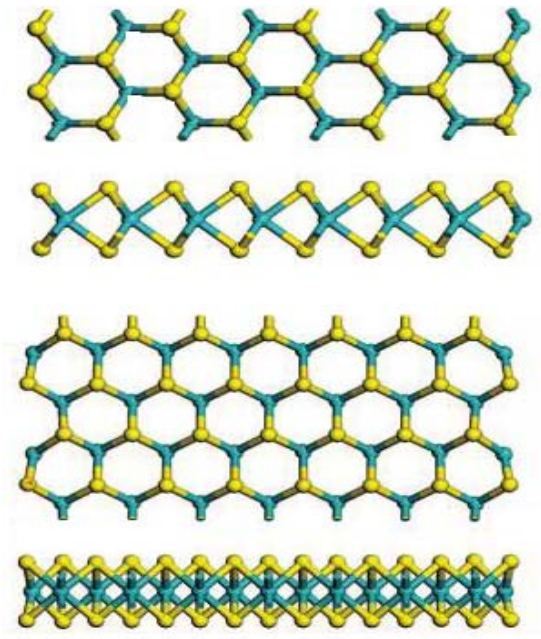
Abstract—*MoS_2 is a new two – dimensional (2D) material which is an extensively researched substance after the super material graphene. Physically it is like a black silver rock similar to graphene It has a layered structure due to which the size of the material can be reduced upto a single layer and being layered its structural integrity is even better than the steel. The layered structure also provides its applicability in the curved screens and panels. The optical reactivity of MoS_2 also changes with number of layers as the luminescence quantum efficiency is dependent over the number of layers. The main reason behind so much of research is not only because of its 2D structure but also many other distinguishable properties like metallic, semiconducting, mechanical strength, optical etc. The most striking benefit of MoS_2 over graphene is that it has a band gap which is a function of the number of layers, which implies that we can tune the energy gap as per the need, as it ranges from direct to indirect. Being electrically active MoS_2 can be used as a gate material in the transistor which can further increase the transistor density over the chip. Before getting into the semiconducting research MoS_2 was used in the lubricants and in the oil refining for the desulphurisation. But due to these electrical and other properties, MoS_2 is proved to be very flexible in many applications like electronics, nanotechnology, sensing, oil refining, chemical etc. In this review we will discuss about the structure, characterisation and its applications.*

1. INTRODUCTION

MoS_2 is a one of the Transition Metal Dichalcogenides (TMD). TMD's are compounds of transition element (Molybdenum (Mo), Tungsten (W)) and elements from chalcogens (Sulphur (S), Selenium (Se), Tellurium (Te)). The research on the 2D materials in the electronics field is going on, from decades but Geim and Novoselov revolutionised it by their work using graphene[1]. They find the simplest and the cheapest method to get the few layers of layered materials by using a simple scotch tape, for which they the noble prize in 2010. Theoretically it is performed by using the density functional theory (DFT), that MoS_2 has the property of spin and valley polarisation due to its more than one conduction and valence band extremes in the momentum space[2]. Valley polarisation can provide a new way for the data to embed in a memory at atomic level [3]. MoS_2 is used as a catalyst for hydrodesulphurisation for removing the sulphur from the oil. Experimentally it is proved that MoS_2 is stable at the temperature of 500°C and at a pressure of 23 GPa [4]. Where as H.Peelaers and C.G. Vander Wall has done the DFT calculations to prove it stable for 35 GPa[5]. MoS_2 is used for the hydrogen evolution reaction (HER) where the catalytic activity of hydrogen evolution is altered by the number of layers of the MoS_2[6]. Recently it is reported that the photoluminescence showed by the few layered structure of MoS_2 increases as number of layers decreases which is mainly connected with its transition from indirect band gap in bulk to the direct band gap in single layer[7]. MoS_2 nanoribbons can also offer a cathode for rechargeable magnesium (Mg) batteries by the adsorption of Mg over the MoS_2 edges[8]. MoS_2 on the surface of PMMA shows high carrier mobility of 470 cm^2/Vs to 480cm^2/Vs with the thickness of 50 nm[9]. The MoS_2 nanoribbons can be characterised as armchair and zigzag as shown in Fig. 1, the former have a direct band gap with non magnetic nature where as the latter was found to be ferromagnetic[10]. Various atoms can easily be attached on the edges with the sulphur or at the sites with the defects where one sulphur atom is attached with only two molybdenum atoms which is different from the usual. In this paper we present the structure, various properties of MoS_2 and the advancement in the research fields where MoS_2 is used.

2. MOLECULAR STRUCTURE

MoS_2 is a 2D layered structure [1-8] with one molybdenum layer covered with two sulphur layers covalently, whereas the many MoS_2 layers are stacked over each other by Vander Waal forces to form a bulk material. In its structure one molybdenum atom is covalently attached with six sulphur atoms and one sulphur atom is attached with three molybdenum atoms, however the scenario is not the same at the edges. At the edges the sulphur atoms are attached with two molybdenum atoms hence leading to an active site for the other atoms to get adsorbed on the surface.



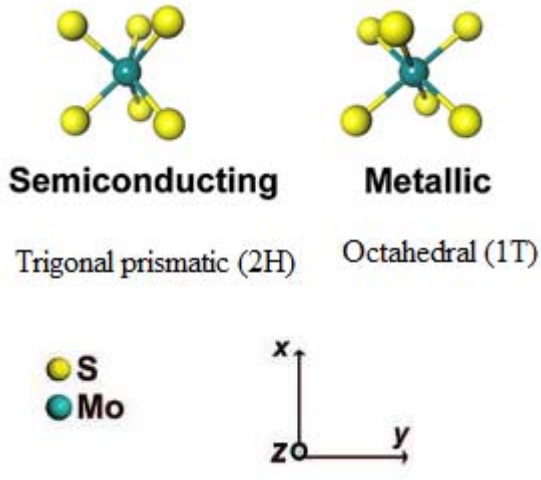
(a)

Fig. 1: (a) The metallic and magnetic zigzag structure of MoS_2 (b) The semiconducting and non-magnetic armchair structure of MoS_2 with top and side view [17].

The extent of adsorption can be increased by creating the defects, reducing the number of layers and even reducing the size of the layers. Adsorption of the element not only depends on these factors but largely on the binding energy [10].

$$E_{binding} = E_{MoS2} + E_{adatom} - E_{MoS2 + adatom}$$

MoS_2 exists in two forms namely as 2H commonly known as trigonal prismatic and 1T which is called as octahedral. The latter is metallic where as the former is a semiconducting most of the research interest as shown in Fig. 2



(b)

Fig. 2: The two forms in which MOS_2 exists as trigonal prismatic (2H) and Octahedral (1T).

The bond length of Mo-S in the crystal structure is 2.4 Å, lattice constant is 3.2 Å and the distance between two sulphur layers is 3.1Å [11, 14]. Being a layered structure the mechanical strength of MoS_2 is greater than steel [12]. The crystal structure of bulk MoS_2 have D_{6h} point group symmetry where as a single layer MoS_2 have D_{3h} point group symmetry [11-12, 14]. The D_{6h} shows inversion symmetry where as D_{3h} does not show inversion symmetry [11, 14]. So it can be characterised using optical second harmonic microscopy.

The layers of MoS_2 stack over each other by the vander wall forces in two ways which we call as AA stacking and AB stacking as shown below in the figure.

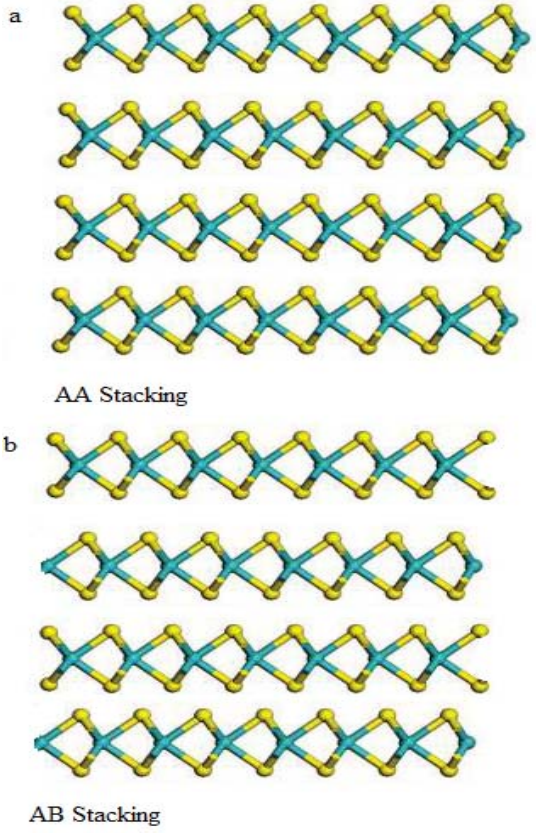


Fig. 3: (a) AA stacking where two layers overlapping are symmetrical to each other. (b) AB stacking where the overlapping layers are asymmetrical[17].

3. BANDSTRUCTURE

One of the most distinguishable property of MoS_2 is having a tuneable band gap, which can be tuned by many ways i.e. by doping, changing number of layers. MoS_2 exhibits a direct band gap of 1.2 eV in the bulk form and an indirect band gap of 1.9 eV in single layer[11,13,15]. So the energy band gap is the function of the number of layers. As the number of layers increases the indirect band gap gets the transition towards the direct band gap i.e. the valence band maxima aligns with the conduction band minima at the Γ-point. This transition in the

material's band gap ensures the interlayer interaction has a great role in determining in band gap of the material[11].

Qihang Liu et. al demonstrated the change in the bandstructure of a bilayer MoS_2 layer in 5 different conformations regarding the arrangement of atoms under the influence of a vertical electric field, which clearly shows a decrease in the energy gap as the electric field is increased[16]. Not only the electric field but the band gap can be altered by inducing strain (as MoS_2 has high young's modulus) over the material as described by Hui Pan and Yong-Wei Zhang[18]. The change in the energy gap with the increase in the number of layers as well as the distance between the two layers in the ABAB confirmation is shown by Tinashu Li and Giulia Galli1[15].

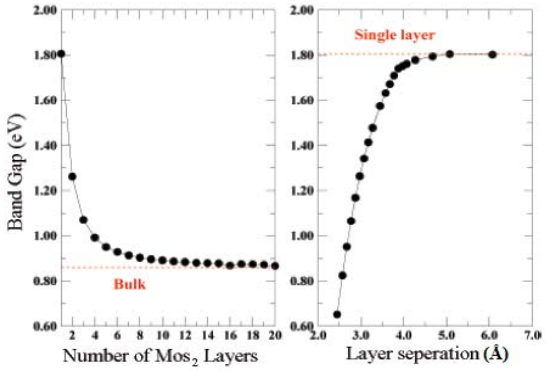


Fig. 4: The decrease in the band gap as number of layers are increased and increase in the band gap by increasing the separation between the two layers[15].

4. CHARACTERISATIONS

The various ways of characterising MoS_2 are described here. The fourier transform infrared spectrum (FTIR) shown by MoS_2 is shown in the Fig. 5[19]. The dispersions of MoS_2 in various solvents for the comparison is done and the peaks of Mo-S bond at 380 cm^{-1} and 478 cm^{-1} are also observed[20].

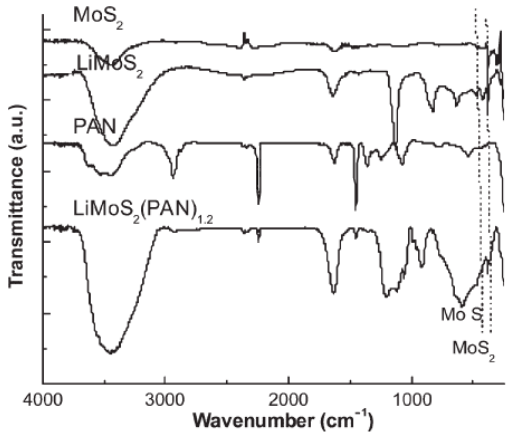


Fig. 5: The FTIR of MoS_2, lithium intercalated MoS_2, Polyacrylonitrile (PAN) and co-intercalated nanocomposite $LiMoS_2(PAN)_{1.2}$[19].

In comparison to ultra violet – visible spectrum of MoS_2 shows clear and significant peaks at 614 nm and 674 nm[21-23] in various dispersions. These two are the characteristic peaks of 2D MoS_2[21]. The absorbance of MoS_2 in the dispersion depends on the concentration of material in the dispersion which depends on many factors like ultrasonic intensities, duration for sonication, method adopted for exfoliation from the bulk, temperature conditions etc. Among the various oil based solvents the maximum solubility shown by MoS_2 is in NMP (N-Methyl Pyrrolidone)[22].

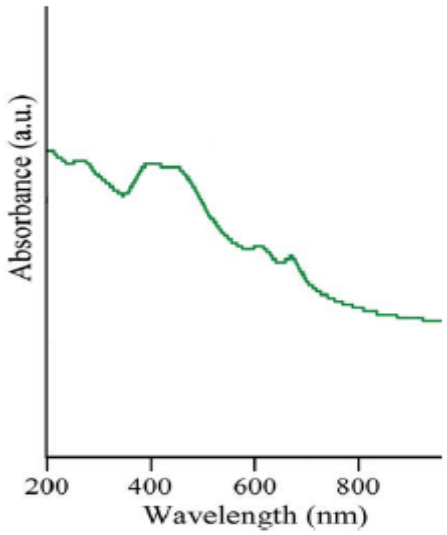


Fig. 6: The UV-Vis spectrum of MoS_2[23]

Another promising method to characterise a material is Raman spectrum. As shown in the Fig. the two peaks of vibration modes A_{1g} and E^1_{2g} are sensitive to number of layers, hence it can be used to get detect the number of layers formed after the exfoliation of the bulk[23,25,26].

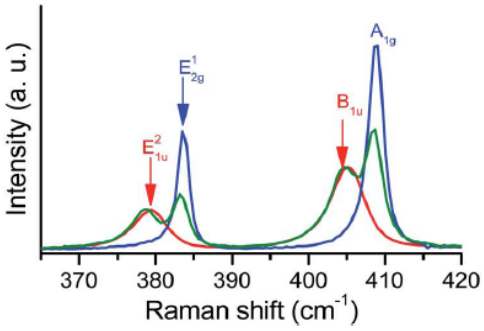


Fig. 7: The phonon vibration modes shown in basal plane (blue), on edges (green) and material exfoliated in Tween 80 (red)[23].

The other two phonon modes i.e. E^2_{1u} and B_{1u} arises when there is a defect in the structure of the material and are then visible in the Raman spectrum[23].

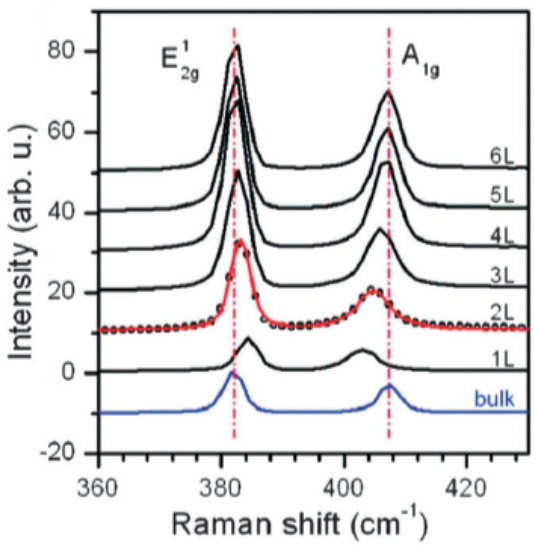


Fig. 8: The Raman spectrum of bulk and some layers of MoS_2 with prominent peaks of E^1_{2g} and A_{1g} vibration modes[24].

5. APPLICATIONS

MoS_2 was used as a catalyst in hydrodesuphurisation in the purification of oil as well as for the hydrogen evolution in the industries from a very long time. MoS2 is used as a gate material in the transistors, as it is immune to the short channel effects if we compare it with the conventional MOSFET, so we can reduce the channel length to a considerable value[27, 28]. MoS_2 is sensitive to most of the spectrum of light which makes it useful in the optical as well as optoelectronic devices[7, 26, 29]. We can not only alter its electronics ability but also can change its magnetic moment by inducing strain into it[18]. But the stand alone feature of MoS_2 is its ability to tune the band gap and an appreciable energy gap as a semiconductor which opens up so many ways to use it in the applications like sensing, switching, memory devices, nano electronics and many more. MoS_2 is now not just a lubricating material anymore, it is about to revolutionise the research many fields.

6. CONCLUSION

MoS_2 has given promising results in various fields due to its versatile properties. To exploit these properties the essential point of research is to make the flakes of MoS_2 of the thickness of few nanometres in large quantities. The biggest challenge is to produce an effective synthesis method for the purpose.

Being semiconducting the most important use is as a gate in transistors which will significantly reduce the channel width without any short channel effects, which can result into higher transistor density on a chip. The possibility of valley and spin polarisation in the material opens the gate towards the new optoelectronic devices.

The hetrostructures of MoS_2 with other 2D materials enhance the existing properties of the material. MoS_2 will become a building block in the ultrathin, ultra small, and power efficient devices in near future.

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