CHAPTER 1

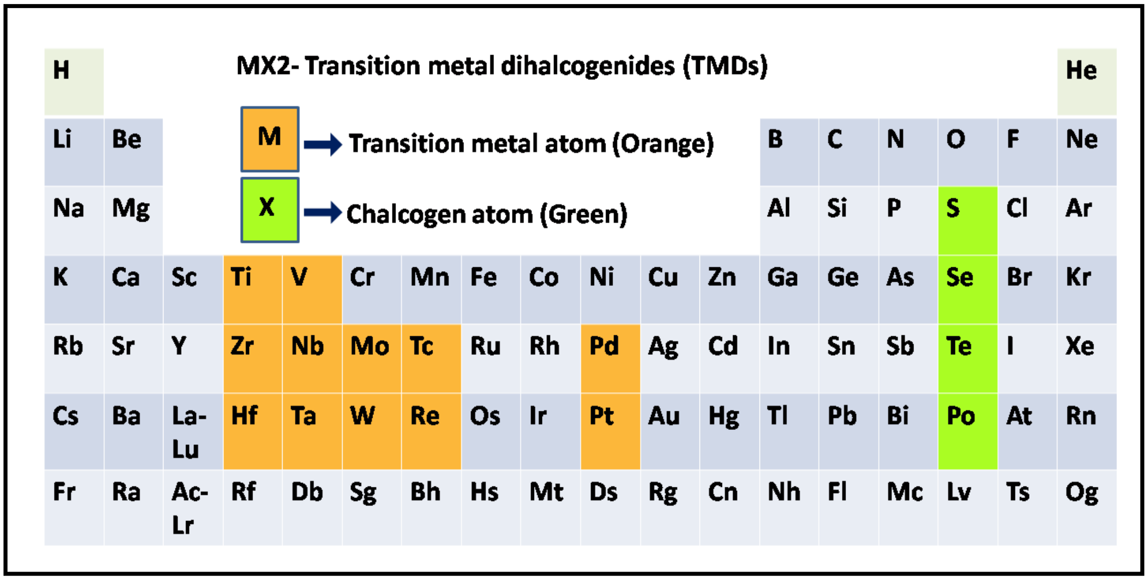
Introduction

1 Introduction

The discovery of two dimensional (2D) inorganic transition metal dichalcogenides (TMDs) and their compounds changed the scenario of electronic and optoelectronic applications in the last few decades. In comparison the semi metallic nature of graphene (2D graphene was prepared using a unique method by Andre Geim and Konstantin Novoselov in 2004 and later they were jointly awarded the Nobel prize in physics in 2010 “for groundbreaking experiments regarding the 2D material graphene”) restricts its application in many potential areas due to its zero band gap energy. This led the researchers to think about other stable 2D materials which have semiconducting nature for the various applications in demand at that time. TMDs were found to be a suitable type of semiconductor (SC) having layered structure like graphene. The layered structure of this inorganic semiconductor gives the opportunity to synthesize few components of devices used in the field of optoelectronics and electronics which are a few layers to even monolayer thickness. Since then, extensive study of TMDs became an attractive area for researchers working in various areas of applications like solid dry lubricants, active components for batteries, photovoltaic (PV) cells, catalysts and superconducting materials, etc. In 2015, Chiya et al. reported on various applications of TMDs such as hydrogen gas evolution, oxygen reduction, flexible solid state capacitors, etc. and the electrochemistry behind these applications [1]. The area of application of TMDs is so broad and diversified that it is very difficult to cover all in a small volume of literature. In this introductory chapter, we will discuss TMD materials, their basic properties and their various applications briefly in the light of reported literature.

1.1 Transition metal dichalcogenides

Chalcogens are chemical elements in group 16 of the periodic table. However, oxygen is treated separately, sometimes even excluded from the chalcogen family because of its very different chemical behavior from other chalcogen elements like sulfur (S), tellurium (Te), selenium (Se) and radioactive polonium (Po). The word chalcogen is derived from the Greek word *khalkós*, principally meaning copper and the Latinized Greek word *genēs*, meaning born. Chalcogenides are chemical compounds having at least one chalcogen



MX2- Transition metal dihalcogenides (TMDs)

M → Transition metal atom (Orange)

X → Chalcogen atom (Green)

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La-Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

Figure 1.1 Figure shows the position of the elements forming TMDs in the modern periodic table.

anion and at least one or more electropositive element. In TMDs the cation is a transition metal ion covalently bound with the chalcogen anion. The general formula that represents TMDs is MX_2 where M is transition metal, e.g. Mo, W, Nb, Hf, V, Ta, Ti, Zr, etc and X is chalcogen atom [2-5]. TMDs have X-M-X layered structure where each layer is attracted by an adjacent layer through Van der Waals force of attraction. The elements in the periodic table forming TMDs are shown in figure 1.1. The main difference between graphene and TMD is that graphene has semi metallic nature having zero band gap (BG) while TMDs are SCs which have a finite BG energy [6-9]. Initially, TMDs, especially MoS_2 and WS_2, were used as dry lubricants due to its slippery nature and robustness [10, 11]. But because of this finite BG, TMDs were further extensively applied in electronics and optoelectronics and many other industrial applications. TMDs are considered as the successor of graphene and inorganic graphene analogues.

1.2 Basic properties of TMDs

1.2.1 Physical structure of TMDs

TMDs are layered structure material and each layer can slip over one another with little external force applied to it. Like graphene, bulk TMDs can be cleaved mechanically, using simple scotch tape, to form atomically thin monolayer [12, 13]. Although, the interaction amongst the atoms within each layer is very strong and the structure is not easily breakable, the weak van der Waals interlayer interaction in TMDs make them slippery and these are, therefore, used as solid and dry lubricant in different machinery appliances [10, 11, 14, 15, 16]. The utilization of MoS_2 as a dry lubricant was extensively done since early 20th century [17]. TMDs basically exist as two stable structures, namely, hexagonal and rhombohedral [3, 5, 18, 19]. MoS_2 and WS_2 generally exist as hexagonal structures. Figure 1.2 shows the basic crystal structure of MX_2 family. In TMDs the metal atom exists in octahedral coordination in a 1T structure and in trigonal prismatic coordination in two layers per unit cell of a 2H structure and three layers per unit cell of a 3R crystal structure as shown in figure 1.2 [1, 3, 20-24]. In monolayer TMDs, the metal atom are sandwiched between chalcogen atoms forming 2D honeycomb structure and generally exist as 1T and 1H structures [24].

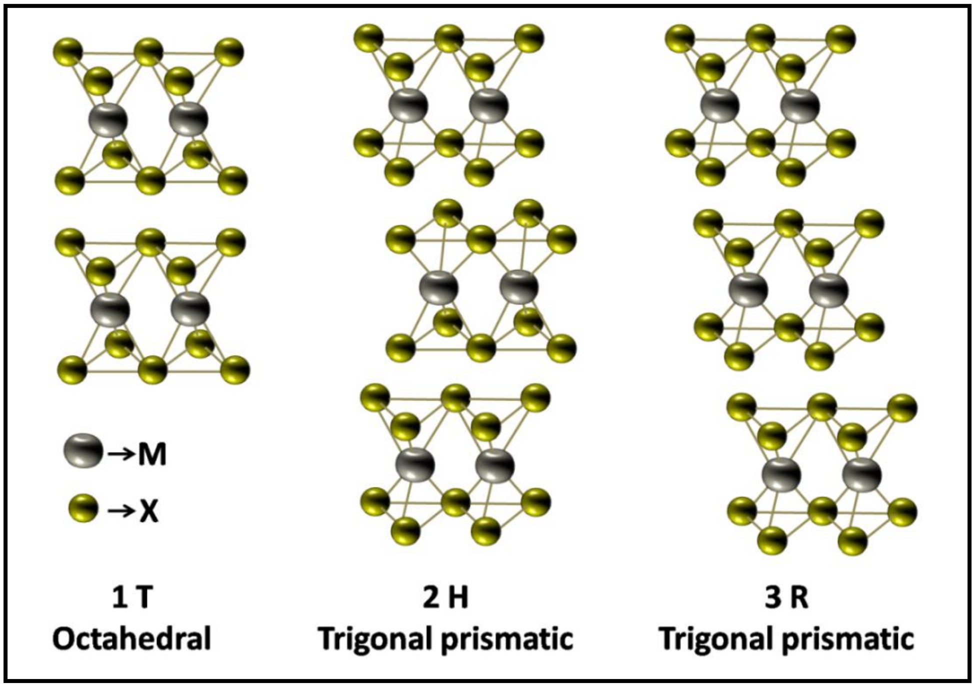


Figure 1.2 Figure shows 1T, 2H and 3R structures of 2D MoS_2. Many other 2D TMDs like WS_2 also exist as these similar structures.

1.2.2 Semi conducting nature of TMDs

The basic property for which TMDs drew constant attention since the last few decades was that TMDs behaved as SCs, unlike graphene. These 2D inorganic materials with finite electronic BG proved to be extremely useful for energy harnessing related research. Among all TMDs, MoS_2 and WS_2 have been studied upon extensively over the decades by researchers of different fields with great attention and enthusiasm. Many researchers have reported that the electronic BG of MoS_2 and WS_2 depends on the thickness of layers, which means that the BG of TMDs is tunable by controlling the layer thickness or dimension of the material [6, 20, 25-28]. The BG of bulk MoS_2 is reported to be 1.29eV while monolayer has BG equal to 1.9eV [2, 6, 23, 28]. Bulk WS_2 has an intrinsic BG of approximately 1.3eV and its monolayer has BG of 2.05eV [8, 28, 29]. Similarly, $MoSe_2$, WSe_2, $MoTe_2$ and WTe_2 in bulk have BG of 1.09eV, 1.20eV, 1.0eV and 0.81eV respectively and as monolayer have BG of 1.58eV, 1.61eV, 1.23eV and 1.18eV respectively [28, 29]. It has been reported that many TMDs such as MoS_2, WS_2, $MoSe_2$, WSe_2 etc. have direct BG in monolayer thickness [2, 6, 8, 20, 25-30]. Due to the presence of such tunable energy BGs, TMD materials have been widely used in electronics, optoelectronics and industrial applications.

1.2.3 Optical properties of TMDs

The presence of a broad range of optical BGs in 2D MX_2 monolayer and their strong light-matter interactions make the TMD a promising and exciting material for novel optoelectronic and PV applications [29]. There is good absorption of light from ultraviolet(UV) to visible range by the TMD materials. Using absorption studies, photoluminescence (PL), and photoconductivity spectroscopy, Mak, K.F. et al., in 2010, reported that with decreasing thickness, there occurred a shift in energy by more than 0.6eV in upward direction in the indirect BG, which lies inside the direct BG of bulk MoS_2 and this leads to a cross over from indirect to a direct-gap material in monolayer MoS_2 [6] . They also reported that monolayer MoS_2 emits light strongly, exhibiting an increase in luminescence quantum efficiency by more than a factor of 10^4, compared with the bulk material [6]. Simillarly, Splendiani, A. et al. have reported the PL property of an ultrathin layer of MoS_2. They found a surprising increase of PL with decreasing layer thickness and observed the strongest luminescence in the MoS_2 monolayer [31]. B. Radisavljevic and few other researchers reported of the fabrication of monolayer MoS_2 transistor with HfO_2 as a gate dielectric engineered by Atomic layer deposition (ALD) and obtaining high mobility (200cm^2/V/s) and substantial ON/OFF current ratio in their device [32]. M. Shanmugam and his colleagues investigated hybrid bulk heterojunction (BJH) solar cells and they employed MoS_2 nanoflakes as a photon harvesting layer with TiO_2 as an electron acceptor and poly3-hexylthiophene (P3HT) as hole conductor. The BHJ solar cell having a stacked structure of ITO/TiO_2/MoS_2/P3HT/Au showed a short circuit current density of 4.7 mA/cm^2, open circuit voltage of 560 mV, and photoconversion efficiency of 1.3 % under an illumination of 100mW/cm^2 [33]**.** Britnell, et al., made a heterostructure of 2D TMDs sandwiched between highly conducting transparent graphene that leads to enhanced photon absorption and creation of exciton pairs. They have, thus, fabricated extremely efficient flexible PV devices with photoresponsivity above 0.1A/watt (corresponding to an external quantum efficiency of above 30%). The cause for this has been reported to be the Van Hove singularities in the electronic density of states of TMDs that enhance light-matter interactions [34]**.** Tongay and his group (2014) demonstrated that in large-area heterostructures of CVD-grown WS_2 and MoS_2 monolayers, due to their strong interlayer coupling, the PL spectrum of the heterostructure gradually changes from additive to “renormalized” [27]. Xue et al. fabricated MoS_2-WS_2 heterostructures having high photoresponsivity for the application of flexible photodetector devices [35]. The light-matter interaction in TMDs is very strong and thus TMDs have proved to be potential material in optoelectronic applications like luminescent devices, thin and flexible parts of solar cells, etc.

1.2.4 Magnetic and superconducting properties of TMDs

Essentially, TMDs show diamagnetism at and above room temperature. However, there are some reports which refer to the tenability of magnetic property of TMDs having a different structure but at a very low temperature. However, the magnetic properties of TMDs are still not completely understood. A comparative study, using experimental methods and theoretical analysis, on the magnetic property of 3d block TMDs with pyrite structure like NiS_2, $NiSe_2$, FeS_2, CoS_2, $CoSe_2$, CuS_2, ZnS_2 etc. was reported by a Japanese scientist S.

Ogawa in 1979. They found many kinds of magnetic states in these crystals [36]. Magnetism at low temperature was also observed in intercalated TMDs [37]. A complex kind of magnetism in intercalated TMDs was reported by R. H. Friend, in 1983 [38]. In 2012, S. Tongay and coworkers reported the ferromagnetic behavior of single crystal MoS_2 from 10K to room temperature which was shown to have originated from the magnetism attributed to the zigzag edges at grain boundaries of the crystal [39]. Many researchers have studied the magnetic behavior of TMDs with different structures constructed theoretically by using density functional theory (DFT) based software. MoS_2 zigzag nanoribbons were reported to be ferromagnetic by Pan and Zhang [40]. P. Lu and coworkers studied the strain-dependent magnetic behavior of MoS_2 having different structures theoretically and observed magnetic property of low dimensional MoS_2 which is tunable through mechanical strain [41]. Zhao et al. reported the magnetic property of Cu-doped WS_2 by using first principle DFT study [42]. The strain-dependent electronic and magnetic behavior of low dimensional WS_2 structure was also reported by H. Zhang et al. [43].

The superconducting nature of TMDs has also been reported by many researchers. In 1983, Ikebe and Muto carried out research to study the effect of alloying and intercalation on superconductivity of TMDs. They observed that the alloy TMDs exhibited anisotropic 3D superconductivity and intercalated TMDs attained quasi 2D superconductivity [44]. Richard A. Klemm reported the superconducting nature of pristine TMDs and TMDs intercalated by organic/inorganic materials. They found that although pristine TMDs did not show superconductivity but intercalated TMDs behave as superconductors [45]. R. Zhang and his research group also reported about the superconducting nature of potassium doped MoS_2 [46]. S. Jo and coworkers achieved superconductivity at the surface of WS_2 crystal by electron accumulation but at a very low temperature of below 4K [47]. Zheliuk et al. in 2017 obtained superconductivity in monolayer WS_2 by static electron doping in a transistor device [48]. As such the potential for superconductivity in TMD materials can be exploited for further advancement.

1.3 Synthesis of TMDs

Different synthesis processes have been reported of synthesis of a monolayer to few layers of TMDs. In the top-down approach, physical exfoliation by mechanically rubbing or using “scotch tape” and ion-intercalation or dispersion by sonication method etc. are mainly adopted. In the bottom-up approach, different techniques such as Chemical vapor deposition (CVD), ALD, solid state reactions, hydrothermal techniques and many other techniques have been reported by many research groups. Mechanical exfoliation using the scotch-tape micromechanical cleavage technique has been employed to produce few layers to monolayer MoS_2, WS_2 and other TMDs since the middle of the 20th century [49,50]. In micromechanical cleavage, layers of TMDs are piled and transferred on to the surface of a substrate and the process is repeated to produce a smaller thickness of 2D structure up to monolayer. Novoselov et al., in 2005, produced flakes of single layers of several TMDs by using a simple procedure of rubbing fresh bulk crystal on another solid surface [51]. Prof. Rao and Nag described exfoliation of bulk MoS_2 and WS_2 by lithium intercalation followed by ultrasonication process to produce monolayer and bilayer of the respective materials [12]. Solid state reaction mechanism and hydrothermal techniques to synthesize few layers TMDs have also been reported by many researchers [12, 52-54]. Duan and his group (2014) synthesized heterostructure of TMDs by using thermal CVD method [55]. In many other works, CVD techniques have been used to synthesize large area TMDs on a solid substrate like silica [27, 56-62]. There are also reports in which uniform high quality and wafer scale TMD films have been deposited by ALD technique [63-65].

1.4 Nanoscale TMDs

The large value of surface to volume ratio and quantum confinement (QC) effects makes the nano dimensional material drastically different from its bulk form. The combination of ionic-covalent interaction within the atoms inside each layer and weak Van der Waals force in TMDs enables the formation of various nanostructures like nanoribbons, nanotubes, nano flakes and nanoparticles (NPs) [28, 66]. The NPs of TMDs have been studied for various application purpose like dry lubrication, catalytic application etc. When the size of the 2D structure decreases, due to the increase in dangling bonds TMDs have a natural tendency to form nanotubes [28]. Tenne and his research group, in 1992, were the first to synthesize synthetic WS_2 nanotubes by heating thin tungsten in hydrogen sulfide [67]. In 1995, Tenne and another group reported the synthesis of MoS_2 inorganic fullerene like NPs and nanotubes [57]. Bertram et al. carried out a theoretical and experimental study of nanoplatelets of MoS_2 and WS_2 [68]. Rao and coworkers, in 2001, also reported the synthesis of MoS_2 and WS_2 nanotubes by using hydrogen treatment in ammonium thiomolybdate and ammonium thiotungstate as precursor [69]. Deepak et al. reported high temperature solid state reaction to synthesize MoS_2 nanotubes and nanoflower having potential application in energy storage and catalysis [70]. The synthesis of fullerenelike NPs and nanoplatelets of MoS_2 using solid state reaction process have also been reported by Frey et al. [52]. They have synthesized NPs in the range 20 to 200nm and nanoplatelets in the range 5 to 500nm in size to study the Raman and resonance Raman spectra of MoS_2. X. C. Song and other two researchers have reported synthesis of spherical shaped MoS_2 particles, named Bucky onions, having size 60nm to 200nm by using MoS_3 as a precursor in high temperature H_2 atmosphere [71].

The electronic and optoelectronic behavior of TMDs has also been seen to be drastically varied as the dimension collapses to nano level. The atomically thin layered heterostructures of different TMDs has been predicted to have great potential applications in different areas. Shanmugam et al. reported the excellent light absorbing property of monolayer/few layer MoS_2 coated TiO_2 NPs in BJH solar cell. Using their heterostructure BJH solar cell, they achieved 1.3% photoconversion efficiency under $100mW/cm^2$ illumination of light. [33]. Xue et al. fabricated MoS_2-WS_2 few layer flexible heterostructure photodetector device [35]. They synthesized the heterostructure by using sulfurization process in CVD method. It has been observed that almost all research in TMDs involve nano scale synthesis for various applications.

1.5 Photocatalytic nature of TMDs

TMDs are found to be a very good absorber of UV and visible (UV-vis) light. The semiconducting property of TMDs allows strong light induced effects; however, the intensity of light-matter interaction depends on the dimension of the material. The absorbed light generates e^--h^+ pairs in the material which actively take part in catalytic and photocatalytic activity through different mechanisms.

Many researchers have reported the evolution of H_2 gas by using TMDs as a catalyst which is a subject undergoing intense study by current researchers. The H_2 evolution by a photocatalytic mechanism using MoS_2/CdS catalyst was studied by Xu Zong and coworkers in 2009 [72]. Q. Xiang et al. (2012) found enhanced H_2 evolution by using TiO_2/MoS_2/Graphene composite as hybrid photocatalyst [73]. The chemical fuel in the form of H_2 gas can be produced by splitting water using visible light photocatalysis. In 2013, Y. Hou and his colleagues investigated the water splitting behavior through photocatalysis by using organic-inorganic layered MoS_2/graphite-carbon nitride as an excellent photocatalyst for H_2 evolution [74]. Han and Hu (2016) reviewed the application of MoS_2 as a potential co-catalyst with other material like CdS, graphene, Carbon Nitride, TiO_2, CdSe etc for water splitting visible light photocatalytic activity [75].

Some members of TMDs like MoS_2, WS_2, etc. have also been utilized for dye degradation. Wingkei Ho and his research group, in 2004, reported the efficient photocatalytic behavior of MoS_2 and WS_2 nanocluster sensitized TiO_2 in the degradation of methylene blue (MB) and 4-chlorophenol [76]. Quinn et al. also carried out visible light photocatalysis by MoS_2 nano sheets to degrade MB [77]. Tan et al. fabricated MoS_2-ZnO nano heterostructure to degrade MB and obtained higher degradation as compared to MoS_2 nanoflower catalyst [78]. P. Wang and his colleagues prepared Ag_3PO_4/MoS_2 composites to study the photocatalytic degradation of Rhodamine B (RB) [79]. They compared its performance with that of bare Ag_3PO_4 and obtained much higher efficiency. Because of the semiconducting nature and good absorption of photons, TMDs have become a potential material for photocatalytic reaction.

1.6 Density functional theory findings on different properties of TMDs

The availability of DFT based software makes possible the study of various properties like electronic, magnetic, optical, structural etc. of chemical structures of any material computationally with proper approximations. Scientist and researchers have promptly applied DFT study on various TMDs materials. Li and Galli reported a first principle DFT study on the QC effect in the electronic structure of MoS_2 NPs [80]. A. Kuc and his group also investigated the QC effect in electronic structure of different TMD models theoretically [81]. From the DFT calculations, they observed that there was spontaneous tuning of electronic band structure depending on the thickness of the material. They reported that MoS_2 and WS_2 showed transition from direct to indirect BG SC on reducing the dimension to monolayer while NbS_2 and ReS_2 remained metallic even with variation of the thickness. Ouyang et al. investigated different properties of WS_2 nanoribbons by using DFT [82]. A. Carvalho and coworkers studied the optical response of 2D TMDs due to band nesting effect using DFT computation [83]. They studied the trigonal form of MoS_2, $MoSe_2$, WS_2 and WSe_2 and octahedral form of TiS_2, ZrS_2, $ZrSe_2$, PdS_2, $PdSe_2$, PtS_2 and $PtSe_2$ and found similarity in band nesting phenomenon in all the samples. S. Tongay and his research group investigated the optical response in MoS_2/WS_2 heterostructures taking into consideration spin-orbit coupling with the help of DFT calculations [27]. Rasmussen and Thygesen, based on DFT first principle computation, reported the electronic structure of several TMDs and correlated them [84]. A. Majid and coworkers have studied electronic properties of MoS_2-CeS_2 alloys and the structural modification with the incorporation of Ce in MoS_2 by using GGA approximation in DFT and discovered metallic transition on the substitution of one Ce atom in MoS_2 [85]. Ouyang, Xiong and Jing have recently reported a theoretical DFT investigation on the TMDs-metal contact resistance. They have achieved different values of interfacial charge transfer for various combination of TMDs-metal contact and their DFT findings suggest that the contact resistance can be manipulated [86]. In the current era, different researchers are studying different properties of TMDs using DFT simulations.

1.7 Intercalation and ternary compounds of TMDs

In case of layered structure material, ions or molecules can be inserted in between the layers in a reversible manner. This process is called intercalation. Electronic, optical, magnetic, etc. properties and the structure of layered materials can be manipulated through intercalation[88]. Since TMDs have layered structure, scientists have tried intercalation of different kinds of organic and inorganic molecules and metal atoms in TMDs to study different properties. Also, intercalation mechanism has been utilized in the synthesis of low dimensional TMDs from the bulk [12, 13, 87]. By intercalation, the stoichiometry and band structure of TMDs can also be manipulated [24]. In 1989, N. Suzuki and coworkers reported about intercalated TMDs [88]. Intercalation with organic donor molecule and alkali metals to study optical and transport properties of TMDs like TaS_2, ZrS_2, $NbSe_2$, MoS_2 etc. was reported by A. D. Yoffe in 1990 [89]. In 1995, E. Figueroa et al. also prepared and characterized intercalated TMDs. R. A. Klemm has reported the superconducting nature of intercalated TMDs [90]. Recently Jung and two others have reported an extensive review on intercalated TMDs and explained the effect of intercalation on various properties [87].

Ternary compound refers to a compound which is composed of three different elements. Ternary TMD alloys having a combination like metal-chalcogen-chalcogen and metal-metal-chalcogen have been studied for investigating different properties. In 1985, B. J. Dalrymple et al. synthesized $Nb_{1-x}Ta_xSe_2$ ternary compound by chemical vapor transport (CVT) technique to study the superconducting behavior [91]. In 1987, Hofmann et al. reported the synthesis of ternary compound $Mo_xW_{1-x}Se_2$ by CVT method to investigate the photoactivity electrochemically [92]. Xu et al. reported the synthesis of $WS_{2(1-x)}Se_{2x}$ nanotubes for H_2 evolution process [93]. Tan and coworkers have also reported the synthesis of $MoS_{2x}Se_{2(1-x)}$ and $Mo_xW_{(1-x)}S_2$ nanosheets and applied as efficient electrocatalyst for dye sensitized solar cell [94]. Tedstone et al. have given a review on the transition metal doped TMDs and reported different applications and properties of such ternary compounds [95]. Recently ternary $WS_{2(1-x)}Se_{2x}$ flakes have been synthesized for catalytic H_2 production by Y. Zhang et al. [96]. The synthesis and applications of ternary TMDs have received good attention from current researchers.

1.8 Scope of the thesis and its objectives

The present doctoral thesis comprises the synthesis of ternary tungsten incorporated MoS_2 compounds in nano-dimensional particle form produced via already existing solid state reactions followed by ultrasonication. A novel approach of utilizing a solid state reaction mechanism to synthesize ternary TMDs has been achieved. It is a low cost and mass producible technique to synthesize the desired materials. Both MoS_2 and WS_2 bare similar structure (metal have trigonal prismatic Mo^{IV} or W^{IV} and chalcogen have pyramidal S^{-2} sites) and hence they have minimum lattice mismatch in their ternary compounds. Though

TMDs, 3d block metal intercalated TMDs and composites of these materials have been explored extensively worldwide, detailed study of ternary sulfide compounds of 4d block element Mo and 5d block element W is extremely rare. The effect of W in W-doped MoS_2 ternary compound system is the subject of current research. The effect of W insertion in MoS_2 lattice is computationally investigated by using DFT based VASP (Vienna Ab initio Simulation Package) software. Already available reports conclude that TMDs show thickness dependent luminescence behavior. In this thesis, a comparative study on PL properties of the as-synthesized ternary compounds with the pristine MoS_2 and WS_2 NPs have also been reported. The outcomes of our experimental observations show that the combining effect of W and Mo also leads to luminescence performance of the ternary TMDs to change. Also, being materials of nano-dimensional semiconductors, their photocatalytic measurements were performed and an enhancement in the photocatalytic behavior of the as-synthesized ternary TMDs was achieved.

Though industrial revolution has solved many problems of mankind and has advanced our lifestyle, the negative impact of industrial byproducts cannot be underestimated. Such type of problems creates harm to the ecological system, directly or indirectly. One such serious problem is the extensive use of dye materials [97-100]. Industrial dye pollution and dye degradation create a serious problem to the environment. Dye degradation by photocatalysis is a promising way to control such pollution. In various industries like paper, rubber, textile, leather, furniture, plastic, automobile, toy, etc., coloring materials are extensively used in large quantities. The released waste water contains an estimated amount of about 2-20% of $7x10^5$ metric tons of dye which is exposed into the environment via obsolete waste disposal methods and faulty drainage systems without any proper treatment [101]. Many such hazardous dyes remain intact in the environment for long periods of time. Some are even carcinogenic, mutagenic to life cycles and are non-self-degradable due to their complex structures [101, 102]. These cause tremendous harm to crops and biological tissues. Thus degradation of dye to control pollution and reusability of waste water is an essential and critical issue for scientists and researchers. The harmful effects of such dyes can be reduced by decomposing them into benign substances. Several conventional methods like filtration, absorption, coagulation-flocculation, solvent extraction, electrochemical techniques, reverse osmosis etc., have been reported to control such pollution, but these are very expensive and require high power consumption [98, 103, 104]. Some of these are even incapable of complete degradation of dyes. Prior studies reveal that photocatalysis is a potentially strong complex multistep process for complete degradation of dyes into benign substances with high cost effectiveness. From the existing literature, it is observed that SC nanomaterials can act as potential candidate to degrade such dye materials through photocatalytic phenomenon [105, 106]. That is why we have performed photocatalytic degradation study of Methyl Orange (MO) and RB as model dyes, both being harmful and non-self-degradable, by using our as-synthesized materials and observing how to overcome such an issue.

On the basis of the above points, the objectives for the research work were selected. In summary the objectives are,

1. Synthesis of ternary compound TMD NPs of Mo, W and S having different Mo:W molar ratio.
2. Application of Solid State Reaction in the synthesis of ternary compound TMDs of Mo, W and S.
3. Characterization of the as-synthesized materials using different analytical techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX or EDS), transmission electron microscopy (TEM), Raman spectroscopy, UV-vis spectroscopy, PL spectroscopy etc.
4. Study of photocatalytic behavior of the as-synthesized nano materials using different dye materials.
5. Computational investigation of the compound material properties basically optical and electronic properties using the DFT based software named VASP.

The thesis reports the work done based on the objectives.

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