Chapter 1.
Introduction

"*Our greatest glory is not in never falling, but in rising every time we fall*"

-Confucius

1.1 Background on nanomaterials

Nanoscale materials have garnered significant interest from researchers, as nanotechnology stands out as one of the most revolutionary technologies of the 21st century [1,2]. Nanotechnology can be described as the systematic investigation of materials whose properties are fundamentally influenced by their nanoscale dimensions and not necessarily by composition. It involves the ability to observe, manipulate, and control matter at the nanometer (nm) scale. These materials, which range in size from around 100 nm down to atomic dimensions (around 0.2 nm), exhibit exceptional physical, chemical, biological properties, etc. that vary remarkably from those of their bulk counterparts [3–5]. Their high surface reactivity is largely attributed to their higher surface-to-volume ratio and ample dangling bonds. The nanomaterials display unique electrical, optical, opto-electronic and magnetic properties at the nanoscale dimension compared to their bulk counterparts. The enhanced and novel characteristics make nanomaterials highly promising for fascinating scientific and technological advancements across various fields, including energy, electronics, photonics, communication, information technology, food engineering and biomedicine [6–8].

The term "nanometer" was first introduced in 1914 by Richard Adolf Zsigmondy [9]. However, the introductory concept of nanotechnology was formally presented by American physicist and Nobel laureate Richard Feynman during a landmark lecture at the annual meeting of the American Physical Society in 1959 [10]. His talk, titled *"There's Plenty of Room at the Bottom,"* is considered the first academic discussion on nanotechnology. In this meeting, Feynman posed a question: "*Why can't we write the entire 24 volumes of the Encyclopaedia Britannica on the head of a pin*?" He proposed the development of machines at the molecular scale and emphasized that the only barrier to manipulating matter at the atomic level was not the laws of physics, but rather the limitations in our tools and techniques. This visionary speech laid the basis for modern nanotechnology. And because of this, Feynman is often acknowledged as the father of modern nanotechnology [11,12].

Nanomaterials are a diverse class of materials that have structural constituents less than 100 nm in at least one dimension [13]. Nanomaterials can be grouped into four categories depending on their size dimensions, namely zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D). In 0D nanomaterials, all three dimensions are in the nanoscale range, close to the bulk Bohr exciton size of a given material system. In 1D nanomaterials, two of their three dimensions are within the nanoscale range. In 2D nanomaterials, one dimension (typically, thickness) is within the nanoscale range and has layered, plate-like shapes and sheet-like morphologies. While in the case of 3D nanomaterials (also classified as bulk materials), no dimension is in the nanoscale regime and is subjected to macroscopic rules in the physical world [14–16].

Quantum confinement effect emerges in nanomaterials when at least one of their dimensions is reduced to the scale of the bulk exciton Bohr radius, leading to spatial restriction of charge carriers. In 2D materials, such as thin films and quantum wells (Q-wells), confinement occurs in one dimension; in 1D materials, or quantum wires (Q-wires), confinement is in two dimensions; and in 0D materials, or quantum dots (Q-dots), all three dimensions are spatially confined. The specific size at which a material begins to exhibit quantum confinement depends on the quantum mechanical behaviour of its electron-hole (e-h) pairs [17].

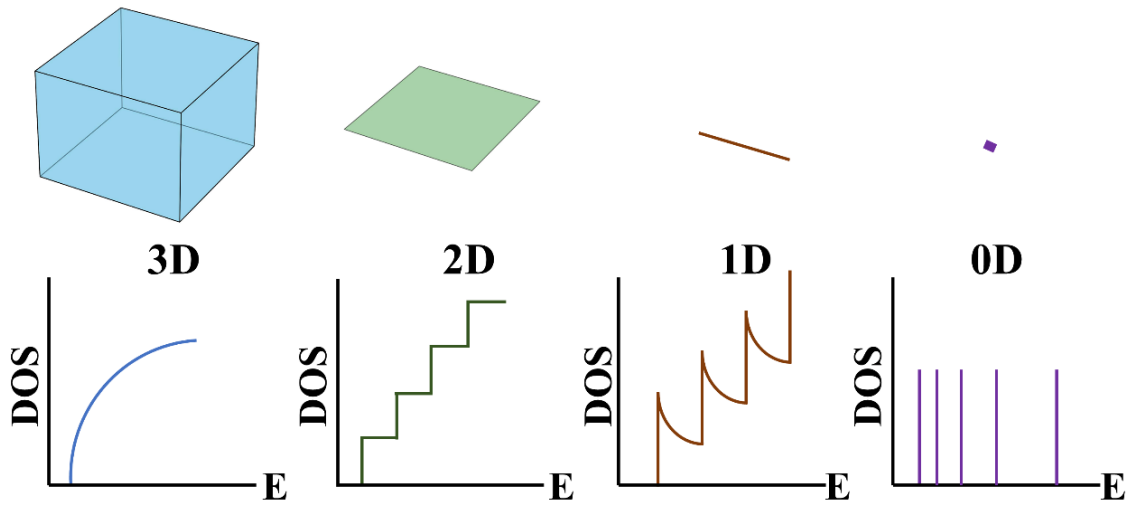

Figure 1.1: A schematic of the density of states of different quantum confined materials as a function of energy.

Quantum dots, being 0D systems, exhibit completely discrete energy levels, and the motion of excitons is restricted to specific quantized states. In 1D systems, carriers are free to move along only one direction, while in 2D systems, electrons and holes have mobility across a surface. This reduced dimensionality and restricted carrier mobility weaken the screening effect, thereby enhancing excitonic interactions, effects that are typically negligible or absent in bulk counterparts [18,19].

To understand the transport properties of these systems, it is essential to examine the density of states (DOS), as variations in DOS resulting from reduced dimensionality have a direct impact on their electrical transport behaviour. The DOS evolving under different confinements, transitioning from the three-dimensional $E^{1/2}$ dependence to the quasi-2D staircase form, then further to the 1D sawtooth pattern ($\sim E^{-1/2}$), and the delta-function peaks characteristic of a 0D system, are illustrated in Fig. 1.1 [20].

1.2 Two-dimensional (2D) layered materials

1.2.1 Graphene and graphene derivatives

Realization of 2D materials came into effect after Konstantin Novoselov and Andre Geim discovered the single atomic layer of graphene from graphite using mechanical exfoliation in 2004 [21–23]. The concept of graphene was first proposed by Wallace in 1947, with a theoretical investigation of its electronic structure [24]. Graphene possesses a flat 2D planar structure and is composed of a single layer of carbon atoms. It is a groundbreaking 2D carbon-based nanomaterial with a hexagonal honeycomb lattice composed of sp^2 hybrid orbitals, which hold π-rich aromatic rings. It can be wrapped up into 0D fullerenes, rolled into 1D nanotubes or stacked into 3D graphite [25,26]. Individual layers of graphene sheets show truly novel transport properties [27]. Graphene is a benchmark material owing to its extraordinary properties such as ultrahigh specific surface area (2630 $m^2 g^{-1}$), higher Young's modulus (1 TPa), quantum Hall effect, excellent optical transparency (97.7%), outstanding thermal conductivity (above 3000 W $m^{-1} K^{-1}$), and superior carrier mobility at room temperature (2.5×10^5 $cm^2 V^{-1} s^{-1}$) [28–30].

A graphene layer is covalently bonded within its planar structure, and it interacts weakly with other materials. The functionalization of graphene is essential to prepare composite materials. Graphene oxide (GO), a derivative of graphene, can serve as a constituent for the creation of 3D graphene with numerous structures that has the ability to associate with diverse functional materials to produce novel 3D-based hierarchical

materials. It is characterized by a high functional group content and with large surface area [31,32]. The GO functionalized with oxygen-containing groups provides chemically stable and surface-modification activity. Graphene and its derivatives are frequently used as a constituent to prepare polymers and inorganic-based composite materials, as it exhibit the highest surface area, enhancing the interaction between the sheets and polymer material. It shows intriguing properties with application prospects in various fields such as electrical and thermal conductivity, structural reinforcement, optics, energy storage, etc. [33–36].

Graphene has been used as a reinforcing filler due to its high theoretical strength and was seen to improve the overall performance and properties of such composites. The addition of graphene can adequately increase the modulus and strength of polyolefin materials. For instance, rGO functionalized-/poly(-vinylidene fluoride) (F-rGO/PVDF) films prepared by Luo *et al.* showed higher mechanical strength with 42% enhancement as compared to the conventional rGO/PVDF films [37–39]. Graphene can also be utilized to improve the thermal and electrical conductivities of polyolefin materials [40,41].

1.2.2 Inorganic layered materials

Motivated by the groundbreaking success of graphene, along with its key limitation of possessing a zero bandgap, the scientific community has increasingly focused on a broad spectrum of graphene-like, ultrathin 2D materials that exhibit finite band gaps. These materials include graphitic carbon nitride (g-C_3N_4), layered metal oxides, MXenes, black phosphorus (BP), and its isostructural counterparts, the transition metal monochalcogenides (TMMCs) such as SnS, SnSe, GeS, GeSe, and SnTe, as well as the transition metal dichalcogenides (TMDCs) including MoS_2, WS_2, WSe_2, $MoSe_2$, and $MoTe_2$ [42–45]. Notably, by controlling the number of layers in these 2D materials, one can tailor their physical, electronic, and optical properties to meet specific functional requirements and application needs.

Layered metal oxides are characterized by anisotropic, stacked crystal structures composed of alternating metal and oxide layers, which offer tunable electronic, ionic, and catalytic properties [46,47]. MXenes, a class of 2D transition metal carbides, nitrides, or carbonitrides with the general formula $M_{n+1}X_nT_x$, exhibit exceptional electrical conductivity, hydrophilicity, and surface functional tunability, making them attractive for energy storage, sensing, and catalytic applications [48]. Black phosphorus is a layered allotrope of phosphorus with a puckered structure, notable for its high carrier mobility and

anisotropic electronic and optical behaviour [49]. TMMCs, with the general formula MX (where M is a transition metal and X is a chalcogen), display strong in-plane anisotropy and hold significant potential in optoelectronic and spintronic applications [50]. TMDCs, on the other hand, have the formula MX_2 and exhibit a wide range of electronic responses, from semiconducting to metallic ones, making them versatile candidates for nanoelectronics, optoelectronics, and catalytic properties [51]. A schematic overview highlighting the key structural and electronic features of various 2D materials is presented in Fig. 1.2. Since this thesis primarily focuses on WS_2 and WSe_2, both members of the TMDC family, a more detailed overview of 2D TMDC materials is provided in the following section.

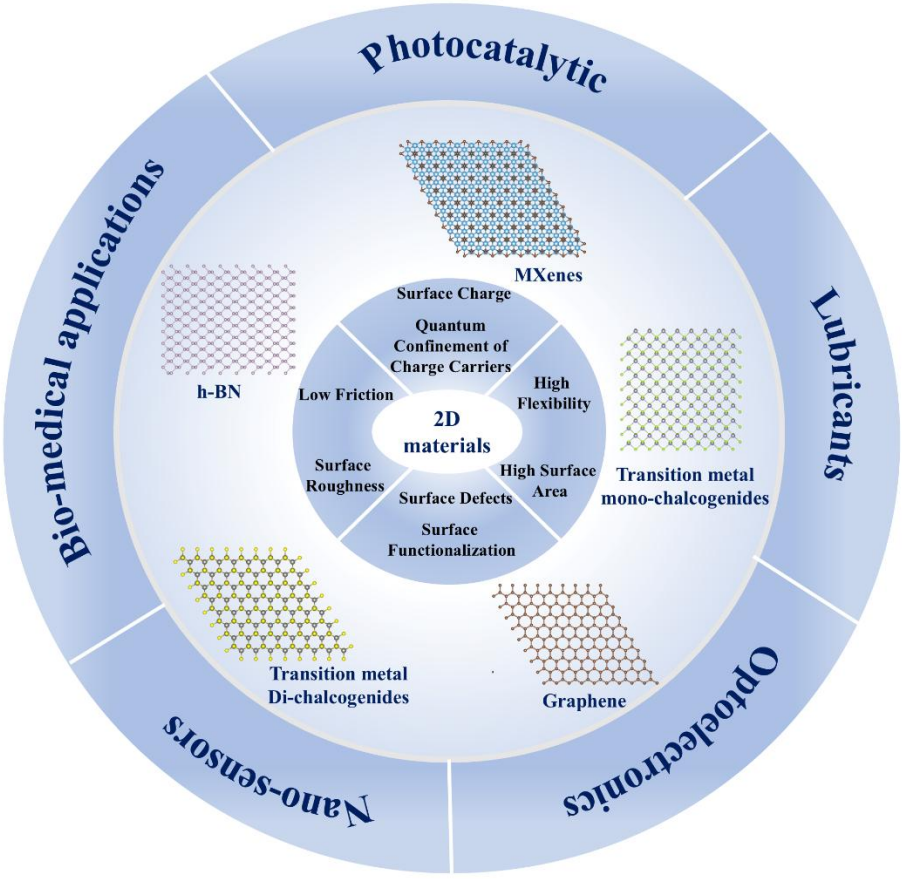

Figure 1.2: An overview of the surface properties and relevance of several 2D materials.

1.2.3 Transitional metal dichalcogenides (TMDCs)

After the discovery of graphene and its derivatives, research into layered nanomaterials, especially 2D TMDCs, has accelerated tremendously owing to their exceptional optical, electronic, and mechanical properties [52]. The structure of TMDCs was first demonstrated by Linus Pauling in 1923 [53]. By the late 1960s, about 60 TMDC compounds had been recognized, with at least 40 exhibiting layered structures. Robert Frindt first reported the creation of ultrathin MoS_2 layers using adhesive tape methods in 1963, and the first successful production of monolayer MoS_2 suspensions was realized in 1986 [54–56]. Since then, the instantaneous progress of graphene research, along with advances in techniques for handling ultrathin layered materials, has created new opportunities for exploring 2D TMDC layers. The TMDCs are often regarded as promising alternatives to graphene and are referred to as graphene-analogous materials. Unlike graphene, which consists of a single atomic layer of carbon, TMDCs are composed of three atomic layers, a layer of transition metal atom (M = Mo, W, Ta, etc.) sandwiched between two layers of chalcogen atoms (X = S, Se, or Te), following the general formula MX_2 [57,58]. The schematic representation of a layered TMDC structure with its interlayer separation of 6-7 Å between two adjacent layers is shown in Fig. 1.3 (a,b). The intralayer X-M-X configuration determines the versatile structural phase of TMDC, offering three atomic layers collectively termed as “monolayer”. The arrangement of atoms within the X-M-X layers produce distinctly different structural phases observed in TMDCs, such as the trigonal prismatic (2H), octahedral (1T), and distorted octahedral (1T′) phases [59,60]. The most prevalent and thermodynamically stable stacking configuration of MoS_2, WS_2, WSe_2, etc. is the 2H phase, where M atoms in one layer are situated directly above X atoms in the adjacent layer (Fig. 1.3 (c)). Further, the layered structure shows unique physical characteristics among many semiconducting TMDCs, such as $MoSe_2$, MoS_2, WSe_2, WS_2, and $MoTe_2$, which are anticipated to display an indirect-to-direct bandgap transition at the monolayer limit, with bandgap energies ranging from ~1.1 to 2.1 eV [61]. The wavelengths comparable to the band gaps of TMDCs fall within the range spanning from the infrared to the visible light region [62–64]. Owing to their distinctive two-dimensional layered structure and exhibiting layer-dependent properties, these systems are currently in focus for potential applications in various fields [65,66]. In this context, 2D TMDCs have gained a wider attention in recent years and are being deeply investigated for use in transistors, photovoltaic devices, lithium-ion batteries, photodetectors, hydrogen evolution catalysis,

and memory devices [67–71]. Moreover, van der Waals heterojunctions made from TMDCs of ultrathin nature exhibit remarkable chemical stability and mechanical flexibility. Most importantly, these heterojunctions integrate the superior properties of two or more materials, resulting in enhanced electrical, optical, and photocatalytic performances. The TMDCs can form both vertical and lateral heterojunctions, which introduce new physical phenomena and improve device functionality [72–74]. These unique features make TMDC heterojunctions highly attractive for fundamental research as well as next-generation applications in electronics, optoelectronics, and energy harvesting [75,76].

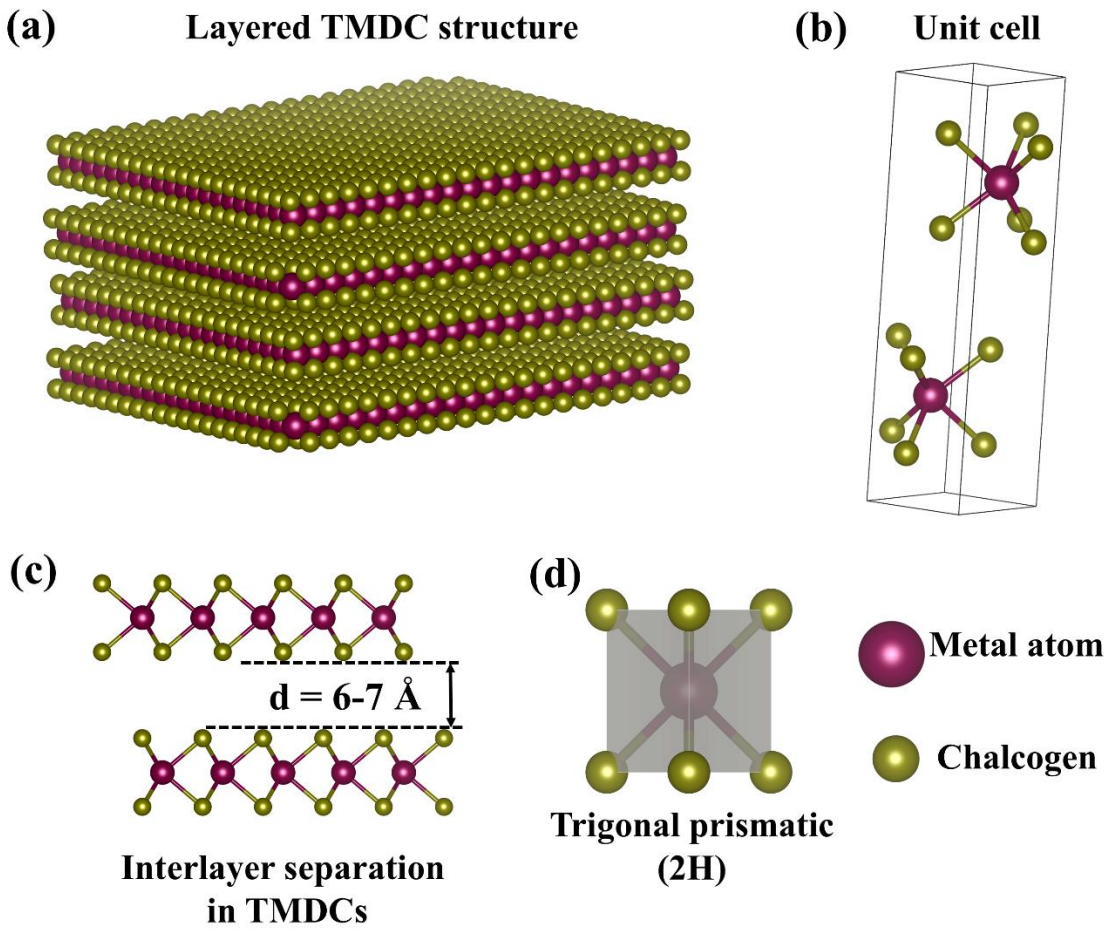

Figure 1.3: Schematic representation of (a) layered TMDC structure, (b) unit cell of TMDC, (c) interlayer separation distance, (d) trigonal prismatic coordination (stable 2H phase).

1.2.3.1 Thermal properties

TMDCs exhibit outstanding mechanical strength and thermal stability, making them potential candidates for next-generation electronic and thermoelectric applications. To fully utilise the potential of electronic devices, one of the most important issues being addressed is heat transfer and management [77]. As device dimensions continue to shrink and operating frequencies rise, thermal energy becomes confined to increasingly smaller regions. When device sizes approach the mean free path of energy carriers, heat transport is no longer governed by the bulk thermal properties of the constituent materials. Instead, it is dominated by energy transfer across material interfaces. Thermal contact resistance, which quantifies the resistance to heat flow at these interfaces, is a fundamental parameter for characterizing interfacial thermal transport [78,79]. Gaining insights into this resistance is crucial for understanding the thermal behaviour of material systems, especially at the micro- and nanoscale, where interface phonon dynamics can significantly influence overall thermal performance compared to bulk materials [80,81].

Recent research has intensified around the thermal properties of graphene and its composites, owing to their exceptional thermal conductivity and applicability in microelectronics. Compared to graphene, TMDCs exhibit significantly lower thermal conductivity, primarily due to differences in band structure, phonon dispersion relations, and dominant scattering mechanisms. Typically, TMDCs show in-plane thermal conductivities on the order of tens of $Wm^{-1}K^{-1}$, with even lower out-of-plane conductivity at room temperature due to their layered structure and the presence of van der Waals gaps [82]. An extensive study on the phonon and thermal properties of thin-film WS_2 deposited on SiO_2/Si substrates by Arkadiusz *et al.* reported that differences in the temperature-dependent phonon responses between bulk and thin-films are related to four-phonon scattering processes and reduced first-order temperature coefficients in Raman modes. The measured thermal conductivity (κ) was 4.3 $Wm^{-1}K^{-1}$, and the thermal interface conductance (g) was 5.5 $MWm^{-2}K^{-1}$. These values are approximately one order of magnitude lower than those observed in single-crystalline mono- and bulk WS_2 [83]. Zulfqar *et al.* provided further insight into TMDC thermal transport by analyzing various monolayers. They reported that WTe_2 exhibits the lowest lattice thermal conductivity (~33.66 $Wm^{-1}K^{-1}$ at 300 K), while WS_2 demonstrates the highest (~113.97 $Wm^{-1}K^{-1}$ at 300 K), attributing this disparity to stronger anharmonicity, isotopic scattering, and lower phonon group velocities in WTe_2 [84]. In addition, thermoelectric power in 1T´ phase of

TMDC, specifically in 1T´-$MoSe_2$, was found to be very large (~6.0×10^{-3} WmK^{-2}) within a temperature range of 100 K-500 K [85].

Beyond thermal properties, another crucial area of investigation in TMDC-based device fabrication involves the interaction between TMDC layers and metal contacts, which significantly influences charge transport efficiency [86–88]. In addition, achieving effective thermal management in TMDC-based devices demands the optimization of interfacial thermal conduction. Tailoring substrate characteristics, such as their interaction strength with TMDC layers and their thickness variations, presents an effective strategy for managing heat dissipation. Consequently, interfacial thermal conduction becomes more influential than in-plane conduction in ensuring efficient thermal regulation in these advanced systems [89].

1.2.3.2 Electrical properties

Research into flexible 2D TMDC devices began in 2012 and has shown superior performance of amorphous, organic, and metal oxide thin-film transistors [90,91]. With their favourable electrical characteristics and extraordinary mechanical flexibility, TMDCs have emerged as promising candidates for the development of high-performance, large-area flexible electronics and circuits [92–94]. A fundamental breakthrough that underscored the potential of 2D semiconductors is the fabrication of a field-effect transistor (FET) with a high ON/OFF ratio using a single layer of MoS_2, which was the first superior device built from a 2D material other than graphene [95,96]. Kaushik *et al.* further demonstrated that FETs based on WS_2 and MoS_2-WS_2 heterostructures exhibit low threshold voltages of -0.28 V and -2.90 V, respectively, at a drain voltage of +1 V, highlighting their suitability for low-power applications [97]. In another study, Cui *et al.* reported that charge carrier mobility in WS_2-based FETs can reach unprecedented values of 83 $cm^2V^{-1}s^{-1}$ at room temperature and 337 $cm^2V^{-1}s^{-1}$ at low temperature (~25 K) by incorporating an Al_2O_3 layer and employing thiol chemical functionalization [98].

The electrical behaviour of TMDCs is highly sensitive to surrounding interfaces and is influenced by both intrinsic and extrinsic defects, including dopants, chalcogen vacancies, and grain boundaries. Depending on the material configuration, TMDCs can form homojunctions (interfaces within the same material but with different charge carrier concentrations), heterojunctions (junctions between two different TMDCs), or Schottky junctions (formed between a TMDC and a metal with a different work function) [99,100].

For instance, an epitaxially grown WS_2-MoS_2 heterojunction reported by Li *et al.* has demonstrated potential in applications such as p-n rectifying diodes, light-emitting diodes, photovoltaic devices, and bipolar junction transistors [99]. In another work by Nguyen *et al.* reported that an Au/WS_2/Ag Schottky diode exhibits high open-circuit voltage (V_{OC}) of 170 mV, a large short-circuit current density (J_{SC}) of 1.45 $mACm^{-2}$, a fill factor of 0.51, and a power conversion efficiency of 5% under illumination with a 625 nm LED.

Furthermore, the electrical properties of TMDCs are strongly governed by charge carrier dynamics, band structure, and transport mechanisms. These characteristics can be further tuned using emerging approaches such as twistronics and valleytronics. Twistronics involves introducing a small rotational misalignment between stacked TMDC layers, which modulates interlayer coupling and electronic band structures [100–103]. In contrast, valleytronics influences the valley degree of freedom, energy extrema in the conduction or valence band, to manipulate material via valley-polarized charge carriers [102,103].

In recent years, considerable efforts have been devoted to synthesizing and exfoliating various TMDC materials, followed by precise structural and compositional tuning to optimize their electronic performance [104–106]. The rich diversity in electronic behaviour of TMDCs has enabled significant advancements in applications such as sensing, energy storage, nanoelectronics, and optoelectronics, etc. [107–109].

1.2.3.3 Mechanical properties

The exceptional mechanical behaviour of 2D materials opens up intriguing opportunities for the development of novel functionalities. These 2D materials exhibit high in-plane stiffness with excellent bending flexibility, which makes them superior to conventional 3D materials. Understanding the mechanical characteristics of 2D materials is therefore critical for the advancement of next-generation flexible electronic and mechanical devices [110–112]. The 2D nanomaterials are often used as reinforcements in polymer nanocomposites due to their distinctive geometry, inherent properties, and multi-functionality. However, achieving effective mechanical reinforcement involves a complex interplay of several factors. It is influenced not only by the intrinsic properties, such as fracture mechanisms, friction, and stress transfer between the 2D layers and the host matrix but also, by various other parameters such as processing techniques, aspect ratio, filler-matrix interfacial property, defect density, volume fraction, and agglomeration aspect [113–115]. Despite these challenges, the incorporation of 2D nanosheets can significantly

enhance not only the mechanical strength but also the thermal, electrical, and optical properties of the composite materials. Thus, nanostructured materials show enhanced features as compared to their bulk counterparts in mechanical aspects such as tensile strength, elastic modulus, hardness, and fracture toughness, along with exhibiting advanced coupled properties, for instance, optomechanical, electromechanical, and thermomechanical responses [116–118]. A few relevant works reported on tensile properties are highlighted. Fares *et al*. explored the impact of γ-irradiation on the mechanical properties of PVC/PANI/TiO_2 nanocomposite films [119]. They reported that the γ-irradiation can initially enhance tensile strength, reaching a maximum of 25 MPa at 100 kGy. Beyond this dose, a declining trend was observed and attributed to polymer chain breakage from excessive irradiation [119]. Sheng *et al.* reported a 37.9% improvement in tensile strength after adding 1.5 wt.% graphene nanosheets (GNSs) in polymethyl methacrylate (PMMA) matrix [120]. Another group, Yang *et al.,* reported that 3.5 wt. % graphene/PVA nanocomposite would offer a 32% increment in the tensile stress [121]. In an article by Sui *et al.*, a gradual reduction in both the ultimate tensile strength and strain at break of polyurethane was reported with γ-ray exposure. When the radiation dose exceeded 300 kGy, the reduction became much slower [122].

On the other hand, following the discoveries of carbon fullerene (C_{60}) by Kroto, Smalley, and Curl in 1985 [123], and carbon nanotubes by Iijima, Reshef Tenne and his group in 1992 [124], proposed that layered inorganic compounds like MoS_2 and WS_2 also adopt non-planar configurations under certain conditions. These materials can transform into closed-cage and hollow-core nanostructures known as inorganic fullerene-like (IF) nanoparticles and multi-walled nanotubes. The mechanical properties of IF-WS_2 and IF-MoS_2 have been extensively studied, primarily due to their excellent solid lubrication behaviour [125,126]. These nanoparticles have demonstrated considerable potential in reducing friction and wear, which has expanded their application in tribological fields. Notably, under moderate pressures (up to 0.5 GPa), the rolling friction of quasi-spherical IF nanoparticles appear to dominate the lubrication mechanism. This effective lubrication is attributed to a synergistic combination of several mechanisms, contributing to their superior performance in reducing wear and interfacial metallic contact [127–131].

1.2.3.4 Optoelectronic and photocatalytic features

Recent studies have focused on developing next-generation optoelectronic devices based on 2D TMDCs, owing to their remarkable optical properties, which differ significantly from those of their bulk counterparts [132,133]. Their exceptionally high exciton binding energy (~300 meV) and large excitonic radii (~1.6 nm), along with distinct excitonic many-body effects and a unique valley degree of freedom, make them highly promising materials for such applications [134]. The focus on investigation of optical properties started after Heinz and Wang, in 2010, who independently showed that a monolayer of MoS_2 possesses a direct band gap and exhibits strong photoluminescence (PL) emission [135,136]. Then, the origins of TMDC-based valleytronics started back in 2012, when valley-selective optical excitation was first observed [137]. The development of van der Waals (vdW) heterostructures began in 2013, enabling the construction of TMD heterostructures and the detection of interlayer excitons. In recent years, research has increasingly focused on the generation of quantum light from localized states and the role of dark exciton states [137].

The optical properties are influenced by modifications in the electronic structure, leading to manifestation in both absorption and luminescence spectra and consequently the lifetime of carriers, excitons and phonons. Their distinctive characteristics, such as sensitivity to light polarization, spectral position, and linewidth, are determined not only by the intrinsic characteristics of the nanomaterial, including its structure, size, shape, and composition, but also by its surrounding environment [138–140].

PL spectroscopy is an efficient technique for exploring the optical emission response of 2D TMDCs arising due to radiative recombination of carriers. It provides valuable insights into events such as the transition from direct to indirect bandgap with increasing layer number, strong Coulomb interactions, and pronounced spin-valley coupling [141]. When a material is illuminated with light with energy greater than the bandgap, electrons are excited from the valence band (VB) to the conduction band (CB), leaving behind holes in the VB. The PL arises when these excited electrons recombine with the holes, emitting light of a certain energy [142]. In 2D materials, reduced dimensionality leads to a weak dielectric screening, which enhances Coulomb interactions and results in stable excitons with large binding energies, even at room temperature [143]. These excitons, consisting of tightly bound electron-hole pairs, which dominate the optical response. Additionally, more complex quasiparticles such as charged excitons (trions),

which possess high binding energies and strong oscillator strengths, play a significant role in determining the optical behaviour of TMDC monolayers [143,144]. A thorough understanding of these phenomena is essential for designing the next-generation electronic and optoelectronic devices. Furthermore, low-temperature PL spectroscopy offers valuable insights into the unique optoelectronic characteristics of TMDCs, primarily influenced by the occurrence of long-lived excitons with strong binding energies reaching several hundred millielectron volts [145]. In addition, 2D TMDCs exhibit remarkable nonlinear light-matter interactions, owing to their giant nonlinear susceptibilities and excellent phase-matching conditions [146]. Nonlinear optical phenomena such as second-harmonic generation (SHG), third-harmonic generation (THG), saturable absorption (SA), four-wave mixing (FWM), and high-harmonic generation (HHG) have been observed in both monolayer and few-layer TMDCs [147–151]. The nonlinear optical properties of 2D materials are of great significance to the design and analysis of photonic applications such as frequency doubling for lasers, microscopy, optical switching, optical bi-stability, wavelength conversion, etc.

In recent years, 2D materials have garnered significant interest for various applications due to their distinctive photoelectrical properties. Among these, photodetectors, which are devices that convert incoming photons into electrical current, play a crucial role in optical communication, image sensing, surveillance, photography, etc. In an article by Kim *et al.*, the group demonstrated that electron beam irradiation (EBI) can enhance the photoelectrical performance of WS_2-based photodetectors [152]. The devices showed responsivities of 0.36, 1.37, and 0.19 mAW^{-1}, and 1.68, 2.45, and 1.09 mAW^{-1} at laser wavelengths of 450, 532, and 635 nm, respectively, after EBI at 1 kV and 3 kV. These findings highlight that WS_2 photodetectors can achieve high responsivity in the visible spectrum, even when processed under low-temperature and rapid EBI conditions [152]. MoS_2-based photodetectors are known for their high photoresponsivity and fast response times. However, their photon absorption is largely limited to the ultraviolet and visible regions due to a relatively wide bandgap (~1.83 eV for monolayer MoS_2), which restricts their application in broadband photodetection. Photodetectors based on heterojunctions, such as WSe_2/MoS_2, $MoSe_2/WSe_2$, and $SnSe_2/MoS_2$, exhibit intrinsic self-powered photo-switching capabilities [153]. For instance, Zhong *et al.* reported that a device utilizing a 9.5 nm-thick α-$MoSe_2$ film achieved a peak photocurrent of 4.60 μA, a

photo-to-dark current ratio (PDCR) of 3067, and a responsivity of 0.94 $mA \cdot W^{-1}$ at zero bias [154].

Monolayer TMDCs materials have emerged as promising platforms for exploring valleytronics due to the breaking of inversion symmetry, which leads to strong coupling between valley and spin degrees of freedom in momentum space. Similar to charge and spin, the valley index can serve as a controllable state variable in electronic devices. Single layers of TMDCs, which are semiconductors with a direct bandgap at the *K*-points, are particularly well-suited for valleytronic applications [155]. There are articles on investigations of spin-valley coupling through optical techniques, and recent advances have begun integrating these methods with transport measurements. Together, these developments point toward promising applications of TMDCs in next-generation electronic and optoelectronic devices [156].

The 2D TMDC-based semiconductors have attracted significant attention for their potential to address global warming and energy issues. Photocatalysis, in particular, has proven to be a promising approach for applications such as wastewater treatment, photo-anodes, water splitting, and pharmaceutical degradation. This process depends on light absorption, charge carrier separation, and surface reaction kinetics [157]. The instantaneous oxidation and reduction of water is a complex, multi-step process and is an energy-consuming reaction involving mixed order kinetics. Improving the efficiency of semiconductors in photocatalysis and solar energy conversion largely depends on increasing the number of surface active sites to facilitate charge carrier absorption. Enhancing photocatalytic performance also involves the construction of semiconducting material to be more porous, thereby increasing its surface area and reactivity [158,159]. In addition, the efficiency of photocatalytic processes is strongly influenced by the light source, as different wavelengths, such as those from daylight or UV light, interact differently with the photocatalyst. For instance, Vattikuti *et al*. reported that the mesoporous WS_2 nanosheets showed enhanced photocatalytic activity with UV light illumination. The optimal concentration of 0.1 wt.% of mesoporous WS_2 resulted in superior catalytic activity carried out in rhodamine B solution, with 97% of degradation within 30 min of UV light exposure [160]. In another article by Aswal *et al*., the photocatalytic efficiency of 2D-2D MoS_2/WS_2 heterostructure exhibited 94 % degradation of methylene blue dye after 180 min of irradiation under visible light [161]. Thus, the

TMDCs are characterised by a high surface area and ample edge-active sites, which facilitate the absorption of photo-generated charge carriers while reducing their recombination rate. Beyond their role as photocatalysts, these 2D materials also find applications in electrochemical devices, sensors, batteries, photo-anodes in dye-sensitized solar cells, and many photocatalytic systems [162,163].

1.3 Irradiation-induced phenomena

Ion beam irradiation technique is well known physical technique for its ability to modify and manifest material properties under a controlled environment [164,165]. Various ion species and a wide range of irradiation conditions can tailor the properties of 2D layered materials at large. The energy of the ion irradiation can be exploited to modify the material properties, extending from low energy (i.e. eV to keV regime) to swift heavy projectile ions (MeV/amu) [166–168]. When an energetic ion traverses through the host material, it transfers energy to the electronic and atomic subsystems in distinct time scales via two ways: nuclear/elastic energy loss (S_n) and electronic/inelastic energy loss (S_e) [169–171]. The energetic charged particles penetrate the target material and undergo multiple collisions. During this process, they interact with both the atoms and electrons within the material. As a result, atomic-scale defects can form when atoms are displaced from their original lattice sites due to the transfer of kinetic energy of projectiles in the target. While at high ion energies, MeV scale energetic ion irradiation of materials results in intense electronic excitations via inelastic energy transfer, which significantly alters structural and physicochemical properties [172–174]. The energy transferred to the target electrons, whether free or bound, generates electron-hole (e-h) pairs, leading to the breaking of ionic and covalent bonds, altered phase transformation dynamics, and increased defect formation and atomic diffusion. The timescales of various ion-induced phenomena occurring within a material are detailed in Table 1.1.

A swift heavy ion (SHI) normally corresponds to the incident ion with energy greater than 1 MeV per nucleon [175,176]. This energy deposited per track length, also known as the electronic energy loss, is typically expressed in terms of S_e. While only a small portion of the energy is transferred through nuclear collisions, conventionally specified as elastic (nuclear) energy loss, S_n [177–179].

An interesting characteristic of the SHI is that it creates columnar type of defects along its path, called ion tracks [180,181]. Depending on the mass and energy of the ion

and the material, SHI can induce a cluster of point defects, defect annealing, defect segregation, and columnar defects in the irradiated material [182]. The various phenomena occurring due to low and high energy irradiation on a target material are shown through a schematic diagram in Fig. 1.4. Accordingly, the role of SHI has become undeniable in defect engineering of materials meant for specific purposes. The energy deposited per unit length and the fluence of the ion beams are extremely critical for defect manifestation, surface patterning and engineering materials [183]. Moreover, a few articles describe the formation of latent ion tracks and its impact on the performance of the devices made in the family of dichalcogenides, such as MoS_2, $MoSe_2$, and graphene, etc. Guo *et al.* investigated the effects of 1 GeV ^{209}Bi and 0.18 GeV ^{56}Fe swift heavy ions for ion fluences 1×10^{10} - 9.4×10^{13} ions/cm^2 on MoS_2 crystals, observing hillock-like latent tracks on the surface of irradiated MoS_2 along with an appearance of a new Raman mode, E^2_{1u}, that occurred near the in-plane E^1_{2g} peak after irradiation [184].

Table 1.1. Typical timescales of ion-induced modifications are summarized [185].

Sl. No.	**Processes occurring**	**Timescale of irradiation-induced phenomena**
1	Electron cascade	10 fs
2	Atomic displacement cascade	200 fs - 2 ps
3	Period of lattice thermal vibration	10 fs
4	Defect clusters and dislocations	ns - stable
5	Defect diffusion	0.1 - 2 ns
6	Chemical effects	fs - stable
7	Thermal heating	100 ns - 10 µs

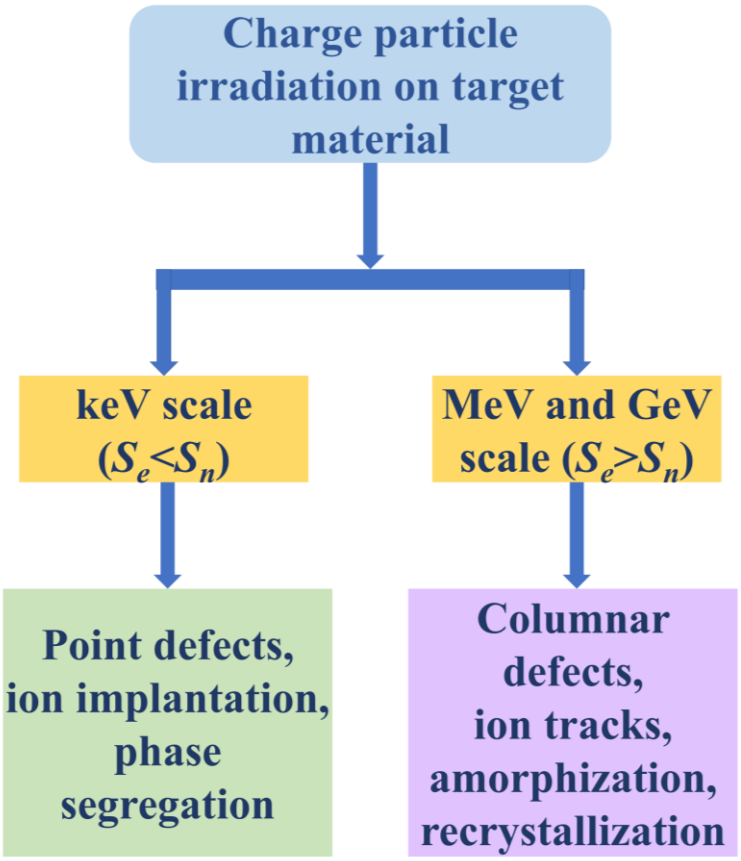

Figure 1.4: Irradiation-induced phenomena occurring at low- and high-energy scales on a target material.

Furthermore, the ion tracks produced due to SHI can be developed into hollow structures with diverse and different shapes through selective etching. Each ion deposits its energy within a narrow cylindrical region, impacting around 10 nm in diameter. Each resulting structure corresponds directly to a single ion track. This technology enables the creation of features with extremely high aspect ratios, up to 10,000 and diameters as small as 10 nm, with lengths extending to several hundred micrometers [186]. Ion track technology possesses several distinctive features. Single-ion tracks have been utilized in various applications, including as apertures for sizing, bio-mimicking devices, and as templates for the electrodeposition of metallic nanowires. While arrays of multiple ion tracks can be employed to create textured materials that exhibit strongly anisotropic permeation and conduction characteristics. These materials enable controlled migration or diffusion of both charged and neutral particles in metals, electrolytes, and semiconductors, and their properties can be tuned in response to changes in temperature, pH, as well as electric and magnetic fields [187,188].

1.4 Theoretical and computational aspects

In addition to experimental studies, researchers frequently rely on theoretical calculations to predict and understand various aspects of nanomaterials, such as phase structure, structural properties, and electronic behaviour. Among the theoretical methods, density functional theory (DFT) has emerged as a powerful and widely used tool [189,190]. By solving the modified Schrödinger equation, known as the Kohn-Sham equation, DFT has proven highly effective in analysing the key characteristics of 2D materials [191].

Theoretical support often enhances the value of experimental observations, providing deeper insights and predictive capabilities. Investigations into the structural and electronic properties of diverse 2D materials, including lattice constants, density of states (DOS), projected density of states (PDOS), band structures, atomic migration, and effective masses of electrons and holes, are essential for physical understanding and to complement experimental validations. For instance, Ma *et al.* experimentally demonstrated that sulfur vacancies in monolayer WS_2 introduce mid-gap states, which enhance saturable absorption in the near-infrared (NIR) region. These findings were corroborated by DFT calculations, which revealed defect-induced states within the bandgap through DOS analysis [192]. In another article, a theoretical study on a SnS/GeSe 2D heterostructure predicted the existence of interlayer excitons with a low binding energy of 0.23 eV. This prediction was later confirmed by the experimental synthesis and characterization of the heterostructure by Sutter *et al.* in 2023 [193,194].

The 2D TMDCs, synthesized via various techniques, commonly exhibit specific types of defects that substantially influence their optical and electronic properties. These defects can alter the crystal structure, affect exciton dynamics, and modify the band structure, impacting device performance eventually. For instance, defect clusters introduced via ion irradiation act as scattering centres, further degrading device efficiency [195,196]. The DFT plays a crucial role in precisely predicting the physical and chemical effects of these defects at the atomic level [197–199]. Beyond its traditional role of interpreting and supporting experimental results, DFT now serves as a predictive tool for assessing the stability and properties of newly discovered materials, making it indispensable in the design and development of next-generation nanomaterials [200].

1.5 Scope of this thesis

There has been a new upsurge of scientific interest in TMDCs because of their atomically thin, layered 2D arrangements. The recent advancements in sample preparation, material transfer, optical characterization, and modification techniques, along with the deeper physical insights gained from studies on graphene, led to the further investigation of TMDC materials. The capability to tune and control the electronic, spin, and optical properties of 2D TMDC materials holds great promise for exploring novel physical phenomena and serves as a valuable candidate for developing next-generation devices. When it comes to ion irradiation of 2D materials, there exists immense potential to investigate their response to a variety of ion types, energies and fluences. Over the past few years, the study of ion track formation by SHI has been a major focus in the field of ion-solid interactions. In particular, for GeV ion irradiation, only a limited number of studies have reported on the formation of latent ion tracks and their impact on the properties of TMDCs.

Motivated by the aspects mentioned above, the following objectives have been proposed for this thesis:

i. To employ liquid phase exfoliation and wet chemical methods for the development of layered transition metal dichalcogenides (TMDCs), namely WS_2 and WSe_2.
ii. To evaluate the mechanical/rheological characteristics of the materials dispersed in suitable carrier fluids (e.g., carboxy methyl cellulose).
iii. To explore the radiation-induced effects of energetic particles on the structural, optical, and optoelectronic properties of the exfoliated nanosystems.
iv. To tailor and compare the physical properties of TMDC systems after ion irradiation at low (keV) and high (MeV-GeV) scale energies, with particular emphasis on excitonic effects of GeV-irradiated systems.
v. To model and predict the physical properties of TMDC materials post-irradiation using DFT, in correlation with the experimental observations.

With the aforementioned objectives in consideration, this thesis work is organised into six subsequent chapters. The experimental processes utilised for developing the WS_2 and WSe_2 materials have been covered in Chapter 2. The mechanical properties of WS_2 systems dispersed in a NaCMC polymeric solution were investigated employing the stress-strain curve at varied concentrations and exposed to gamma rays, as detailed in Chapter 3.

The effect of UV- and β-ray irradiation on the porosity and photocatalytic activity of WS_2 nanosystems were evaluated in Chapter 4. In Chapter 5, the relevance of low-energy 15 keV He^{2+}, 15 keV C^{2+}, and high-energy 0.85 GeV U^{28+} ions on WS_2 systems are discussed, with an emphasis on morphological evolution, luminescence and excitonic characteristics. The effect of low-energy 15 keV He^{2+}, 15 keV C^{2+}, and SHI 60 MeV N^{5+} ions, and γ-irradiation on the morphological and rheological properties of WSe_2 systems are discussed in Chapter 6. Lastly, the concluding remarks of each chapter and the potential future scope of this thesis work are summarized in Chapter 7.

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