



Ultrathin Transition Metal Dichalcogenides for Quantum Sensing: Synthesis, Properties, and Prospects

By

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Abstract

Transition metal Dichalcogenides (TMDs), particularly in their monolayer and ultrathin forms, are emerging as significant materials in quantum sensing due to their distinct quantum attributes. This review delves into the synthesis methods, intrinsic characteristics, and transformative potential of TMDs within quantum sensing technology. Beginning with an overview of TMDs' structural and electronic properties, it covers advanced synthesis techniques vital for achieving high-quality monolayers. Key quantum traits, such as direct band gaps, excitonic behavior, and spin-valley coupling, are analyzed for their applicability in quantum sensing. Despite notable attributes, TMDs face challenges including material stability, scalability, and coherence preservation. The review concludes by examining TMDs' future potential and their anticipated role in advancing next-generation quantum technologies.

Keywords: Transition Metal Dichalcogenides (TMDs), Quantum Sensing, Monolayer Material, Spin-Valley Coupling, Excitonic Properties,

1.1 Introduction

Quantum information science and engineering (QISE)—which entails the use of quantum mechanical states for information processing, communications, and sensing—and the area of nanoscience and nanotechnology have dominated condensed matter physics and materials science research in the 21st century[1] Quantum sensing, in particular, has the potential to revolutionize precision measurement by enabling the detection of extremely weak signals, such as subtle changes in magnetic fields or electric currents. Quantum sensing is typically defined as the use of a quantum system, quantum properties, or quantum phenomena to perform a measurement of a physical quantity and the quantum sensors are defined as systems engineered to enable precise measurements of these physical quantities. It deals with the optimal estimation of classical parameters encoded in quantum transformations, offering maximum precision at the fundamental limits. In this context, discovering new materials that enhance quantum interactions is crucial. [2, 3].

Common quantum sensing platforms include atomic vapors[4], trapped ions[5], superconducting qubits[6],

superconducting quantum interference devices (SQUIDS)[7], and solid state quantum sensors. Solid-state quantum sensors attract much attention given their potential for high sensitivity and nano applications.[8] Solid-state quantum emitters are considered as the forefront of quantum computing and sensing, owing to their prospects of scalability, robustness, and ease of handling since these are probe to weak, fluctuating magnetic fields under ambient conditions and at sub micrometer scales, which cannot typically be accessed by existing techniques such as nuclear magnetic resonance. Graphene quantum dots (QDs) have also attracted interest in the scientific community due to their high transparency and large surface area but its lack of an electronic bandgap has stimulated the search for 2D materials with semiconducting character.[9] Likewise diamonds has also been studied for quantum sensing applications owing to nitrogen vacancy defects in quantum sensors[10]. However, Nitrogen-vacancy (NV) centers in diamond face limitations like reduced coherence times at higher temperatures and sensitivity to environmental noise, impacting their performance in quantum applications. [11, 12]. Transition metal Dichalcogenides (TMDs), which are semiconductors of

the type MX_2 , provide a promising alternative. Transition metal Dichalcogenides (TMDs) possess unique electronic properties and high sensitivity to external fields, making them ideal candidates for quantum sensing applications.

1.2 Transition Metal Dichalcogenides; An Overview

Two-dimensional transition metal Dichalcogenides (TMDCs) are an emerging class of materials with properties like atomic-scale thickness, direct bandgap, strong spin-orbit coupling and favorable electronic and mechanical properties that make them highly attractive for fundamental studies of novel physical phenomena and for applications ranging from Nano electronics and Nano photonics to sensing and actuation at the nanoscale. [13]. There are more than 40 kinds of stable 2D TMDs that have been found. All of these materials have common structural properties: their bulk form is stacked by X–M–X layers and their neighboring layers are connected via interlamination van der Waals forces. According to their electrical band structures, bulk TMDs range from semiconductors such as MoS_2 [14] and MoSe_2 , to semimetals such as WTe_2 and VS_2 , to metals such as TaS_2 and NbS_2 [15]. Their bandgap lies in the visible and near-IR range, and they possess strong Excitonic resonances, high oscillator strengths, and valley-selective response. Coupling these materials to optical Nano cavities enhances the quantum yield of exciton emission, enabling advanced quantum optics and Nano photonics devices [16].

1.3 Ultrathin TMDS;

Since, tailoring the dimension of nanomaterials to achieve precise control of electronic, optical, and catalytic properties has been the major goals of researchers for decades. Since the discovery of graphene in 2004, many efforts have been devoted to developing other 2D materials, like graphene derivatives, hexagonal boron nitride, metal oxides, and transition-metal Dichalcogenides (TMDCs). This is due to their excellent physical and chemical properties [17]. As the thickness of TiSe_2 film increases from 1 to 6 layers, more quantum well valence states emerge [18].

These ultrathin 2D materials also acts as potent candidates in quantum sensing as in two-dimensional nanomaterials (2D), quantum confinement occurs in one direction exhibiting plate-like shapes. However, in bulk or 3D materials, there is no confinement in any dimension. When compared to bulk materials, layered 2D materials have a variety of unique features, including a high aspect ratio (surface-area-to-volume ratio) that is strongly related to the number of layers. From a scientific and technological standpoint, 2D materials have a number of benefits over bulk 3D materials because their properties may be dynamically tuned via electrical, chemical, electrochemical, and other methods. [19] When TMDs are thinned down to monolayers, they undergo significant changes in their electronic and optical properties. Bulk TMDs typically exhibit indirect bandgaps, but in their monolayer form, these materials transition to direct bandgaps, resulting in enhanced photoluminescence. This makes monolayer TMDs particularly useful in optoelectronic and quantum sensing applications [20]. Despite being atomically thin, monolayer TMDs are stable in normal conditions and mechanically

robust due to strong in-plane covalent bonding, and can be handled with ease compared to more sensitive 2D materials such as phosphorene [21]. Moreover, Ultrathin TMDs are intrinsically capable of sustaining much larger mechanical strain when compared to their bulk counterparts. The surface area per gram (SAPG) of TMDs increases substantially when reduced to a few layers from bulk. MoS_2 shows a SAPG value increase from 8.4 to 25 m^2 per gram. The increase in the active surface site density increases the probability of binding of analytes to the sites of the sensing transducer elements and hence, causing the modulation of opto-electronic properties, which results in highly sensitive biosensors with improved detection limit [22]. One important consequence of exfoliation is freeing the adjacent MX_2 layers from s–p π orbital interaction, which causes the bandgap to widen. Changes in orbital hybridization also transform the single-layer MX_2 from indirect-bandgap to direct-bandgap semiconductors, thus giving rise to enhanced photoluminescence compared with the bulk material [23].

The diverse and intrinsic properties of TMDs nanostructures are highly dependent on their sizes and morphologies, and so far the unique preparation methods and properties of various TMDs dimensionalities, making an important contribution to the practical sensing application. The monolayer TMDs are particularly interesting due to their direct energy band gaps and non-centrosymmetric lattice structure. MoS_2 exhibit tunable bandgaps that can undergo transition from an indirect band gap in bulk crystals to a direct band gap in monolayer Nano sheets and great properties of 2D TMDs nanostructures make their counterparts of different dimensionalities, such as zero-dimensional (0D) and one-dimensional (1D) TMDs structures, highly attractive. 0D TMDs including the dot structures with the sizes of below 100 nm in all dimensions, such as TMDs quantum dots (QDs), small Nano flakes, and nanoparticles, have been prepared and widely applied in the sensing field. [24] Likewise, metallic or semi conducting behavior of TMDs is also dependent on thickness as the monolayer PtSe_2 is semiconductor with the indirect band gap of ≈ 1.2 eV, while the thicker layers of PtSe_2 becomes metal without a band gap [25].

1.4 Structure of TMDs

Many TMDs crystallize in a graphite-like layered structure that leads to strong anisotropy in their electrical, chemical, mechanical and thermal properties. Group 4–7 TMDs are predominantly layered, whereas some of group 8–10 TMDs are commonly found in non-layered structures. In layered structures, each layer typically has a thickness of 6–7 Å which consists of a hexagonally packed layer of metal atoms sandwiched between two layers of chalcogen atoms [26].

In each X–M–X layer, the M–X bond is strongly covalent, while adjacent layers are weakly coupled by van der Waals (vdW) interactions, resulting in a distinctive easy slippage and easy cleavage of planes in TMDs. TMDs contain group VI transition metal having a chemical structure of MX_2 (M: Mo, W and X: S, Se, Te) are naturally found in their semiconducting phase and can be readily exfoliated to yield 2D sheets that exhibit layer-dependent electronic structure,

strong excitonic effects, spin-valley physics, and nonlinear optical phenomena. They have an indirect gap in the bulk form but becomes a direct gap material when thinned down to a monolayer [27].

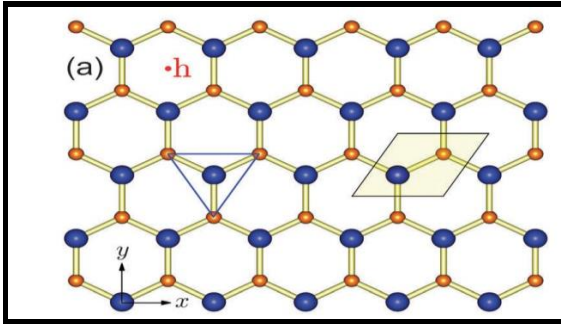


Figure 1 : (a) Top views of group-VIB TMD monolayers. The blue and orange spheres represent M and X atoms respectively. The light yellow diamond region is the 2D unit cell with lattice constant a .

The metal atoms provide four electrons to fill the bonding states of TMDs such that the oxidation states of the metal (M) and chalcogen (X) atoms are +4 and -2, respectively. The lone-pair electrons of the chalcogen atoms terminate the surfaces of the layers, and the absence of dangling bonds renders those layers stable against reactions with environmental species. The metal coordination of layered TMDs can be either trigonal prismatic or octahedral (typically distorted and sometimes referred to as trigonal-antiprismatic). Depending on the combination of the metal and chalcogen elements, one of the two coordination modes is thermodynamically preferred. In contrast to graphite, bulk TMDs exhibit a wide variety of polymorphs and stacking polytypes (a specific case of polymorphism) because an individual MX_2 monolayer, which itself contains three layers of atoms (X-M-X), can be in either one of the two phases. Most commonly encountered polymorphs are 1T, 2H and 3R where the letters stand for trigonal, hexagonal and rhombohedral, respectively, and the digit indicates the number of X-M-X units in the unit cell. [28]. When MX_2 is exfoliated into thin sheets, the prismatic edges and basal planes are exposed, and edge termination by either M or X atoms is possible depending on the chemical potential of the growth environment and the resulting monolayer TMDs exhibit only two polymorphs: trigonal prismatic and octahedral phases. The former belongs to the D_{3h} point group whereas the latter belongs to the D_{3d} group that are referred to as monolayer 1H (or D_{3h})- and 1T (or D_{3d})- MX_2 , respectively.

A single layer of semiconducting TMDs for instance MoX_2 , schematically shown in Fig. 19(a), consists of a plane of transition metal atoms sandwiched by layers of chalcogen atoms. Analogous to graphene, monolayer TMD materials exhibit strong intralayer bonding but weak interlayer bonding, and can subsequently be peeled apart to achieve a single monolayer (1L). The Brillouin zone of this system is shown in Fig. (b) In single layer form, the direct gap occurs at the K-point, and the optical properties of these materials are governed by strong excitonic transitions, both neutral and

charged. In addition to being optically active with strong photoluminescence (PL), they also have unique optical selection rules. Time reversal symmetry and strong orbital-hybridization couples the valley and spin indices [29].

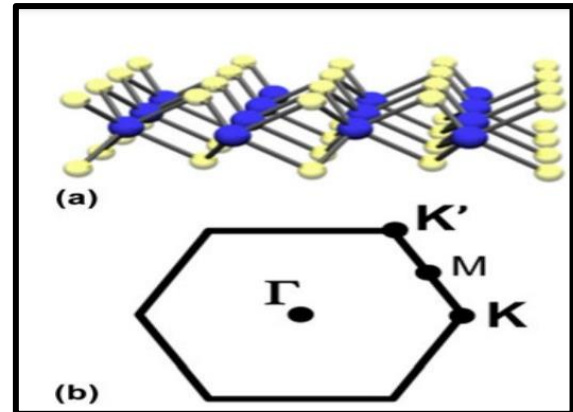


Figure 2: Crystal structure of a single-layer transition-metal dichalcogenide. A central layer of transition metal atoms is sandwiched by layers of chalcogens. (b) Brillouin zone for a reduced dimensional hexagonal lattice. Some relevant high symmetry points are indicated.

1.5 Electronic Structure of TMDs

The electronic structure of TMDs strongly depends on the coordination environment of the transition metal and its d-electron count; this gives rise to an array of electronic and magnetic properties. The basic electronic properties of TMDs can be, however, predicted from the ligand field splitting of the nonbonding transition metal d-orbitals and the filling of these orbitals. In both 1H and 1T phases, the nonbonding d bands of the TMDs are located within the gap between the bonding (σ) and antibonding (σ^*) bands of M-X bonds. Octahedrally coordinated transition metal centers (D^3d) of TMDs form degenerate d_{z^2}, x^2-y^2 (e_g) and d_{yz}, xz, xy (t_2g) orbitals that can together accommodate the TMDs' d electrons (a maximum of 6, for group 10 TMDs). On the other hand, the d orbitals of transition metals with trigonal prismatic coordination (D^3h) split into three groups, d_{z^2} (a_1), $d_{x^2-y^2}, xy$ (e), and d_{xz}, yz (e'), with a sizeable gap (~ 1 eV) between the first two groups of orbitals.

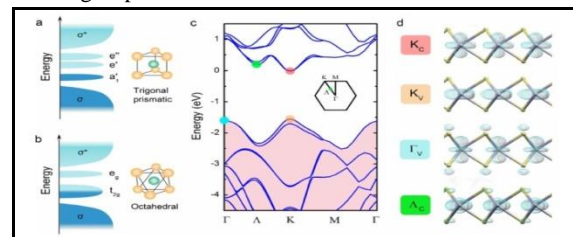


Figure 3: Schematic illustration of orbital filling of group 6 TMDs with trigonal prismatic (a) and octahedral (b) coordination. In trigonal prismatic (2H) coordination, the d orbitals split into three groups, namely, d_{z^2} (a_1'), $d_{x^2-y^2}, xy$ (e') and d_{xz}, yz (e''). These orbitals are located within the bonding (σ) and antibonding (σ^*) states. In octahedral (1T) coordination, the d orbitals split into d_{xy}, yz, zx (t_{2g}) and $d_{x^2-y^2}, xz$ (e_g) bands. (c) Calculated electronic band structure of monolayer MoS_2 . (d) Electron distribution for states at the

four extrema in the band structure indicated by colored dots in panel c[30].

When the orbitals are partially filled, as in the case of 2H-NbSe₂ and 1T-ReS₂, TMDs exhibit metallic conductivity as the orbitals are fully occupied, such as in 1T-HfS₂, 2H-MoS₂ and 1T-PtS₂, the materials are semiconductors. In general, MoX₂ and WX₂ compounds are semiconducting whereas NbX₂ and TaX₂ are metallic.

The wave functions at different points in the Brillouin zone (BZ) include a mix of transition metal d-orbitals and chalcogen pz orbitals. For example, the conduction band valley at the Λ point (Λ_c) and the valence band hill at the Γ point (Γ_v) show admixture, while K_c and K_v have a predominantly d-orbital character. In monolayers, the pz orbitals extend to the outer surfaces, while the d-electrons remain centered in the middle of the X–M–X sandwich structure. This distribution is important in understanding the electronic properties and interactions of TMDs with external stimuli [31].

1.6 Valley Index and Valley Polarization in Monolayer TMDs

In monolayer TMDs, the conduction band minimum (CBM) and valence band maximum (VBM) are at the corners of the first Brillouin zone (BZ), denoted by K and K'. The six corners split into two inequivalent groups (K and K') under time-reversal symmetry where each group has three equivalent corners related to each other by reciprocal lattice vectors. The energetically degenerate but inequivalent band extrema at K and K' constitute a discrete index of carriers, known as the valley index or pseudospin. Low-energy electrons and holes therefore have this extra valley degree of freedom in addition to spin. This extra degree of freedom is instrumental in valleytronics and quantum sensing.

K and K' transform into each other under the time reversal operation. Hereafter we use K_c and K_v to denote the CBM and VBM at the K points respectively. The CB also has six local minima at the low symmetry Q points while the VB has a local maximum at the Γ points, which are referred to as Q_c and Γ_v respectively hereafter. These critical points are also important because they are energetically close to K_c and K_v respectively, and in cases such as under strain or in multilayers, Q_c may become the global CBM or Γ_v the global VBM. K and Γ are high symmetry point [32]

1.7 Properties Enabling Ultrathin TMDs for Quantum Sensing

TMDs are particularly attractive for quantum applications because of their tunable electronic, optical, and mechanical properties. The quantum confinement effect, direct bandgaps in monolayer form, strong spin-valley coupling, and potential for excitonic behavior make them versatile platforms for quantum sensing

1.7.1. Quantum Confinement

In nanomaterials with dimension shaped into 2D structure, the electronic structure is significantly affected by the quantum confinement effects (QCEs) arising from thickness reduction.

The term quantum confinement mainly deals with energy of confined electrons (electrons and holes). The energy level of electrons will not remain continuous as in case of bulk materials compared to nano crystal. Moreover obtaining the confined electrons wave function, they become a, discrete set of energy level. Such kinds of effects appear when dimensions of potential approach near to de Broglie wavelength of electrons resulting in changes or discrete levels of energy this effect is called quantum confinement.

Due to the strong quantum confinement in the perpendicular direction, the energy bandgaps in single- and few-layer are always enlarged compared to their bulk counterparts. They possess indirect bandgaps in their bulk and few-layer forms; when the thickness decreased to single layer limit, the bandgaps abruptly turn into direct ones. Such indirect-direct-gap crossover originates from the perpendicular quantum confinement with decreasing layer number (N) [33]. Transition metal Dichalcogenides (TMDs) with atomically thin 2D structures, such as WSe₂, WS₂, MoSe₂, and MoS₂ have a wide range of unique electronic and optical properties, which is due to quantum confinement. [20] All MoX₂ and WX₂ compounds are expected to undergo a similar indirect- to direct-bandgap transformation with decreasing layer numbers, covering the bandgap energy range 1.1–1.9 eV as shown in figure [34].

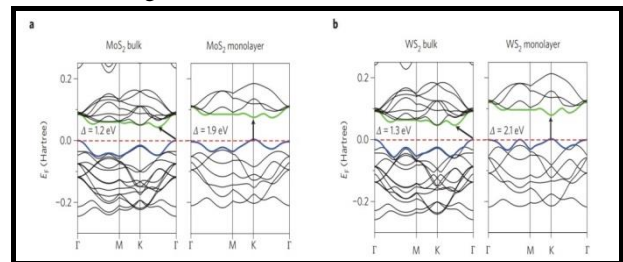


Figure 4: Band structures calculated from first-principles density functional theory (DFT) for bulk and monolayer MoS₂ (a) and WS₂ (b). The horizontal dashed lines indicate the Fermi level. The arrows indicate the fundamental bandgap (direct or indirect). The top of the valence band (blue) and bottom of the conduction band (green) are highlighted [35].

Quantum dots (QDs) are three-dimensionally confined semiconductor nanocrystals, quantum rods (QRs) have two-dimensional confinement and one-dimensional confined nanocrystals are often called quantum plates, sheets, or wells. Thus, quantum confinement is most prominently observed in quantum dots (QDs), which are nanoscale semiconductor particles. Quantum confinement effects give rise to unique optical and electronic properties in QDs [36] and optically active self-assembled quantum dots with deep electron and hole confinement allow for the realization of highly efficient single-photon source, all-optical manipulation of confined spins and a spin–photon quantum interface, the random nature of their growth seems to be the biggest hindrance to their use in scalable quantum information processing. In contrast, electrically defined single or double quantum dots hosting one or two excess electrons have been shown to exhibit long spin coherence times together with a clear path towards integrated scalable devices. However, weaker

confinement has precluded the possibility to reliably transfer quantum information from spins to photons in these systems. Quantum dots in monolayer transition-metal Dichalcogenides (TMDs) have the potential to combine the desirable features of both optically active and electrically defined quantum dots [37].

The work of Heinz's group, also studied the effect of size induced quantum confinement in MoS₂ that displayed a layer-dependent bandgap, which changed from an indirect bandgap in the bulk material to a direct bandgap in the semiconductor. In addition, the PL quantum yield (QY) improved with decreasing thickness. With regard to few-layered MoS₂, the QY was of the order of 10⁻⁵–10⁻⁶. Even for the monolayer MoS₂ Nano sheets, the QY was only about 4 × 10⁻³. Through the disintegration of Nano sheets, TMD QDs were obtained and the corresponding QY was obviously enhanced [38].

As the change of spectra absorption in QDs of PbSe₂ owing to enhance quantum confinement with decrease in diameter so PbSe QDs with average radius that varies from about 3 to 8 nm. The lowest absorption feature blue-shifts as a function of reduced diameter. The upper right diagram depicts how the ground state wave function experiences increased confinement, explaining this shift in the lowest-energy transition. The kinetic energy increases and the separation between states increase as the QD size decreases [39].

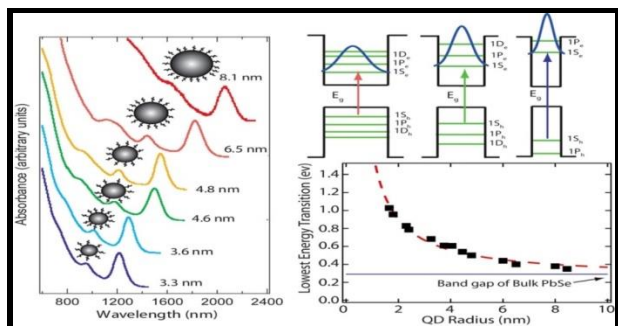


Fig 5: Absorption spectra of PbSe QDs spanning the range from 3.3 nm to 8.1 nm show strong quantum-confined 1st exciton shifted absorption. Several discrete transitions are observable and represent discrete excitonic transitions. Bottom right shows that for PbSe QDs E_g varies approximately as $1/r$. Top right depicts the increased quantum confinement that the 1st exciton experiences as the particle size decreases [40].

Quantum confinement enhances quantum sensing by modifying the electronic and optical properties of materials, which leads to increased exciton stability and sensitivity to external stimuli. This capability enables precise measurements and advancements in sensor technologies, particularly in applications like single-photon detection and quantum metrology.

1.7.2. Optical Properties: Excitons, Trions, and Plasmons

The optical properties of TMDs are dominated by excitons, which are formed when electrons in the conduction band bind with holes in the valence band. The excitonic binding energy

in TMDs is much larger than in bulk semiconductors, leading to stable exciton formation at room temperature [41]. Additionally, TMDs support trions (charged excitons) and plasmonic resonances, both of which can enhance light-matter interactions and improve the sensitivity of quantum sensors.

1.7.3. Spin Valley Coupling

In a crystalline solid, a local energy minimum in the conduction band (CB) or a local energy maximum in the valence band (VB) in the momentum space is known as a valley. In addition to charge and spin, a carrier is assigned a valley degree of freedom, indicating the valley that the carrier occupies. Thus in addition to spin, charge carriers also exhibit a valley degree of freedom (DOF), which behaves like a pseudospin and these two valleys can be optically addressed using circularly polarized light, opening up exciting possibilities for "valleytronics" [42]. Electrons, holes, or excitons can populate the valleys to store and carry information and form the basis of the so-called valleytronics [43]. Graphene and TMDCs which have hexagonal crystal structures possess inequivalent valleys at the K and K' points. Like charge and spin, valley information can also be transported through materials. There are many carriers of valley pseudospin, such as free electrons and holes, doped electrons and holes, and quasi-particles such as neutral, charged, and bound excitons. Thus in addition to spin, charge carriers in TMDs and graphene exhibit a valley DOF, which behaves like a pseudospin.

1.7.4. Defects in TMDs

Solid-state spin defects have garnered significant interest in recent years due to their potential for various quantum applications, ranging from sensing, and simulation to communications. Point defects in solids are analogues of atomic systems 'trapped' in their host materials. Some point defects exhibit unique optical and spin properties, leading to applications in quantum science and technology. To date, spin color centers in diamond and silicon carbide have been extensively studied. However, one of the drawbacks of diamond is the difficulty in creating high-quality NV centers near the diamond surface due to surface charge and spin noise. Quantum defects in two-dimensional (2D) van der Waals (vdW) materials offer new opportunities to address these limitations. 2D vdW materials can be stable even at the monolayer limit and essentially have no dangling bonds on the surface, which effectively avoids the problems encountered by diamond surfaces [44]. A specific advantage is that these defects can be implanted into more complex, electronic device heterostructures, allowing for the electrical control of quantum emission the crystalline structures of TMDCs are enriched by a variety of intrinsic defects, including vacancies, atoms, grain boundaries, and substitutional impurities. Customized design and engineering of the interfaces and defects provides an effective way to modulate the properties of TMDCs. Various interface engineering approaches for TMDCs are overviewed, including surface charge transfer doping, TMDC/metal contact engineering, and TMDC/dielectric interface engineering [45].

1.8 Synthesis of ultrathin TMDs

At present, a variety of preparation methods including mechanical exfoliation, liquid phase exfoliation, chemical exfoliation, chemical vapor deposition, and solvothermal synthesis, have been developed to synthesize 2D TMDs with single or few layers so these methods can be divided into two categories: top-down (get layered nanomaterials from bulk crystals through different exfoliation ways) and bottom-up approaches (use atoms or molecules as precursors to grow into layered nanomaterials under special conditions) [46].

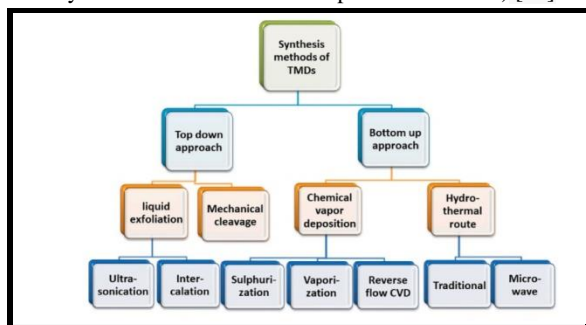


Figure 6: Categorization of various methods for the synthesis of TMDs into top-down and bottom-up approaches[47].

1.8.1. Bottom –up Approaches

In recent years, much progress has been made in the synthesis of TMDs through solution-phase bottom-up processes. The properties of the as-prepared TMDs vary widely with the use of different synthetic regimes, precursors, and stabilizing ligands, giving rise to TMDs with a wide range of morphologies, phases and applications. Chemical vapor deposition and solvothermal/hydrothermal approaches are more prominent and popular in this category for synthesizing TMDs.

1.8.1.1 Chemical Vapor Deposition (CVD) Methods

Chemical Vapor Deposition (CVD) is the most widely used method for synthesizing high-quality monolayer TMDs. The CVD process involves vaporizing metal precursors (such as Mo or W compounds) along with chalcogen precursors (like sulfur or selenium), which then react on a substrate at elevated temperatures to form ultrathin TMD films. CVD allows for precise control over the growth parameters, such as thickness, domain size, and crystal quality, which are crucial for applications in quantum sensing [48]. CVD growth of TMDs can be performed by two ways, first is by sulfurization/selenization of transition metal an effective approach for synthesizing MoS₂ flakes in rhomboid shape with controlled number of layers by the layer-by-layer sulfurization of MoO₂ microcrystals through CVD techniques [49] or metal oxide thin film, and the second way is the vapor phase reaction between the precursors [50] But the synthesis of many m-TMDs is difficult because their precursors including metals and metal oxides usually have relatively high melting points and low vapor pressure which limits the reaction especially for IVB group and VB group transition metal oxides. To solve this issue, salt-assisted CVD is introduced [51] In the formation of high quality atomically thin TMD layers via CVD technique, synthesis parameters such as precursor type, precursor ratio, temperature, position

of the substrate from precursor, flow rate of carrier gas, type of substrate etc., play an important role [52].

1.8.1.2. Hydrothermal/Solvothermal Techniques

Hydro/solvothermal methods refer to the synthesis of materials in closed vessels at high temperatures and pressures, carried out in water (hydrothermal) or other non-aqueous solvents (solvothermal)—Hydro/solvothermal methods are commonly used in the synthesis of a variety of nanomaterials. They are also widely reported methods in the wet-chemical, bottom-up synthesis of TMD-based nanomaterial [53]. The solvothermal and hydrothermal approaches to the synthesis of nanoscale TMDs date back to the years 1998 and 2000, respectively. During the hydrothermal process, the reaction temperature is one of the most important reaction parameters, which can significantly affect the morphology and crystallinity of TMDs [54].

1.8.2. Top-Down Approach

1.8.2.1 Mechanical and Liquid Exfoliation Techniques

This method is popularly known as ‘scotch tape method’. A high-quality mono- and few- layers of 2D materials including TMDs have been achieved in a very quick way. Typically, a lamellar crystal is attached between two pieces of adhesive tape, repeatedly peeled off, and transferred onto a desired substrate, which leaves an ultrathin mono layer of TMD on the substrate. Castellanos-Gomez et al. reported a modified scotch tape method using a ‘visco-elastic silicone stamp’ for the exfoliation of MoS₂, NbSe₂, and TaSe₂, having lateral dimension of the order of few micrometers. Modified scotch tape method has extra benefits over simple scotch tape method, as the stamp does not leave traces of adhesive bound to the surface of the sheets, thereby enhances the quality of exfoliated TMD layers.

In contrast, liquid-phase exfoliation offers a scalable solution by dispersing bulk TMD powders in solvents and applying shear forces to isolate monolayers [55]. Both techniques produce high-quality ultrathin TMDs with minimal defects, making them ideal for quantum sensing applications where material quality is paramount.

1.9. Attributes of a Quantum Sensor;

Experimental realizations of quantum sensors can be compared by some key physical characteristics. One characteristic is to what kind of external parameter(s) the quantum sensor responds to. Charged systems, like trapped ions, will be sensitive to electrical fields, while spin-based systems will mainly respond to magnetic fields. Some quantum sensors may respond to several physical parameters. A second important characteristic is a quantum sensor’s “intrinsic sensitivity.” On the one hand, a quantum sensor is expected to provide a strong response to wanted signals, while on the other hand, it should be minimally affected by unwanted noise.

1.10. TMDs as quantum sensors

1.10.1. Photo detectors and Optoelectronic Sensors

TMD-based photo detectors have demonstrated enhanced performance in terms of photoresponsivity and sensitivity due

to their strong light-matter interaction and direct bandgap. These properties make TMDs ideal for optoelectronic quantum sensors, which can detect minute changes in light intensity or wavelength with high precision [56].

1.10.2 Spin-Based Quantum Sensors

TMDs exhibit strong spin-orbit coupling, which leads to spin-valley coupling, a phenomenon where the electron spin is linked to its momentum in the crystal lattice. This property enables the use of TMDs in spin-based quantum sensors, which can detect changes in magnetic fields or spin states with extreme precision [57].

1.11. Challenges and Future Prospects

1.11.1 Challenges in Material Stability and Scalability

Despite their potential, TMD-based quantum sensors face several challenges, particularly regarding material stability and scalability. TMDs are prone to degradation under ambient conditions, and large-scale production of defect-free monolayers remains challenging. Addressing these issues will be critical for the commercial adoption of TMD-based quantum sensors.

1.11.2 Future Directions in TMD-Based Quantum Sensing

Advancements in quantum technologies, which deploy the properties of quantum physics, promise to take a step further and revolutionize virtually all of industry and daily life. The result could yield more powerful and energy-efficient devices. But to do so requires that physicists get creative about how they exploit the weird ways atoms interact with each other.

Transition metal Dichalcogenides have a diverse range of quantum properties, making them especially attractive for scientific investigation. Researchers in the field have said that the unique materials have "virtually unlimited potential in various fields, including electronic, optoelectronic, sensing, and energy storage applications.

Ultrathin TMDs, with their distinctive quantum properties such as quantum confinement, quantum defects, and spin-valley coupling, show significant promise in advancing quantum sensing technology across various fields. As synthesis techniques and experimental methods evolve, the potential applications and performance capabilities of TMD-based quantum sensors continue to expand. The following outlines some key future directions and applications where TMDs could have a transformative impact.

The future of TMDs in quantum sensing lies in the development of novel fabrication techniques that improve material quality and scalability. Additionally, integrating TMDs with other quantum materials, such as graphene or topological insulators, could open up new possibilities for hybrid quantum sensing devices. With ongoing advancements in nanofabrication and quantum engineering, TMDs are poised to play a significant role in the next generation of quantum sensors [58].

Conclusion

Transition metal Dichalcogenides (TMDs) exhibit exceptional properties that position them as prime candidates for quantum sensing applications. Their adaptable electronic, optical, and spin characteristics, alongside the capacity for defect engineering to create tailored quantum states, place TMDs at the forefront of advanced quantum sensor technologies. Nevertheless, challenges such as material stability and scalability must be addressed to unlock the full potential of TMD-based quantum sensors. Future research in this field is expected to emphasize enhancements in fabrication techniques, the discovery of novel sensing mechanisms, and the integration of TMDs into increasingly sophisticated quantum devices.

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