Transition metal dichalcogenides based 2 D materials: Structure properties and applications-A Review

Manukrishna V R
Assistant Professor
Electronics and Communication Engineering Department
Cochin University College of Engineering, Alappuzha, India

Abstract: The 2D materials can exhibit fascinating and technologically useful properties. This article review the state of art of 2D materials beyond grapheme. This category includes mainly Transition Metal Dichalcogenides (TMDs) (e.g. MoS_2, WS_2, $MoSe_2$, and WSe_2) which can provide different immense applications in the areas of Nano electronics, photonics, sensing, energy storage, and opto-electronics This article briefly discuss the structure, properties and applications of TMD based 2 D materials.

***Index Terms* – 2 D materials, Nano electronics, Transition Metal Dichalcogenides (TMDs)**

I. Introduction

The interest in transition metal halide based 2D materials is driven by the study of low dimensional physics and the design of functional heterostructures. They can be represented as MX2 and MX_3 where *M* is a metal citation and *X* is a halogen anion often form such structures.2D materials made of single atom or single polyhedral layer can be grouped into various categories. The first category consists of atomically flat Vander walls solids like graphene TMD's etc. The second category is made of ionic solid formed by sandwiching polyhedral layer and halide or hydroxide. Surface-assisted Nano layered solids such as silicene, germanene etc forms the third category. This paper limited the discussion to category 1 due to it wide range of applications in Nano electronics and photon ics. The rapid increase in research activities [1] on 2D materials is reflected in the number of publications in last 1 decade as indicated in Fig (1).The remaining section of the paper is organized as follows. Section 2 describes the structure of TMD material. Section 3 deals with the properties and section 4 deals with applications of 2 D materials. The section 5 is conclusion and 6 is references

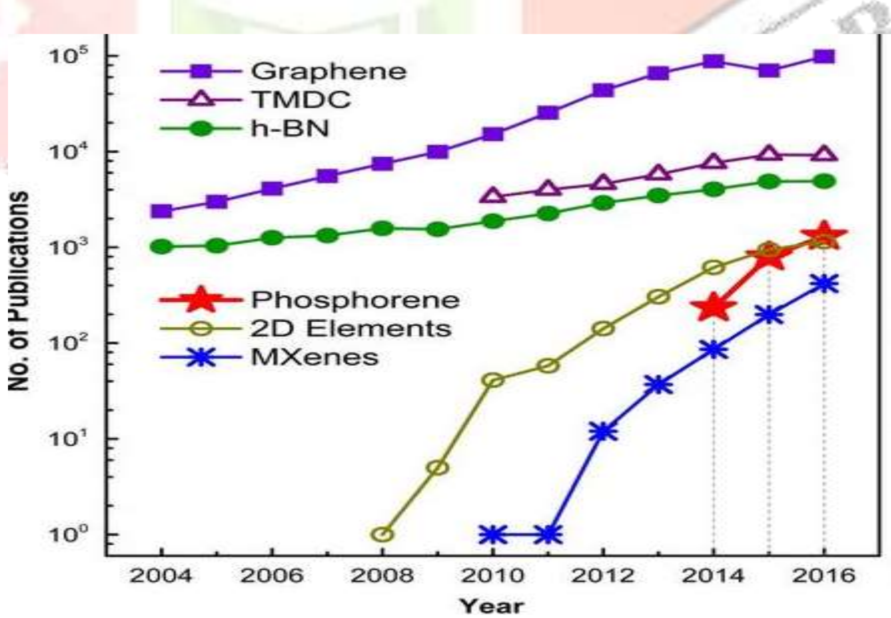

Fig-1:year wise publication of articles on 2 D materials(adapted from [1])

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II. CRYSTAL STRUCTURE

Molybdenum Disulfide (MoS2) belongs to the group of TMDC materials denoted by MX2, where M may be a transition metal element of group IV (Ti, Zr, Hf), group V (V, Nb, Ta), or group VI (Mo, W), and X is a chalcogen (S, Se, Te). These materials can make layered structures of the form X–M–X, with the chalcogen atoms in two hexagonal planes separated by a plane of transition metal atoms [2].The properties of crystal can be explained based on the structure of crystal. The TM monolayers can be fabricated by a three step process which involves Exfoliation, Chemical vapour depositation and Epitaxy.The structure of primitive cell of Tungsten sellinede is given in Fig 2

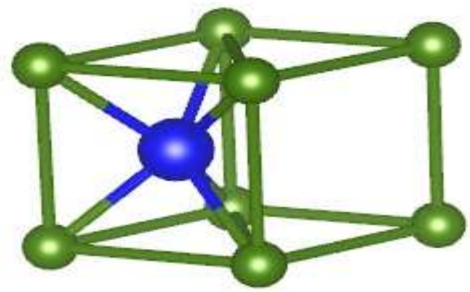

Fig-2:Crystal structure of WSe2(adapted source[2])

If the structure has even number of mono layers, then it has an inversion at the center. If the number of monolayers is odd no inversion at the center. Due to this structure the crystal exhibits non linear behavior. If it is excited by laser the frequency of the output doubled. Second phenomenon to be noticed in the structure is it has electronic band structure with direct band gap. This features indicate that TMD can explore spin and valley physics with numerous optical and electronic applications.

III. PROPERTIES

Mechanical properties: Mechanical properties is estimated on the basis of Young's modulus.The measurement is conducted on suspended monolayer membrane of MoS_2.Measurements shows that the tensile strengths of the material is comparable with that of stainless steel. This property enables single layer MoS_2 for nano mechanical applications and multilayer MoS_2 in multilayer transistors.[7]

Electronic properties:

One of the key requirement of basic electronic devices like field effect transistor is the ability to turn on and off by applying suitable voltage at gate. The schematic drawing of energy band of bulk MoS_2 and monolayer MoS_2 is shown in the figure 3(a) and 3(b) below[7].

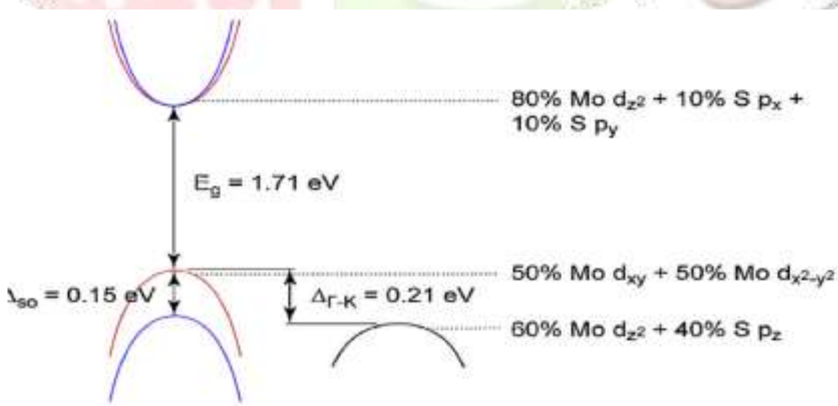

Fig 3(a) Energy gap of bulk MoS_2 [7]

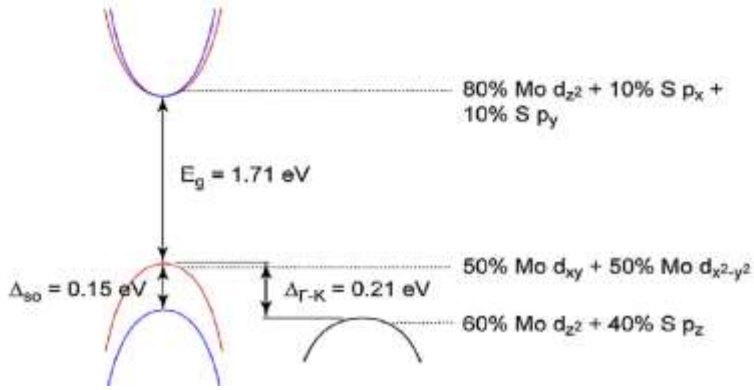

Fig 3(b) Energy gap of monolayer MoS_2 [7]

Table -1 showing the electronic properties of commonly used Mo and W based TMD's[7][8]

1.

Metal	Halide	2 D material	Band gap (ev)	properties
Mo	S	MoS_2	1.67	Semiconducting
Mo	Se	$MoSe_2$	1.44	Semiconducting
Mo	Te	$MoTe_2$	1.07	Semi metallic
W	S	WS_2	1.81	Semiconducting
W	Se	WSe_2	1.55	Semiconducting
W	Te	WTe_2	1.06	Semi metallic

Values are calculated using calculated from first principles using density functional theory (DFT) within the generalized gradient approximation (GGA)[7]

Optical Properties: The band gap of bulk TMD material down to a thickness of two monolayers is still indirect, so the emission efficiency is lower compared to monolayered materials. The emission efficiency is about 10^4greater for TMD monolayer than for bulk material [6]. The band gaps of TMD monolayers are in the visible range (between 400 nm and 700 nm). The direct emission shows two transitions called A and B, separated by the spin-orbit coupling energy[7]. Owing to their direct band gap, TMD monolayers are promising materials for optoelectronics applications. Multilayer MoS_2 show higher photoresponsivities enables them for making phototransistors.[8]

Transport Properties: The transport property is described on the basis of mobility.Graphene have very high mobility but the zero band gap property limits its application in FET's and switches.The TMD structurs have mobility comparable to that of silicon. High carrier mobility, high on/off ratio and small thickness (one monolayer) of TMD devices are potentially interesting for such applications.

IV. APPLICATIONS:

Graphene as well as MoS2 exhibits remarkably unique and diverse range of properties.Due to this the hybrids of graphene and MoS2 are currently the focus of many research groups across the globe. Highlight of top priority application is given in the given section.

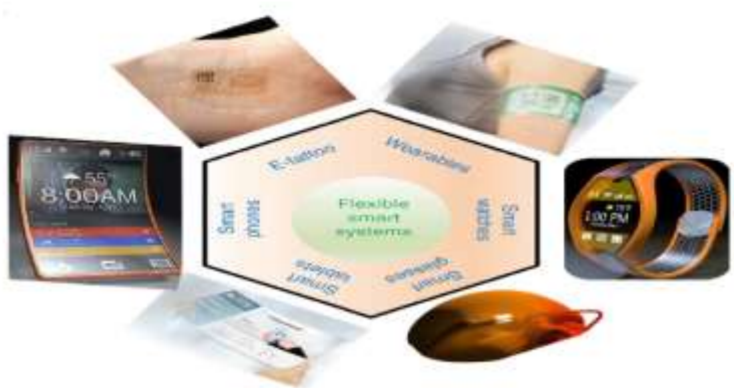

Fig 4-Application of 2 D materials

Electronic Applications: Owing to its excellent semiconducting properties with a direct bandgap of 1.83 eV, single-layer MoS2 nanosheets are used for fabricating low power electronic devices.The performance of FET fabricated using MoS_2 is almost double compared to that of conventional FET.[8]If we use multi-layered structures instead of single layer we get added advantage[10].This MoS_2 based FET's can be integrated to form different logic gates, Random access memory and oscillators.

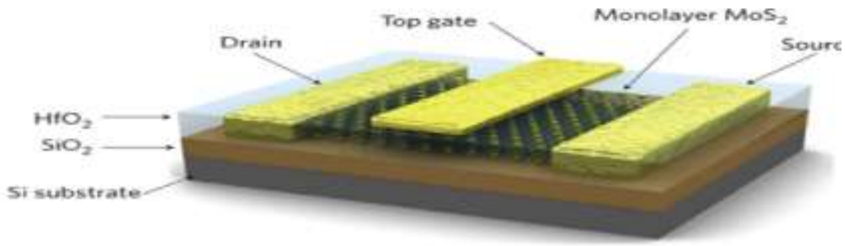

Fig 5:Schematic view of MoS_2 based FET[10]

Optoelectronic Applications:

2D materials also provide an enormous scope to study the fundamental principles of light absorption and emission in atomically thin materials with the ultimate goal to realize high performance optoelectronic devices like light emitting diodes (LEDs), photo detectors, lasers, and optical cavities, among others. MoS_2 have thickness dependent band gap. Recently a single layer MoS_2 based photo transistor having excellent ON OFF ratio and mobility of 0.11 $cm^2/V\,S$ has been invented.1.65 eV band gap photo transistors are used for green light detection and 1.35 eV band gap photo transistors are used for red-light detection.MoS_2 is also used for the fabrication of LED's.[8]

Rechargeable batteries:

Rechargeable batteries are very popular in portable electronic devices.Graphene and TMD structures can be used as anode of rechargeable batteries. If we use grapheme there is a chance of occurring aggregation problem. So to avoid this, we use TMD structures as anode. For improving stability, graphene is hybridized by electrochemically similar material to form composite electrode.They have higher current density and specific capacity[7].

Super capacitors:

Super capacitors are next generation energy storage devices. Supercapacitor requires electrode material with better surface area and electrical conductivity ,Present experiments shows that .graphene is a right candidate for it. They have high energy density and power density and are used in portable electronic devices. Since MoS2 have low intrinsic conductivity, they are not widely used. To make electron transport faster To get better conductivity super capacitor electrodes can be prepared by directly bonding layered MoS_2 on GO substrate.[7]

Gas Sensors:

Chemical, biological and gas sensors utilizing FET-device structures. The change in resistance of FET channel allows them detection. Single and multi-layered MoS_2 Nano sheets are used for making sensors for NO detection. Single layer usually gives unstable response. Sensing capability can be increased by functionalization of MoS_2 with Pt nano particles.[8]

V. CONCLUSION

The emergence of 2D materials has led to increased attention on correlating the structural, optical, and optoelectronic properties of thin MoS2 layers In this paper we discussed about the structure, properties and application of TMD based 2 D materials. Advancement in the main themes of this review_theory, synthesis, characterization, and devices will continue be as we move forward in 2D materials science and technology

VI. REFRENCES

[1] Akhtar, M., Anderson, G., Zhao, R., Alruqi, A., Mroczkowska, J.E., Sumanasekera, G. and Jasinski, J.B., 2017. Recent advances in synthesis, properties, and applications of phosphorene. *npj 2D Materials and Applications*, *1*(1), p.5.

[2] Transition metal dichalcogenide monolayers-wikiwind.

[3] *Kumar, N.; Najmaei, S.; Cui, Q.; Ceballos, F.; Ajayan, P.; Lou, J.; Zhao, H. (2013). "Second harmonic microscopy of monolayer MoS_2". Physical Review B.* ***87*** *(16). arXiv:1302.3935v2*

[4] Malard, L. M.; Alencar, T. V.; Barboza, A. P. M.; Mak, K. F.; De Paula, A. M. (2013). "Observation of intense second harmonic generation from MoS_2 atomic crystals". *Physical Review B*. **87** (20).

[5] Malard, L. M.; Alencar, T. V.; Barboza, A. P. M.; Mak, K. F.; De Paula, A. M. (2013). "Observation of intense second harmonic generation from MoS_2 atomic crystals". *Physical Review B*. **87** (20).

[6] Malard, L. M.; Alencar, T. V.; Barboza, A. P. M.; Mak, K. F.; De Paula, A. M. (2013). "Observation of intense second harmonic generation from MoS_2 atomic crystals". *Physical Review B*. **87** (20).

[7] Yazyev, O.V. and Kis, A., 2015. MoS2 and semiconductors in the flatland. *Materials Today*, *18*(1), pp.20-30.

[8] Han, S.A., Bhatia, R. and Kim, S.W., 2015. Synthesis, properties and potential applications of two-dimensional transition metal dichalcogenides. *Nano Convergence*, *2*(1), p.17.

[9] Radisavljevic, B.; Radenovic, A.; Brivio, J.; Giacometti, V.; Kis, A. (2011). "Single-layer MoS_2transistors". *Nature Nanotechnology*. **6** (3)

[10] Li, X. and Zhu, H., 2015. Two-dimensional MoS 2: Properties, preparation, and applications. *Journal of Materiomics*, *1*(1), pp.33-44.