Bachelor's thesis 2017

Band Structure Study of Graphene and Transition Metal Dichalcogenides Heterostructures

A Thesis Submitted to the

Department of Electrical and Electronic Engineering

Of

BRAC University

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In partial fulfillment of the requirements for the degree of

Bachelor of Science in Electrical and Electronic Engineering

Summer 2017

BRAC University, Dhaka

An Undergraduate Thesis on Band Structure Study of Graphene and Transition Metal Dichalcogenides Heterostructures for Future Nano Electronic Devices

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Declaration

We hereby declare that the research work titled "Band Structure Study of Graphene and Transition Metal Dichalcogenides Heterostructures" is our own work. The work has not been presented elsewhere for assessment. Where material has been used from other sources it has been properly acknowledged/referred.

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Abstract

According to Moore's Law, it is predicted that the number of transistors –the building blocks of any modern electronic device– on integrated circuits per square inch will double every year. However studies show that the limit would be reached within the next three years as the size of Silicon based transistors, already reduced to a few tens of nanometers, can no longer be further reduced. This is not the only challenge for the semiconductor industry. Besides the transistor size, engineers are also not being able to decrease the minimum voltage required to turn on a device, making it tough for us to build even low power consuming devices. This has compelled us to focus on different alternatives. Graphene has turned out to be the wonder material in the scientific community recently, and its applications are innumerable. It is only an atomically thick 2 dimensional material with very high electron mobility. However, the only reason that acts as the barrier to fully utilize the great potential of this material is its missing band gap. This is when the role of transition metal dichalcogenides (TMDCs) comes into play, another atomically thick 2 dimensional set of materials, which, unlike Graphene, has direct band gap but low mobility i.e. characteristics that can compensate for those missing in Graphene. Scientists have recently combined Graphene with TMDCs to extract the best possible characteristics from both the materials in quest for a substitution for traditional Silicon based transistors in the industry and the results are promising; however, the low current on/off ratio of such devices is still a challenge that needs to be overcome. In our thesis we have simulated band structures of Graphene and different TMDCs like MoS_2, $MoTe_2$ etc. Additionally we have simulated band structures of Graphene interfaced with various TMDCs and also Graphene sandwiched between various TMDCs. Through literature review, we have also found out the spin orbit coupling – a phenomenon that allows us to control electricity through orientation of electrons' polarization rather than the flow of charge – of Graphene and various TMDCs. We have then graphically analyzed our data and finally proposed that by combining the electronic band gap and the spin orbit coupling of a material simultaneously in the future, we may be able to create devices which will be much smaller in size and run with much lower power than current transistors and simultaneously have a high current on/off ratio.

Keywords: Graphene, transition metal dichalcogenides, band structure, spin orbit coupling, heterostructures.

Acknowledgements

We would like to sincerely thank our Supervisor Dr. Md. Mosaddequr Rahman, Professor, Department of Electrical and Electronic Engineering, BRAC University, and Cosupervisor Md. Anamul Hoque, Lecturer, Department of Electrical and Electronic Engineering, BRAC University, for carefully supervising our thesis throughout the three semesters, pushing our limits and bringing the best out of us. Additionally, Saif Ahmed would especially like to cordially thank his teacher Mr. Rachaen M. Huq, Lecturer, Department of Electrical and Electronic Engineering, BRAC University and his friend Rutba Ahmed for their great moral support throughout the period of the thesis; on the other hand, Nafisa Nowshin Ahmed would like to express her heartfelt gratitude to Mohaimin Al Aoun for his unconditional support in every way possible. Moreover, we are very grateful to the other faculty members of the department along with our peers for guiding us during times of need. Last but not the least, we would want to draw attention to the unprecedented support that we got from our family members and friends that encouraged us to be focused and goal oriented.

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Introduction

This chapter gives an introduction to our thesis to give readers an overview, followed by the future possibilities of the field we have conducted our research on.

1.1 Introduction

Digital and analog electronics are the two classified divisions of the semiconductor technology. Silicon based MOSFETs are mostly utilized for digital electronics and have a great investment made on them, especially in the last four decades. This has given a tremendous advantage to the Si CMOS technology, making any new technology difficult to survive after an entry into the industry. In contrast, the scenario tends to be opposite for analog electronic circuits as it is not as highly integrated as the former one and thus seems to be more adaptive towards newer forms of technology in transistors. [1] There are two types of semi conductors which we mainly work with. One is an N type semiconductor, mainly responsible for the transfer of negatively charged electrons, while a P type semi conductor deals with holes, known as electron deficiencies. Among many examples, Silicon based ones have proven to be the best semiconductor is use, which forms the basis of most integrated circuits in the industry.

To cope up with the continuously increasing demand of technological advancement, designers have sought out ways to decrease the sizes of these transistors until recently where their sizes, already being reduced to nano-scale, cannot be further reduced, violating Moore's law: Gordon Moore, co founder of Intel made an observation in 1965 stating that the

number of transistors present on integrated circuits per square inch had increased by a double each year since its discovery. By following the prediction of this law, for a very long time, a dynamic evolution took place, profiting the industry as there was a reduction of 25 percent per year in the cost of a transistor. This led to a boom of almost 17 percent and the main reason responsible for this was the continuous nano scaling of Silicon based MOSFETs. The International Technology Roadmap for Semiconductors (ITRS) requires 10nm MOSFETS by 2020 however, till date 20nm gate transistors have been in mass production. [2] On the other hand, for some time many scientists have been able to confirm that as technology advances, Moore's law may be valid for more decades and not indefinitely, making the size of transistors saturated. It has been well estimated by research and many studies strongly suggest that the physical limit of Moore's Law will be reached around 2020.

This brings our attention to think of newer materials to be used in MOSFETs that can follow the Moore's Law. Among many characteristics required for an ideal semiconductor, having great carrier transport properties, high thermal conductivity and a sufficient band gap stand out to be the most important ones. All these qualities are rare to find in one material, which has compelled us to think of combining two materials: Graphene and TMDCs (transition metal dicalcogenides). Termed as a wonder material because of its 2D nature after its first discovery in 2004, Graphene, a semi metal, has a very high mobility compared to that of the other type of materials: TMDCs. However, Graphene has a zero band gap and a low spin orbit coupling SOC -a phenomenon that allows us to control electricity through orientation of electrons' polarization rather than the flow of charge .[2] Unfortunately, not having a band gap takes away its chances of creating efficient Graphene based transistors. The semi metallic nature causes the current on-off ratio in Graphene based transistors much lower than the required minimum. Nevertheless, apart from this drawback, Graphene shows great promise in high speed analog electronics because the current gain of transistors has more of an importance than the on-off ratio. [3] To cope up with the limitations of Graphene in digital electronics, the characteristics of TMDCs (such as MoS_2,$MoTe_2$,$WS_2MoS_2WSe_2$, $MoSe_2$) play a great role because they have a

much higher SOC than Graphene. However, TMDCs have very low relative mobility. But, When scientists have combined TMDCs with Graphene and created an interface – such as Graphene + MoS_2, Graphene + WS_2 and so on – the results were promising. This is measurably higher than when we only work with Graphene and helps in driving a device at a much lower supply voltage. Thus, a newer proposition of transistors for the next generation can be a combination of Graphene with TMDCs. Furthermore, the spin can be controlled using the combination of these two together, causing us to choose and work with this topic and explore its true potential.

1.2 Scope of the Thesis

The scope of our thesis is to conduct a thorough research on the band structures of the of Graphene and its interface with various TMDCs, as well as a sandiwiched heterostucture with Graphene in between two TMDCs, and to combine the band gaps obtained with the intrinsic spin orbit coupling of these very materials for higher efficiency and current on off ratio in our proposed Graphene/TMDC based field effect transistors. For years, we have gained the benefits of using traditional field effect transistors, such as MOSFET (metal oxide semiconductor field effect transistors) in our electronic devices, however certain limitations of MOSFET has compelled us to explore various materials and features for a better performance. Our thesis proposes the addition of the band gap and the SOC (spin orbit coupling) for each of these combinations, which would contribute to generate similar on off current ratios to that of ideal MOSFETs. This in turn would ensure that a lower voltage would be required to turn on a device, which will be much smaller in size than traditional MOSFETs, making better transistors with higher efficiency in integrated circuits for the upcoming generation. We certainly believe that, with time and with proper research, Graphene/TMDC based field effect transistors would prove to be better alternatives in terms of size and have its implementation in a variety of devices with respect to the Moore's Law. To be more precise, in addition to finding the band gaps, our thesis hopes to make relevant comparisons of SOC with the change of its mobility

and temperature in different topological insulators and semiconductors. Throughout our research, we studied the combinations of materials, such as WeS_2, MoS_2, $MoSe_2$ WS_2 with Graphene. Our thesis sets out to generate and simulate their band structures to find out their band gaps and how each factor can be manipulated to reach the best possible output for integrated circuits. As we progressed, we found out the theoretical spin orbit coupling values from various scientific papers (given as references at the end of the thesis) along with band gaps for individual, sandwiched and interfaced materials (Graphene with various TMDCs, such as MoS_2, WS_2 and so on) through simulation software. Our research helps in producing theoretical and simulated results and hopes to provide enough data and information for future study in this subject arena and encourage more attention to be given to this proposition.

2

Literature Review

This chapter starts with a brief overview field effect transistor (FET), followed by the limitation of traditional MOSFET, followed by its alternatives: Graphene-FET and spin FETs, which relies on the applications of spintronics. The chapter also discusses how spintronics is implemented in Graphene.

2.1 Field-Effect Transistors (FETS)

A semiconductor device, having three terminals where the source and gain (two electrodes) have voltage applied on them, is known as a Field Effect Transistor (FET). A channel is formed under the gate which controls the flow of charge carriers between the source and the drain (the third electrode). The source and gate control how much of conductivity does the semiconductor have. An n-channel FET has a channel formed in the n type semiconductor, while a p type semiconductor is referred to as a p-channel FET. MOSFET (metal oxide semiconductor field effect transistor) is the most commonly used FET in the semiconductor industry. MOSFETs are embedded in microprocessors and memory devices in numbers of thousands to millions for implementing logic gates and data storage, which act as the basic switching functions. Along with this, they are also used for amplifying electronic signals. There are two types of MOSFETs known as depletion mode and enhancement mode. The current on-off ratio for typical FETs is around 10^6 to 10^{10}, which is the ratio for the current of accumulation current over the depletion mode. [4]

Moore's law predicts that the number of transistors in an integrated circuit will double every two years. Over the years, the size of these devices have been made smaller and smaller and thus the number of transistors have increased in an integrated circuits. But conventional silicon based MOSFETS are reaching its limits as sizes of these transistors can no further be reduced than a few tens of nanometers and the performance of these devices cannot further be enhanced.

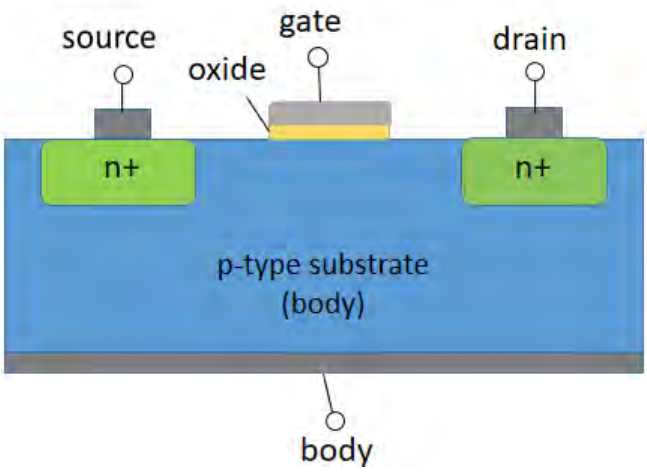


Figure 2.1: Traditional charge-based MOSFET

Thus further researches needs to be conducted to model out substitute forms of transistors with significant reduction in size according to the Moore's Law.

2.2 Graphene FET

In this era, a large number of chip makers have been involved in Graphene research and fabricating Graphene transistors and they are doing it quite successfully. Graphene has become a better alternative for making transistors instead of Silicon.[5, 6]

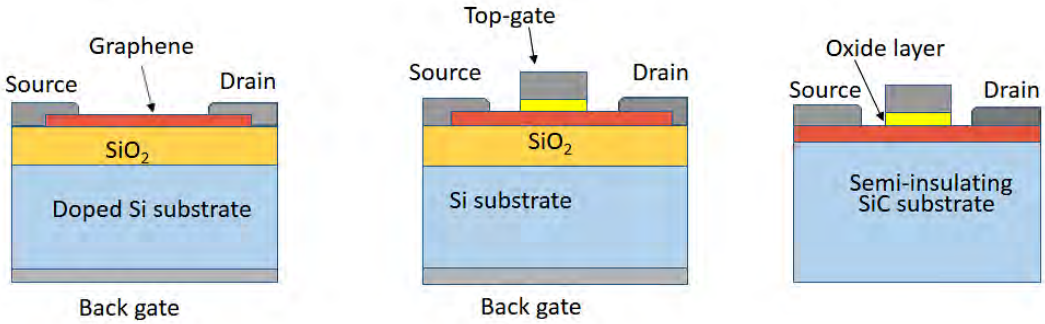


Figure 2.2: This figure represents various types of Graphene MOSFET: the figure at left shows back-gated Graphene MOSFET; the figure at the center shows top-gated Graphene MOSFET where a channel of Graphene is exfoliated or grown on metal and transferred to a Si wafer covered in SiO_2; the fiure at the right shows top-gated Graphene MOSFET with an epitaxial-Graphene channel. Either large-area Graphene or Graphene Nanorribon can be used to make the channel shown in red.

The above diagram is of different types of Graphene FET like top gated, back gated, Silicon substrate, SiC substrate etc. [5] In spite of many properties and functions, Graphene is still undetermined. Although the high mobility of Graphene in room temperature is highly advantageous, the ultimate challenge lies with its absence of band gap which makes the practical implementation of these devices very challenging.

2.2.1 Challenges of Graphene FET

Graphene has a zero band gap but a huge area. The huge area of Graphene channel can be used in any device, but the transistor/device would be unable to switch off because of Graphene having a zero band gap. One of the prominent properties of Graphene is its high carrier mobility at room temperature. It has a mobility of around 10,000- 15,000 cm^2/Vs for Graphene on Si wafers (covered by SiO_2). By choosing the gate dielectric properly (of Graphene FET), a high mobility can be achieved. Now, although the mobility achieved for Graphene is very high, the band is gapless and this is a problem that is faced in Graphene FET transistors. [5]

However, the band structure can be modified. This is the reason, fabrication of bilayer Graphene FET is introduced and it is found that the band gap can be increased up to 130 meV in bilayer Graphene. [5, 7]

To determine speed carrier transport effectively on a FET, the carrier's mobility is a good option. The mobility depends on the electric field. A top gate is needed for Graphene transistors. There is a large positive gate voltage that produces electron accumulation in n-type channels and negative gate voltage for p-type channels. As mentioned already, the practical Graphene transistors have large area with no band gap, so switching them off is a challenge. The on/off ratio which is reported is in the boundary of 2-200 [5] and is very low. According to [7], in bilayer Graphene, the current on/off ratio observed is 100 and in single layer Graphene, it is 4, so in bilayer Graphene the ratio is almost 25 times larger (this was considered in room temperature and when drain voltage is 1V and source voltage is grounded). Here, the maximum current on/off ratio can be gained when the back gate bias is at its optimum, by modulating the top gate bias.

In case of 2-D bilayer Graphene, if we can introduce spin-FET (pseudospin) between two Graphene layers using thin dielectric layers and under some bias condition, we can shorten the tunneling resistance between two layers effectively. If it is done, the FET would supply high current and if the

tunneling resistance gets high, it would shut the current off and would deliver both much faster. [5]

2.3 Spin-FET

Another promising alternative device seems to be spin field-effect transistors or spin-FETs or simply spin transistors, devices which are still under development and utilize the application of spintronics or electronic spin transport technology to operate.

Quantum mechanics define electronic spin as one of the two inherent forms of angular momentum present in electrons. Semiconductor devices have depended on the charge of the electrons and ignored the electronic spin degree of freedom until lately. After realizing the existence and thus the possibility of practical implementation of the phenomenon, scientists are using electronic spin transport property to store and process information, thereby giving rise to spin transistors which combine the existing microelectronics with interaction between the magnetic property of the materials and their spin carriers [8]. If the spin degree of freedom is successfully implemented in coherence with the electronic charge transport depended transistors, or even if solely the spin degree of freedom can be implemented in modern microelectronic devices i.e. the spin-FETs, the result will be the production of far more superior and capable information processing and storage devices with higher efficiency in terms of power consumption, much higher data processing speeds and increased density of integrated circuits [8].

Spin-FET in semiconductors introduced high performance and low power consumption of electronic devices. Efficient injection, detection, transportation and manipulation, being the fundamental prerequisites for the application of spintronics in transistors, an equally vital factor is the choice of material being used to build these devices because spin currents must be transported over a relatively long path (transport length) at room temperature, for which the orientation of the electron spin must be suitable and needs to have an undisturbed alignment over a long range for a long period of time (spin lifetime) [9]. Silicon has caught the attention for spintronic applications besides metal. With spin lifetime and diffusion length of electrons, orders of magnitude higher than metals [10, 11, 12], semiconductors are good candidates for spin transport, especially silicon whose low spin-scattering and lattice inversion symmetry contribute to a better spin lifetime and longer electron diffusion length [10].

2.3.1 Spin Transfer-torque-Switch MOSFET

Spin-Transfer-torque-Switching MOSFET (STS-MOSFET), as shown in figure 2.3, is a proposed, improved silicon spin based MOSFET with better transport properties than other silicon based MOSFETs which lack spin manipulation and control due to silicon's low spin orbit coupling. STS MOSFET is better because in STS, one can utilize spin manipulation due to the presence of magnetic multilayers. It is also known as magnetic tunnel junctions (MTJ) that controls the spin while reducing contact resistance. Spin manipulation can be utilized in magnetic tunnel junctions (MTJ) or giant magneto resistance (GMR) on the source and/or drain using tunnel barrier. The area of Magnet Tunnel Junction(MTJ) determines the current while small MTJ can be involved in manipulation of the direction of spin.

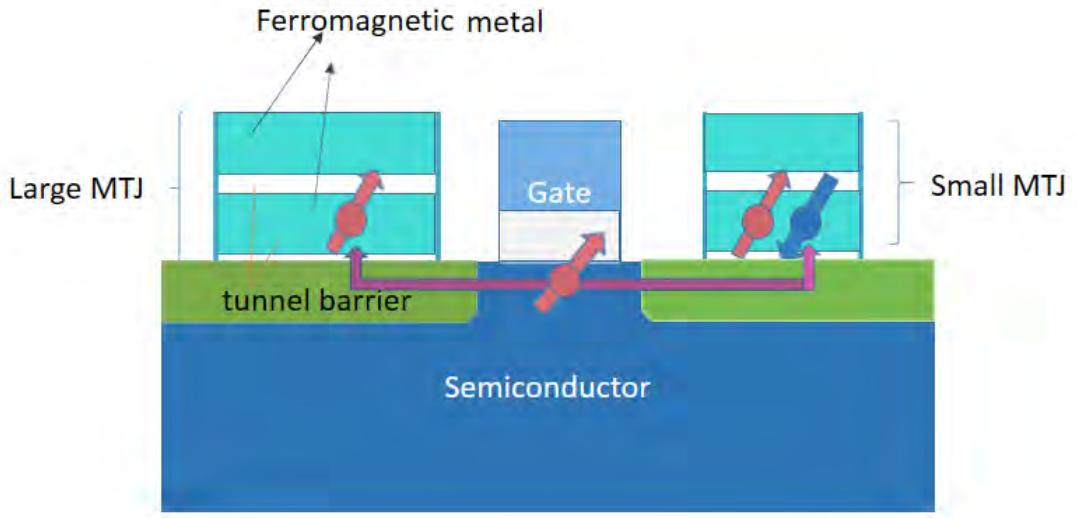


Figure 2.3: Spin Transfer-torque-Switching MOSFET (STS-MOSFET) in which magnetic tunnel junction (MTJ) is contacted to source and drain electrodes

The prime application for spin–MOSFET is in programmable logic chips which is possible due to its fast writing time along with transistor functions, non-volatile memory, high longevity and CMOS compatibility. One of the advantages of STS-MOSFETs includes large on/off current flow ratio which is gained by using Silicon based p/n junction to control the gate voltage. [13] Such devices are still in initial stage of development.

2.4 Spintronics in Graphene

Graphene possesses many amazing physical properties which make Graphene a better choice for spintronic applications compared to STS-MOSFETs. However, just like in any application of spintronic devices, major challenges in spintronics in Graphene also lies in the following four areas :

- Spin Injection
- Spin Detection
- Spin Transportation
- Spin Modulation

2.4.1 Spin Injection and Detection in Graphene

Graphene has effective spin injection and detection which occurs in it simultaneously. For spin injection and detection in Graphene, two processes can be followed : Non-Local and Local measurements.

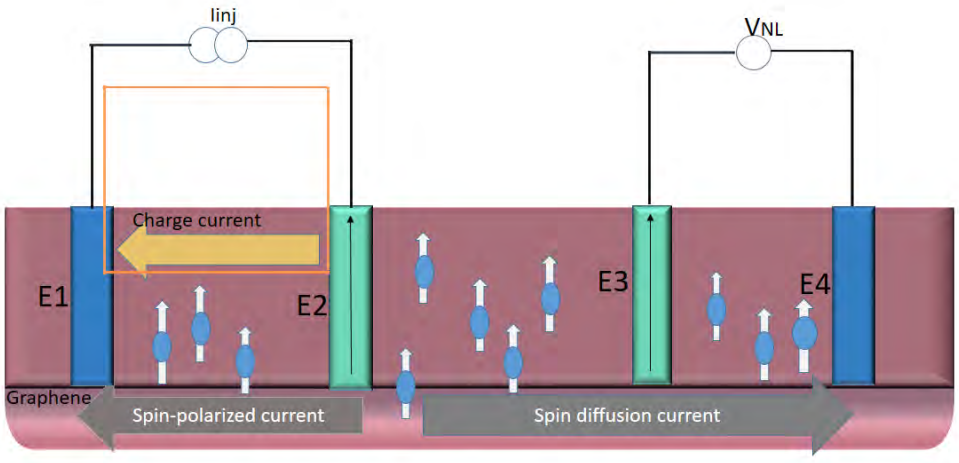


Figure 2.4: Figure 2.2: E1, E2 and E3, E4 are two pair of electrodes. E2 is used as spin injector and E3 as Spin detector

In figure 2.2 the local measurement in shown. There are two separate electrode pairs E1, E2 and E3, E4. After spin injection occurs in E2, E2 will be considered as the spin injector and E3 will

behave as the spin detector. Spin will diffuse from E2 to both E1 and E3. Our focus here will be on spin diffusion from E2 to E3. There is a current source between E1 and E2 which produces the spin current (Iinj) and will later be used to supply injection of spin in E2. [14, 9]

In figure 2.2 the non-local measurement is also shown. A voltage source is shown in figure, measuring voltage between E3 and E4. The diffused spin moves to the detector E3 and because of the parallel and anti-parallel spins, two kinds of voltage is achieved : let us assume Vpar and Vanti; then VNL is the magnitude of the difference of these two voltages, which is found in the voltage source and we get the resistance : RNL(Vnl/I).This (Rnl with magnetic field) provides an idea of numerical value of spin polarization of detector and also injector. From RNL, we can detect the undistorted spin signal. [14, 9]

Because the spin from E2 is moved to E3 due to spin diffusion, the spin detection occurs in E3 electrode and thus, E3 is the spin detector. However, it is difficult to measure spin using non-local measurement process because of high mobility of Graphene. So we can use the local measurement process for spin detection (the diffused spin from E2 to E3).

From figure 2.2 we can also see that in the process of local measurement, two electrodes have been used and only a voltage source is used to detect the voltage achieved due to the diffused spin from E2 to E3. Let us say that the resistance here is Rl and This Rl is not effective enough to measure to detect undistorted spin signal.[14]

2.4.2 Spin Transportation in Graphene

Graphene's spin transport system is a very impressive property because of its long spin lifetime and long distance spin propagation. It also has a long spin diffusion length which makes the spin transport of Graphene very promising in recent studies. As previously discussed, it is difficult to observe the transport using non-local process. In local process, E1 is the spin injector and E2 is the spin detector. The movement of spin from E1 to E2 is the spin transport. Spin transport in Graphene is observed in large area of Graphene and it has higher mobility. Manufacturing in large area is done by chemical vapor's installation. In room temperature, the spin diffusion length is several micrometers. [14]

Referring to figure 2.2, when the spin moves from injector to detector it is called spin transport.

The non-local resistance RNL gives a proper idea on how to quantify spin lifetime and diffusion length of Graphene channel.

2.4.3 Spin Modulation in Graphene

Spin modulation is the most challenging part of spintronics. The idea of spin modulation in spin-FETs is based on spin orbit coupling. The manipulation of the magnetic properties of spin with electric field in nanostructures has been an attraction in spintronics. Recently, it has been shown that spin states of anti-ferromagnetic field can be modulated by internal electric field. A new phenomenon that gives a new dimension to electronic devices is by using modulated spin current by either electric or magnetic field. The spin is predicted to make a new revolution in the next generation because of logic and memory functions. Spin in Graphene catches the interest even more and the reason is the propagation of spin of Graphene covering long distances due to its small spin orbit coupling and negligible interaction. However, it also infers that the spin of Graphene cannot be modulated by external electric field but it can be modulated by magnetic field, which is known as Hanle spin precession [9, 15] and an alternate way of spin modulation by magnetic field is to use adjacent ferromagnetic insulator. It has been predicted that if the spin of Graphene can be modulated, it will take spintronics to a new level.

3

Materials

The main idea of our thesis is discussed here as properties of materials like Graphene and Transition Metal Dichalcogenides (TMDCs) are studied.

3.1 Graphene

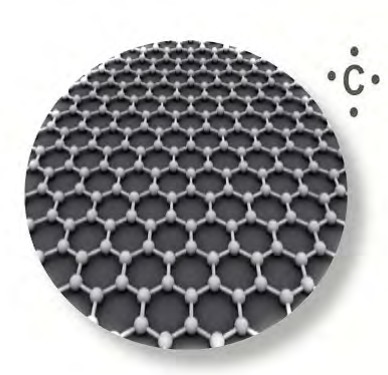


Figure 3.1: A single layer of graphene

Scientists have long depended on Silicon for making Silicon based semiconductor devices such as Metal Oxide Field Effect Transistors (MOSFET), which are the building blocks of any modern digital system until recently, as the sizes of these devices cannot further be reduced. Hence, the new focus has been on Graphene and transition metal dichalcogenides (TMDCs) which not only have great electronic transport properties but also can be used to make spintronic devices.These devices would depend on how efficiently the spin-polarized currents can be generated and how well the electric field can be manipulated.

A 2D material [16], Graphene is an excellent choice for the development of minimal power consum-

ing spintronic devices due to its long spin relaxation length [17, 18, 19], gate tunnability [17, 20], ballistic charge transport property at room temperature [17, 21]. Topological / quantum spin hall effect and spin hall effect are among other intriguing phenomena [16, 22, 23, 24] that are being difficult to achieve in Graphene due to its extremely limited spin orbit coupling.

However, despite having an excellent carrier mobility, [25, 26], Graphene's practical implementation is difficult due to its missing band gap and very weak inherent spin orbit coupling [16]. Missing band gap leads to have high off current [27], an undesirable property of transistors that leads to increased power loss (I^2R loss) while weak spin orbit coupling makes it difficult to control the spin through electric field. Even though spin manipulation can be done in Graphene, it requires a large amount of voltage, which is not practically convenient to implement in nano-scaled devices. This is because it will use up a significant amount of power and hence increase I^2R loss even further. In order to overcome this barrier, various theories have been proposed [28, 29, 30, 14] and experiments have been conducted but not without compromising Graphene's inherent electronic or lattice structure and material quality [28, 14, 16, 17, 31]. If these qualities are not kept intact and unaffected,Graphene is no more special than other materials that are already in widespread use.

For instance, the spin orbit coupling of Graphene can be sharply increased by weak hydrogenation of Graphene [17, 16]. But this converts the sp_2 to sp_3 bonds [16], significantly decreasing the mobility of the electrons as structural disorder is introduced [17, 20]. Due to electronic (Anderson) localization [16], [16, 32] and clustering of hydrogen atoms [16], [16, 33], Graphene loses its semi-metallic property [16]. Simultaneously, carbon-hydrogen hybridization introduces sp_3 defects by inducing a Rashba type spin orbit coupling which breaks the inversion symmetry of the lattice [17], [17, 34]. Similar approaches such as lateral confinement into nanoribbons have been initiated to induce band gap in Graphene but it has led to considerable reduction of carrier mobility, loss of coherence and increased off-current compared to that of Graphene [27]. Another unsuccessful effort to enhance Graphene's intrinsic spin orbit coupling includes injecting heavy atoms such as Gold (Au), Thallium (Tl) or Indium (In) as impurity [17, 30, 35], but this too jeopardizes the intrinsic structure of Graphene and hence the charge and spin transport properties [17, 36]. However, in all the cases, ultimately the mobility of Graphene is severely compromised, nullifying the entire concept of using Graphene because then, we can opt for more convenient high spin orbit coupling heterostructrures such as transition metal dichalcogenides (TMDCs).

3.2 Transition Metal Dichalcogenides

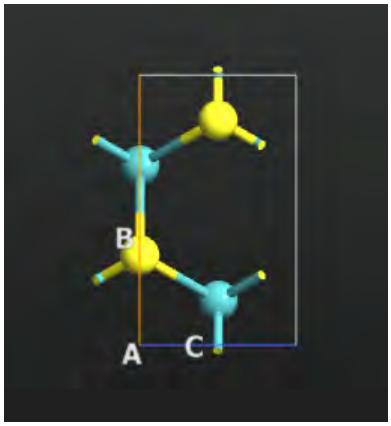


Figure 3.2: Atomic model of MoS_2, a TMDC

Like Graphene, transition metal dichalcogenides are atomically thin 2D materials with diversified electronic properties [25, 37, 20]. TMDC monolayers have molecular formula MX_2 where M refers to a transition metal and X refers to dichalcogenides [25]. Examples of widely studied transition metal dichalcogenides include Molybdenum Disulphide (MoS_2), Tungsten Disulphide (WS_2), Molybdenum Diselenide ($MoSe_2$) and Molybdenum Ditelluride ($MoTe_2$). These materials are of particular interest to us due to having direct band gaps [25, 29], [25, 29, 38, 39, 40], unlike Graphene, making it suitable for use in field effect transistors [41] for future nano-electronic device applications as this leads to demonstration of better gate controllability [27]. TMDCs have spectacular mobility at room temperature [37], which makes it an ideal choice for application in electronics and optoelectronics [37]. TMDCs are chemically inert and atomically flat, an extremely important characteristic to retain quality transport properties [28]. However, the mobility in a MX_2 monolayer like WS_2 is still much lower than that of Graphene [28], due to the presence of prevalent, inherent defects in the structure of WS_2.

Importantly, the lattice structures of monolayers MX_2 are found to remain constant as that of bulk MX_2; band structures of two-dimensional (2D) transition metal dichalcogenide are calculated along with investigation of monolayer transition metal dichalcogenide transistors using ab-initio theory. [27] With valence and conduction band edges, chiefly contributed by dx_2, dxy_2 and dx_2-y_2 orbitals of M atoms, placed at the two corners of the first brillouin zone (i.e. K and – K points) transition metal dichalcogenides can thus be deemed similar to that of Graphene [37]. This, combined with large spin orbit coupling in MX_2 monolayers and absence of inverse symmetry, another interesting

property of MX_2, give rise to the strong splitting between the spin which are quintessential in spintronics. [37]This makes MX_2 an almost ideal material for spintronic applications [17] only to be hindered by the relatively much lower mobility when juxtaposed with that of Graphene.

3.3 Graphene on Transition Metal Dichalcogenides

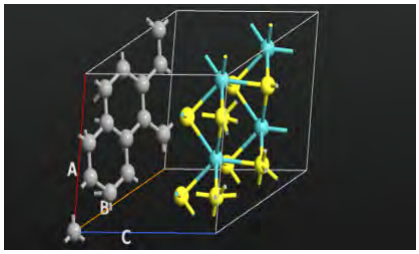


Figure 3.3: Atomic model of an interface between Graphene and MoS_2

Despite having an extraordinary potential for not only spintronic applications but also optoelectronics in the near future, both Graphene and TMDCs have their own limitations that prevent their revolutionizing phenomenon to be practically implemented in the world of electronics. Therefore, another promising alternative has been proposed to significantly increase the spin orbit coupling in Graphene, without affecting its inherent properties. It is possible to simultaneously retain only the high charge carrier mobility of Graphene and prominent spin orbit coupling of TMDCs by combining Graphene with TMDCs. " Graphene on TMDCs has already been grown and investigated for transport as well as considered for technological applications." [42] It has been experimentally shown that the retention of high charge carrier mobility of Graphene and large spin orbit coupling of TMDCs is possible by exploiting the proximity effect between Graphene on TMDCs, which, even at room temperature, will eventually result in a gate tunnable spin hall effect, a key to spintronic application. [17]

The ultimate focus being, reduction in transistor size, although the performances of all the different monolayer MoX_2 transistors are similar due to the similarity in the electron effective masses, Tungsten Disulphide (WS_2), one of the more promising members of the TMDC family, has the best performance within ballistic regime for use as transistors [27]. WS_2 transistors outperform 2D-Silicon transistors in terms of on-current by about 28.3 percent, exhibiting good gate control and resulting in high on current, making it a tough competitor to replace Silicon field effect transistors, added to the fact that the lack of dangling bonds in MX_2 prevents the formation of native oxide

on the surface of monolayer MX_2. This otherwise results in a further increase in the total gate insulator thickness in 2D-Silicon transistors but cannot do so in MX_2 transistors.[27] Due to a similar work function between Graphene and Tungsten Disulphide (WS_2), the charge neutrality point of Graphene is roughly centered at middle energy gap of WS_2, which in this case acts as an inert substrate, much like Silicon Dioxide or Boron Nitride. [17] Interestingly, the very presence of intrinsic defects in WS_2 limits its charge carrier mobility and hence the practical use, as discussed earlier, acts as a sink for electronic charges. This enables a gate-biased independent conductivity when WS_2 is used as a substrate on Graphene, provided the substrate is thick enough to have to create a large number of defects. [17]

4

Results

In this chapter, the simulated and studied results are discussed in details. We have comprehensively simulated the band structures of Graphene, all relevant Transition Metal Dichalcogenides (TMDCs) and their interfaces. We have also simulated the band structures of sandwiched heterostructures, where we have put Graphene in the middle of two exact layers of TMDCs and observed higher band gaps compared to that of simple interfaces.

4.1 Atomic Structures of Graphene and TMDC Heterostructures

Figure 4.1a represents a 2D structure of Graphene. It is a unit cell representation with A and B vectors perpendicular to the C vector, which is parallel to Z. Initially, we obtained an orthogonal unit cell of Graphene with Z direction pointing out of the Graphene cell, but it should lie on the plane. Hence, we swapped the axes by interchanging A and C followed by interchanging Z and X.

Figure 4.1b is the 2D configuration of Molybdenite or MoS_2 represented in unit cell with similar vector representation as that of Graphene. We have performed the same axes transformation on MoS_2 as we did for Graphene. Here, the yellow spheres represent the Sulfhur (S) atom while the blue sphere represents the Molybdenum (Mo) atom.

Figure 4.1c represents the interface between Graphene and MoS_2. The grey spheres represent the Graphene atoms while the yellow and blue spheres represent the Sulfur and Molybdenum atoms, respectively. We can notice the formation of new bonds between Graphene and MoS_2. This is giving the structure more stability as internal bonds are formed between Graphene and MoS_2, as observed from the diagram. Graphene + $MoSe_2$, Graphene + $MoTe_2$, Graphene + WS_2,

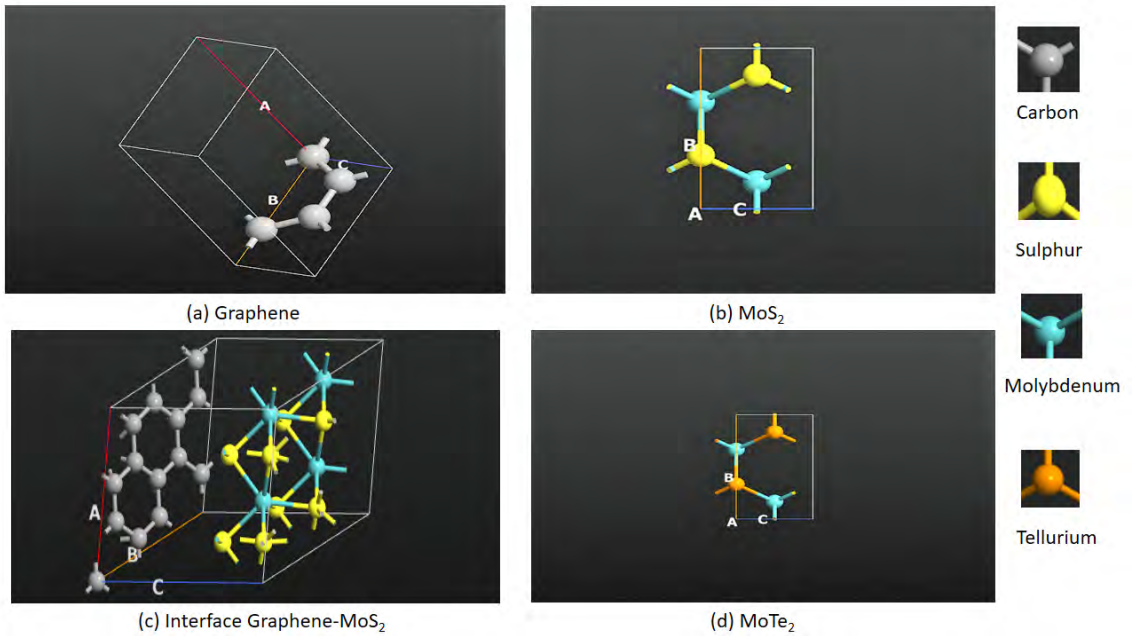
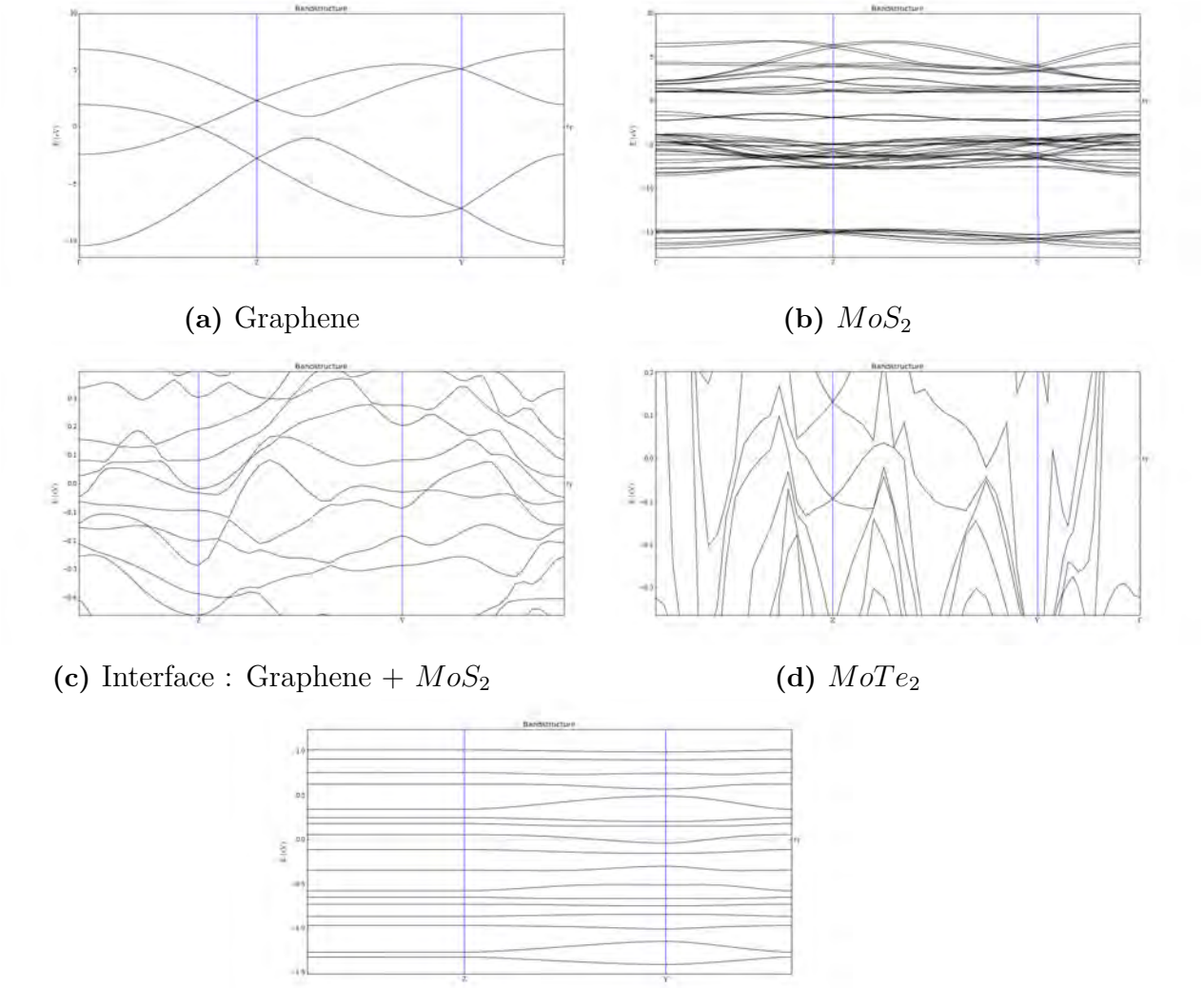


Figure 4.1: Figure 4.1a represents the atomic structure of Graphene comprising of carbon atoms only. Figures 4.1b and 4.1d represent MoS_2 and $MoTe_2$, respectively with blue atoms representing Molybdenum (Mo) and the yellow and brown atoms representing Sulfur and Tellurium, respectively. Figure 4.1c shows how carbon in Graphene attaches itself to form a bond with TMDCs, which, in this case is MoS_2.

Graphene + WSe_2 interfaces produced very similar structures.

Figure 4.1d depicts the atomic orbital of $MoTe_2$, where we can see that this is a 2D material, very similar to that of MoS_2. The lattice distance of $MoTe_2$ from B to C is higher than that in MoS_2, however WS_2, WSe_2, $MoSe_2$ share very similar atomic structures with $MoTe_2$ and MoS_2.

4.1.1 Band Structures of Graphene and TMDC Heterostructures



(a) Graphene

(b) MoS_2

(c) Interface : Graphene + MoS_2

(d) $MoTe_2$

(e) Interface: Graphene + WS_2

Figure 4.2: Figure 4.2a represents the band structure of Graphene with apparently no direct band gap. Figures 4.1.2-b,c,d and e represent the band structures of MoS_2, Graphene + MoS_2 interface, $MoTe_2$ and Graphene + WS_2 interface with calculated band gaps of 2.174 eV, 0.071 eV, 0.225 eV and 0.170 eV, respectively. In all cases, the upper band represents the conduction band and the lower band represents the valence band.

In figure 4.2a, as expected, it can be observed that there is no direct band gap in Graphene, which is the underlying problem of the material. The bruillouin zone can be identified from the diagram, which demonstrates the energy dispersion relationship for Graphene.

In figure 4.2b, we obtained a direct band gap of 2.174 eV in MoS_2 as observed in the figure, with the conduction band being closer to the Fermi level than the valence band. This is a sizable band gap for manipulation but due to low mobility, its direct practical implementation is hindered. WS_2, WSe_2, $MoSe_2$ share very similar band structures with MoS_2 but $MoTe_2$ does not.

In figure 4.2c, the interface between Graphene + MoS_2 generates a value of 0.071 eV. Compared to the initial band gap obtained for Graphene, the interface gives us a much higher band gap, but the gap is still considerably lower than that of MoS_2 only. The energy gaps in the conduction band are much closer compared to that in the valence band. There are quite evident differences in the band gap in the valence band while they are negligible for the conduction band. Graphene + $MoSe_2$, Graphene + $MoTe_2$, Graphene + WS_2, Graphene + WSe_2 interfaces produced very similar band structures. The data has been tabulated and a graph has been plotted in one of the latter sections.

In figure 4.2d, a direct band gap of only 0.225 eV is observed in $MoTe_2$, which, though still much higher than that for Graphene, falls much short to its MoS_2 ¬ counter. Also, the band structure seems to be haphazard when compared to thats of other TMDCs, which usually have a clear gap between the valence and the conduction band. It can thus be inferred that $MoTe_2$ is probably not the best choice for interfacing with Graphene.

In figure 4.2e, a value of 0.170 eV is obtained for the interface of Graphene and WS_2 which indicates a value higher than that for Graphene individually. An opposite scenario was noticed when compared with the individual structure of WS_2. The band gaps in both conduction and valence bands get narrower eventually as we can see from the diagram. The energy gaps in the conduction band had a straight lined pattern compared to the wavy one found individually, before making the interface. Unlike Graphene + MoS_2 interface, the bands observed in Graphene + WS_2 are straight parallel lines although the value is fairly smaller than that for the interface between Graphene + MoS_2. It is also observed that just like MoS_2, the conduction band is closer to the Fermi level than the valence band.

4.1.2 Graphical Representation of Band Structures of Graphene and TMDC Heterostructures

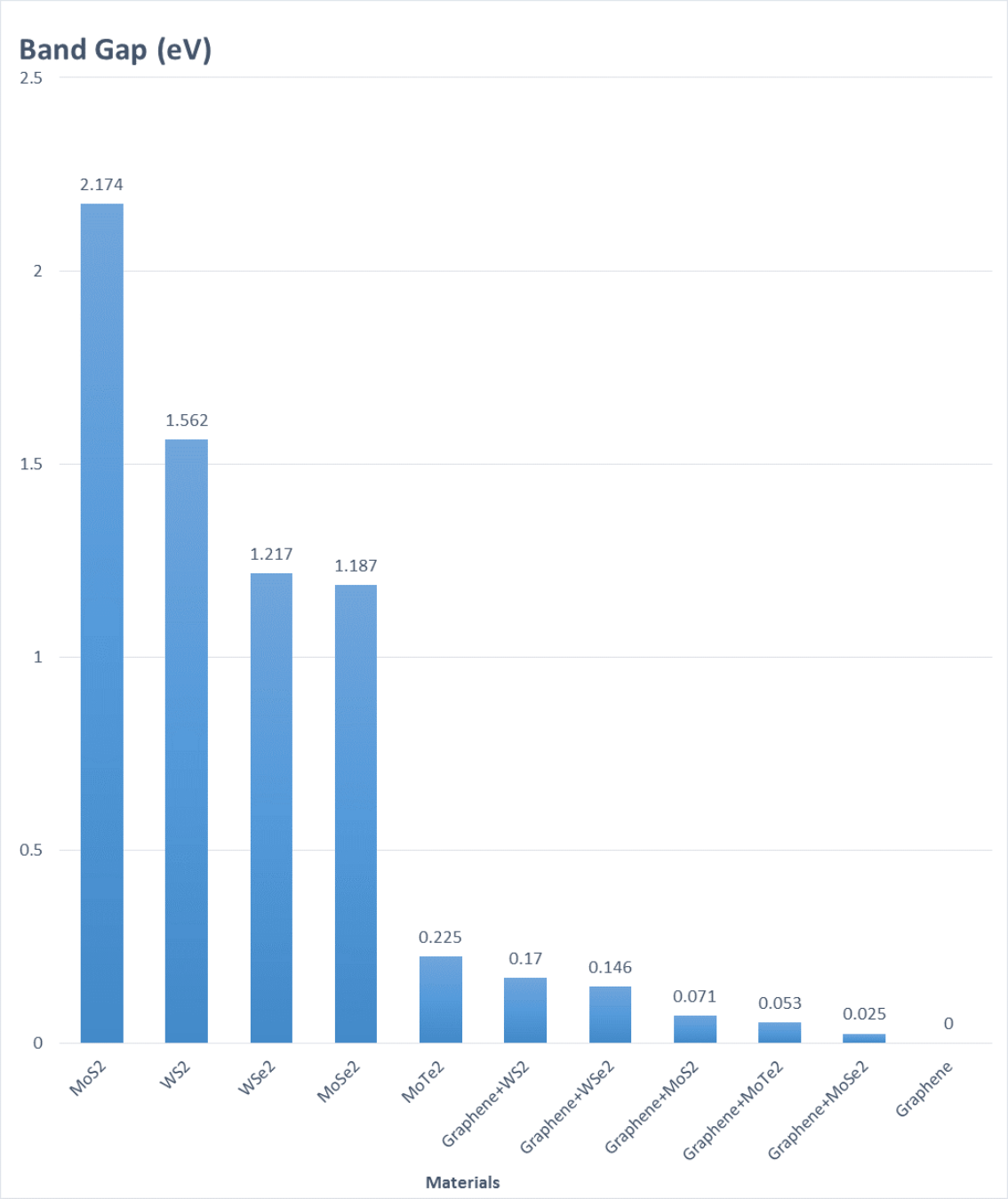


Figure 4.3: Graphical representation of band structure of Graphene and TMDC heterostructures in descending order

Figure 4.3 is the graphical representation of band strucutures of Graphene and TMDC heterostructures i.e band gap versus material. It is observed that the band gap of Graphene is zero. On the other hand, the band gapa of TMDCs are higher compared to that of Graphene. We also see that the Graphene + TMDC interface band gap is in between the band gap of Graphene and TMDCs separately. Among the TMDCs, MoS_2 has the highest band gap and $MoTe_2$ has the lowest band gap. However, when TMDCs are interfaced with Graphene, WS_2 has the highest band gap and $MoSe_2$ has the lowest band gap.

The graphical data are tabulated in table 4.1

Table 4.1: Tabular Representation of Band Structures of Graphene and TMDC Heterostructures

Materials	Band Gap (eV)
MoS_2	2.174
WS_2	1.562
WSe_2	1.217
$MoSe_2$	1.187
$MoTe_2$	0.225
Graphene + WS_2	0.170
Graphene + WSe_2	0.146
Graphene + MoS_2	0.069
Graphene + $MoTe_2$	0.050
Graphene + $MoSe_2$	0.036
Graphene	0.000024

4.2 Atomic Structures of Sandwiched Heterostructure Models

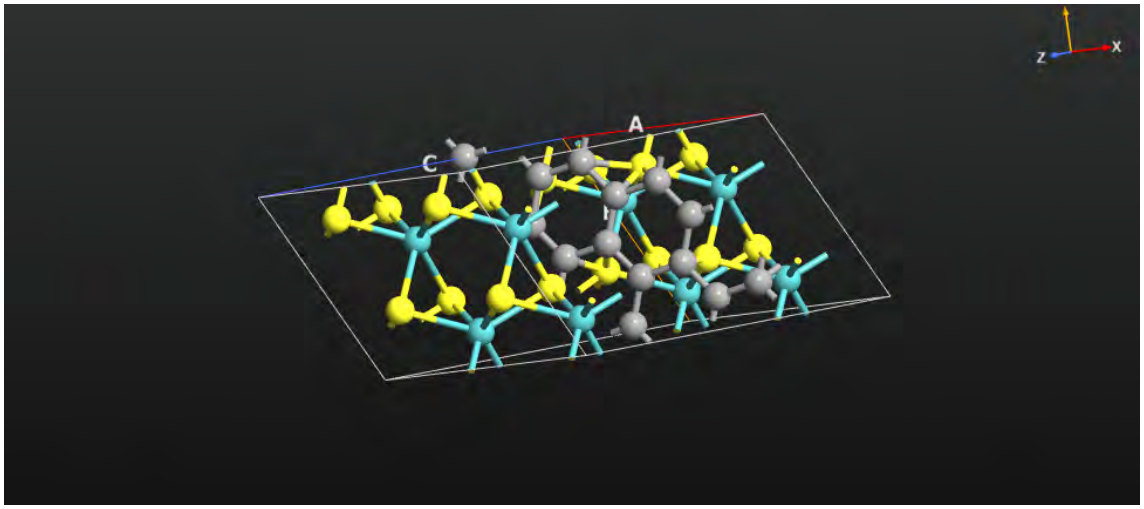
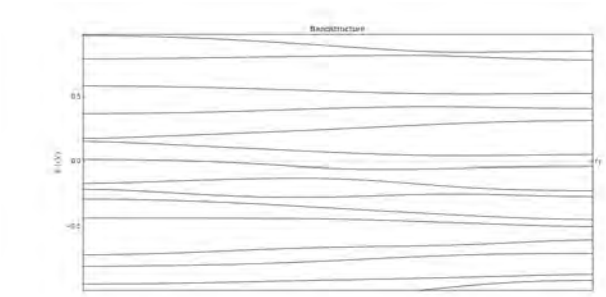


Figure 4.4: Figure 4.4 represents the 3D view of the sandwiched atomic structure $MoSe_2$ + Graphene + $MoSe_2$. A silver sphere represents carbon making up Graphene, the blue represent Molybdenum (Mo) while the other spheres represents Sulfur (S) .

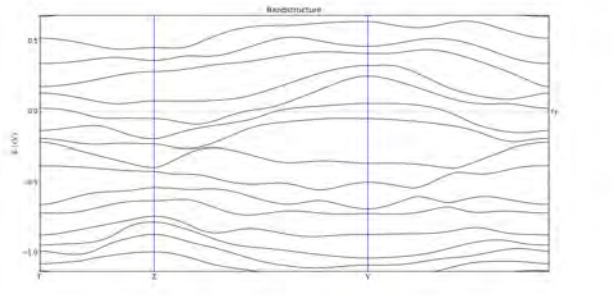
In figure 4.4 the silver spheres represent the carbon atoms making up Graphene while the blue and yellow spheres represent the Mo and S atoms, respectively. Thus, a single layer of Graphene is sandwiched between two single layers of MoS_2.

$MoSe_2$ + Graphene + $MoSe_2$, $MoTe_2$ + Graphene + $MoTe_2$, WS_2 + Graphene + WS_2 and WSe_2 + Graphene + WSe_2 were exactly similar in structure except Graphene being sandwiched between two layers of MoS_2 ; they were sandwiched between two layers of $MoSe_2$,$MoTe_2$, WS_2 and WSe_2 were used, respectively.

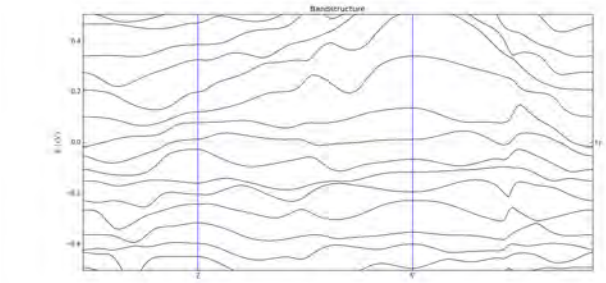
4.2.1 Band Structures of Sandwiched Heterostructure Models



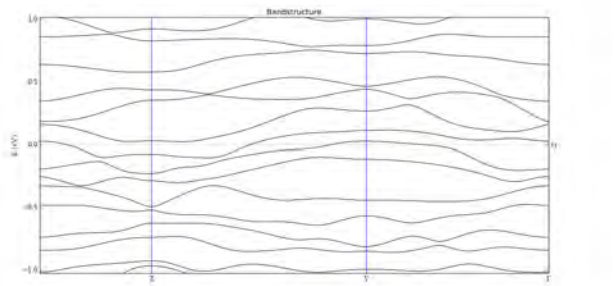
(a) Interface:MoS_2 + Graphene + MoS_2



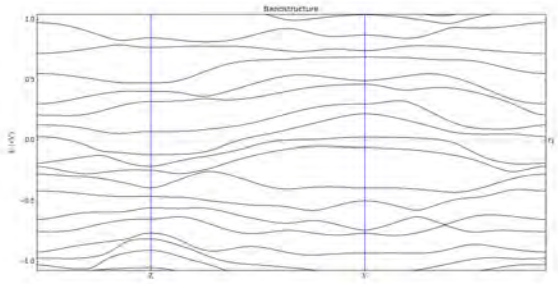
(b) Interface : $MoSe_2$ + Graphene + $MoSe_2$



(c) Interface : $MoTe_2$ + Graphene + $MoTe_2$



(d) Interface : WS_2 + Graphene + WS_2



(e) Interface : WSe_2 + Graphene + WSe_2

Figure 4.5: Figures 4.5-a,b,c,d and e represent the band structures of Graphene sandwiched between two layers of MoS_2, $MoSe_2$, $MoTe_2$, WS_2 and WSe_2 with calculated band gaps of 88.56 meV, 108.7 meV, 363.8 meV, 104.7 meV and 85.08 meV, respectively. In all cases, the upper band represents the conduction band and the lower band represents the valence band.

Figure 4.5a represents the band structure of the sandwiched materials : MoS_2 + Graphene + MoS_2, exhibiting a band gap of 0.0886 eV. On the contrary, the previously mentioned bilayer

heterostructure of Graphne + MoS_2 had a band gap of 0.071 eV. Therefore, in this sandwiched structure we have an increase in the band gap by 0.0176 eV.

Figure 4.5b depicts the band structure of the sandwiched materials : $MoSe_2$ + Graphene + $MoSe_2$, exhibiting a band gap of 0.1087 eV. On the contrary, the previously mentioned bilayer heterostructure of Graphene + $MoSe_2$ had a band gap of 0.025 eV. Therefore, in this sandwiched structure, we have an increase in the band gap by 0.0837 eV.

Figure 4.5c depicts the band structure of the sandwiched materials : $MoTe_2$ + Graphene + $MoTe_2$, exhibiting a band gap of 0.3638 eV. On the contrary, the previously mentioned bilayer heterostructure of Graphene + $MoTe_2$ had a band gap of 0.053 eV. Therefore, in this sandwiched structure, we have an increase in the band gap by 0.3108 eV. This is a relatively significant improvement.

Figure 4.5d shows the band structure of the sandwiched materials : WS_2 + Graphene + WS_2, exhibiting a band gap of 0.1047 eV. On the contrary, the previously mentioned bilayer heterostructure of Graphene + WS_2 had a band gap of 0.170 eV. Surprisingly, unlike the other cases, in this sandwiched structure, we have a decrease in the band gap by 0.0653 eV.

Figure 4.5e represents the band structure of the sandwiched materials : WSe_2 + Graphene + WSe_2, exhibiting a band gap of 0.0851 eV. On the contrary, the previously mentioned bilayer heterostructure of Graphne + WSe_2 had a band gap of 0.146 eV. Again surprisingly, in this sandwiched structure, we have a decrease in the band gap by 0.0609 eV.

Hence from our data analysis, we can conclude that the sandwiched structures comprising of Graphene and bilayers of TMDCs containing Tungsten (W) has a deteriorated band gap when compared to the heterostructure consisting of only Graphene and that material. In all other cases, sandwiched structures showed an improvement in band gap with $MoTe_2$ + Graphene + $MoTe_2$ having the most significant improvement.

4.2.2 Graphical Representation of Band Structures of Graphene TMDC Sandwiched Heterostructure Models

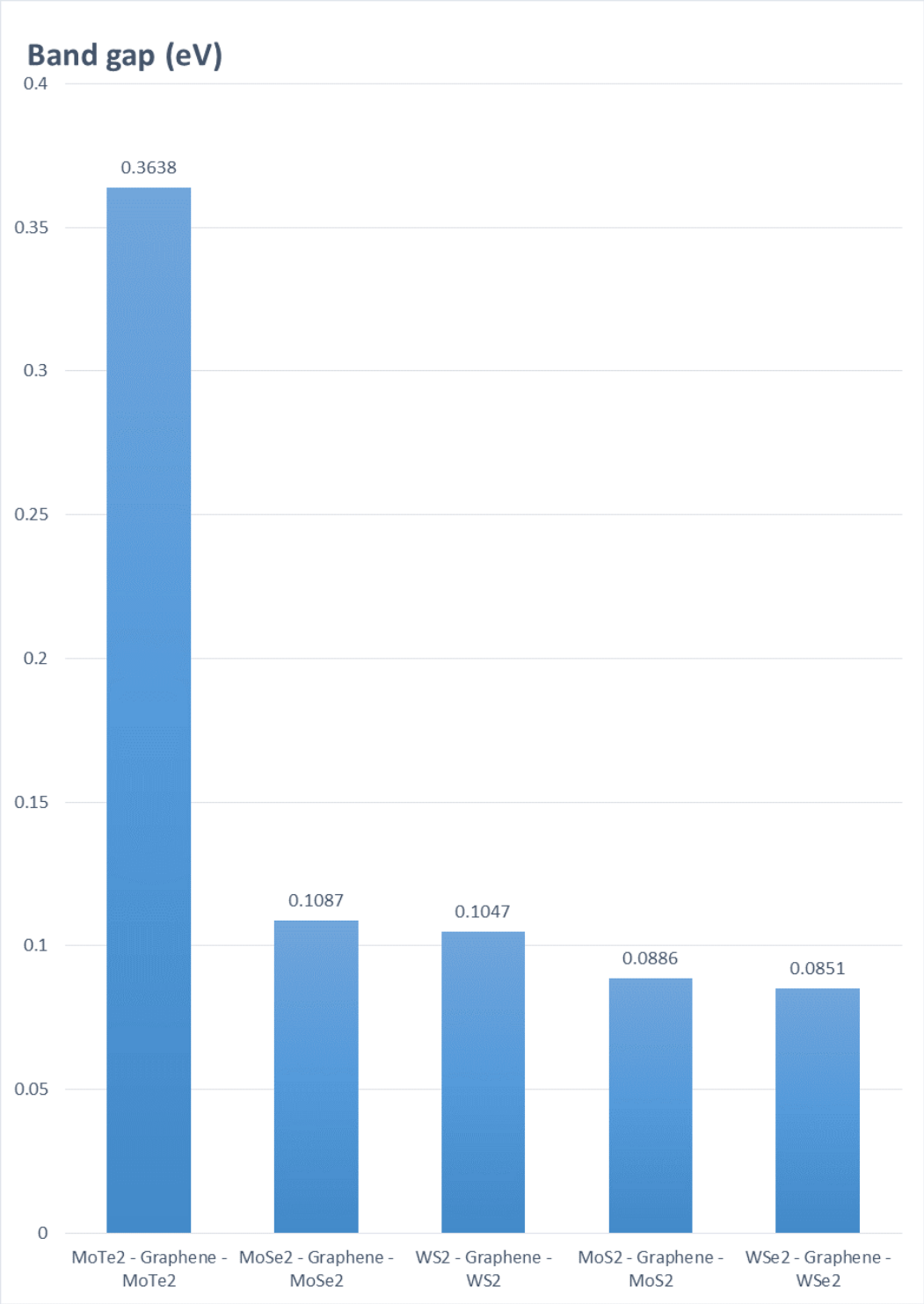


Figure 4.6: Graphical representation of band structures of Graphene TMDC sandwiched heterostructure models in descending order

The graph in figure 4.6 of band gap versus sandwiched heterostructures gives a clearer idea on the band gap of different sandwiched structures. Clearly, $MoTe_2$ + Graphene + $MoTe_2$ is the winner in case of sandwiched heterostructures.

Table 4.2 below tabulates the graphical data.

Table 4.2: Tabular representation of band Structures of Graphene TMDC sandwiched Heterostructure models

Compound	Band Gap (eV)
$MoTe_2$ + Graphene + $MoTe_2$	0.3638
$MoSe_2$ + Graphene + $MoSe_2$	0.1087
WS_2 + Graphene + WS_2	0.1047
MoS_2 + Graphene + MoS_2	0.0886
WSe_2 + Graphene + WSe_2	0.0851

4.2.3 Comparison of Band Gaps between Graphene, Graphene and TMDC Heterostructures, and Graphene and TMDC Sandwiched Heterostructure Models

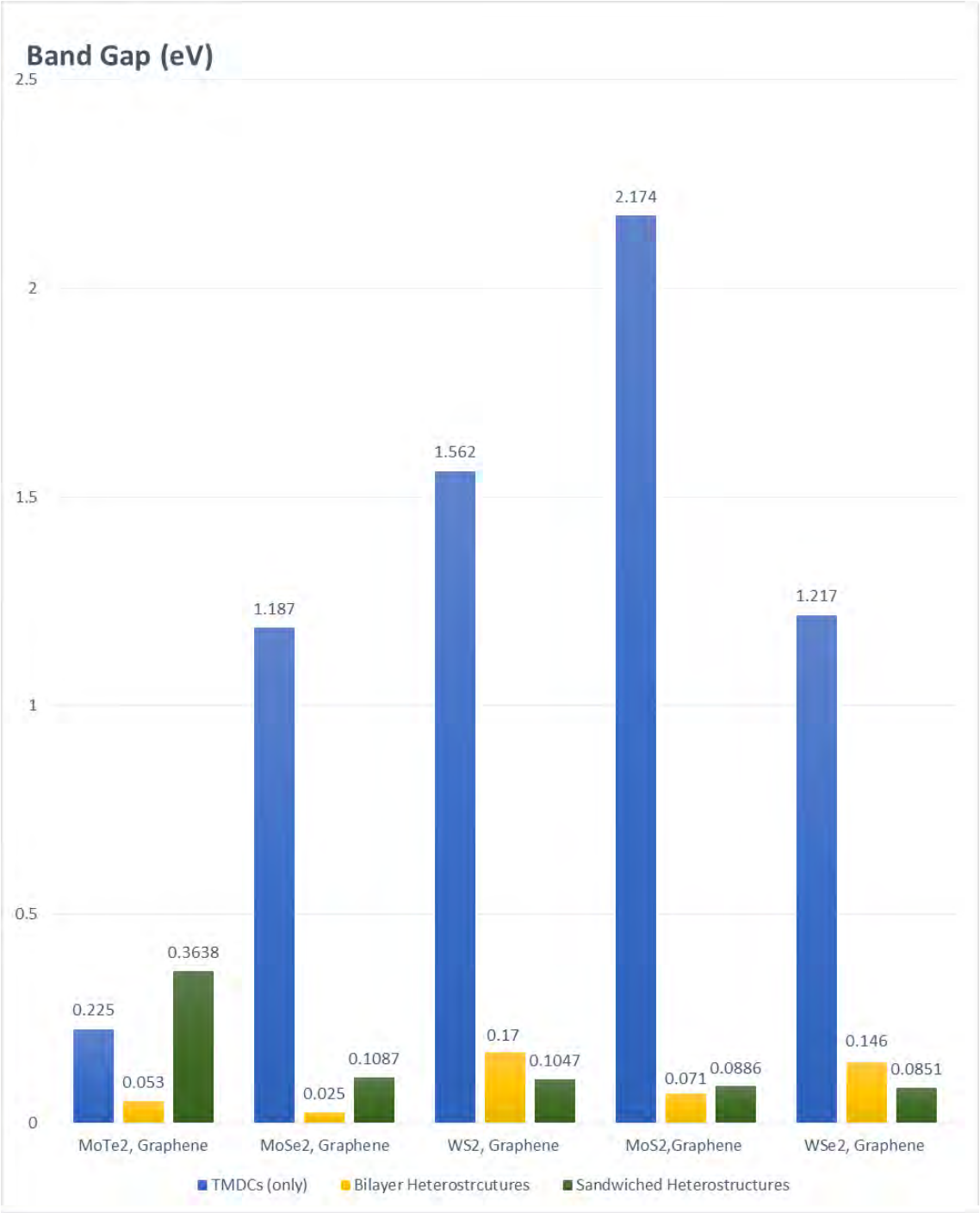


Figure 4.7: Graphical representation of band gap comparison between Graphene, Graphene and TMDC heterostructures, and Graphene and TMDC sandwiched heterostructure models

Figure 4.7 gives us an excellent graphical representation of all the data we have obtained from our simulation. We can clearly see the drastic fall in band gap for TMDCs the moment they are paired with Graphene in a heterostructure, followed by a slight improvement when in sandwiched heterostructures. The only exception is in case of $MoTe_2$ where the band gap of sandwiched structure supersedes that of only $MoTe_2$. Also, of all the possible heterostructured combinations we have worked with, sandwiched $MoTe_2$ + Graphene + $MoTe_2$ heterostructure produced the most promising result with the highest band gap of 0.3638 eV.

The graphical data have been tabulated below in table 4.3.

Table 4.3: Tabular representation of band gap comparison between Graphene, Graphene and TMDC heterostructures, and Graphene and TMDC sandwiched heterostructure models

Materials	TMDC only	Bilayer Heterostrcutures	Sandwiched Heterostructures
$MoTe_2$, Graphene	0.225	0.053	0.3638
$MoSe_2$, Graphene	1.187	0.025	0.1087
WS_2, Graphene	1.562	0.17	0.1047
MoS_2,Graphene	2.174	0.071	0.0886
WSe_2, Graphene	1.217	0.146	0.0851

4.3 Results Found from Studies

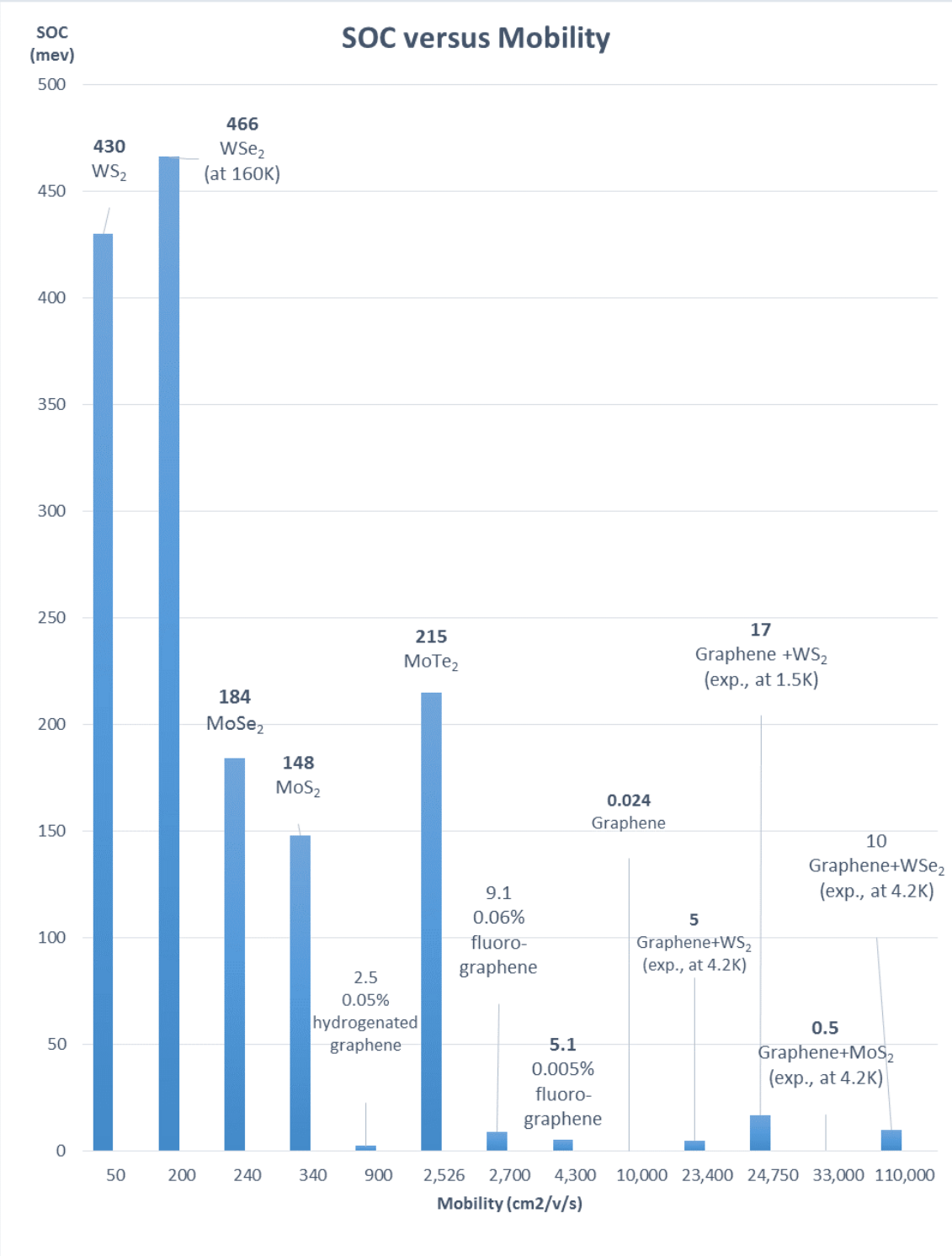


Figure 4.8: A graph of spin orbit coupling (SOC) versus mobility of Graphene and its interfaces with TMDCs.

At first, we have tried to analyze the relationship between spin orbit coupling and mobility as found from studying various articles.

Figure 4.8 includes the graph representing data about mobility and spin orbit coupling of Graphene, TMDCs and Graphene on different TMDC materials. We can see that there is no correlation between spin orbit coupling and mobility of materials. From this graph, we can have a clear idea that Graphene has the lowest spin orbit coupling of them all and TMDCs have a much higher spin orbit coupling than Graphene. MoS_2 has the lowest spin orbit coupling among TMDCs. We want a higher spin orbit coupling of Graphene for it to be used for different purposes. So, we tried to observe what will happen to the spin orbit coupling of Graphene if combined with TMDC materials. We can see that in different temperatures, new spin orbit coupling values of Graphene on different TMDCs are in between the previous individual values of Graphene and TMDCs. For example, pristine Graphene's spin orbit coupling increased from 0.024 to 10 when we used Graphene on WSe_2 (at 4.2 Kelvin). We also observed that the spin orbit coupling of different kinds of Graphene like fluorographene and hydrogenated Graphene have higher significantly higher spin orbit coupling than the pristined one.
In case of mobility, we can see that Graphene has a much higher mobility than TMDCs. While experimenting Graphene on different TMDCs this mobility has increased even more.

The graphical data are tabulated below in table 4.4.

Table 4.4: A graph of spin orbit coupling (SOC) versus mobility of Graphene and its interfaces with TMDCs.

Materials	Mobility (cm^2/Vs)	SOC(meV)	References
WS_2	50	430	[37],[43]
WSe_2	200	466	[37], [44]
$MoSe_2$	240	184	[37], [45]
MoS_2	340	148	[37], [45]
0.05height$MoTe_2$	2,526	215	[37], [45]
0.06height0.006heightGraphene	10,000	0.024	[43], [27]
Graphene + WS_2 [4.2 K]	23,400	5	[28], [46]
Graphene + WS_2 [1.5 K]	24,750	17	[17]
Graphene + MOS_2 [4.2 K]	33,000	0.5	[46], [43]
Graphene + WSe_2 [4.2 K]	110,000	10	[46]

Next, we have conducted a temperature dependence study of spin orbit coupling, found from

studying various articles.

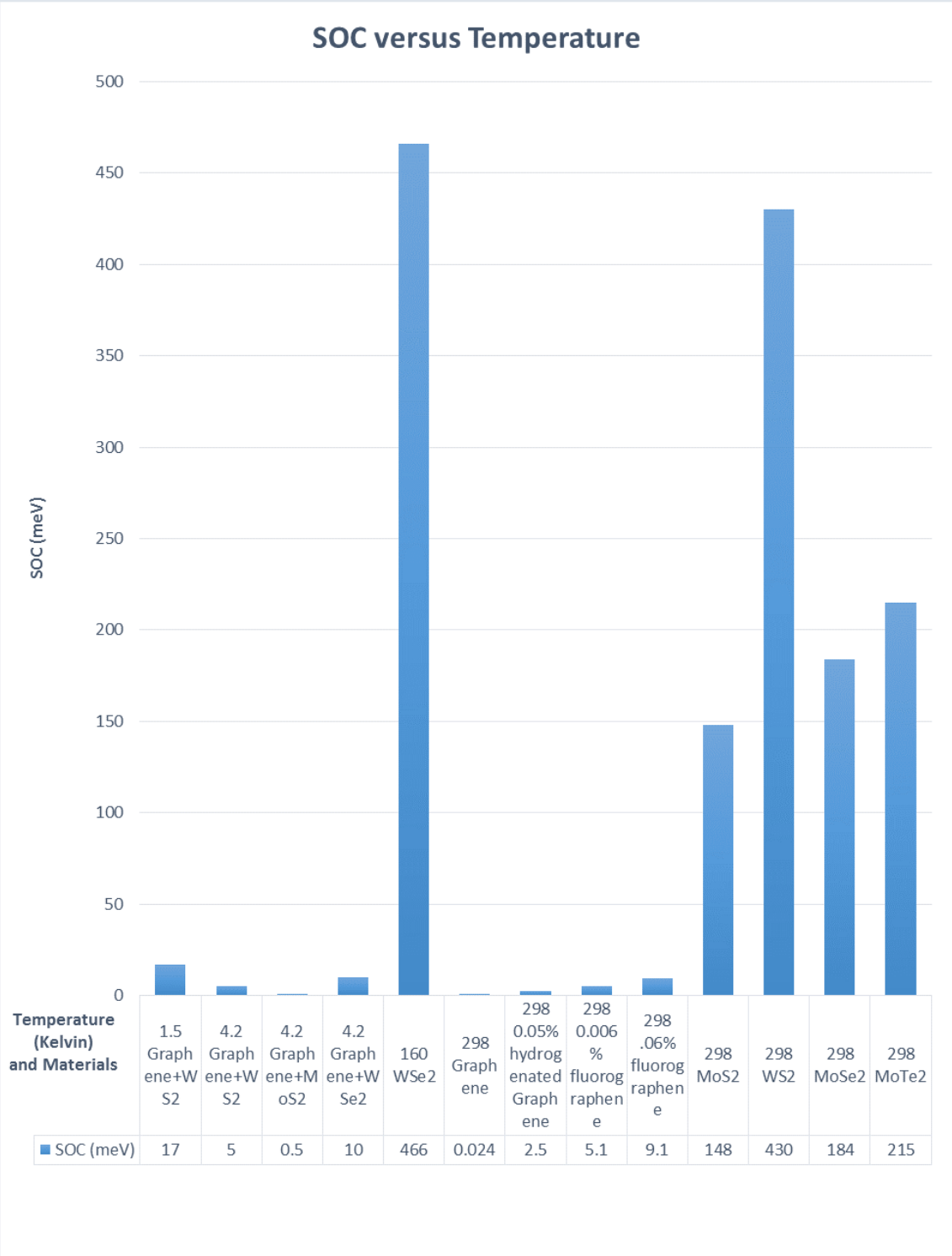


Figure 4.9: A graph of spin orbit coupling versus temperature of Graphene and TMDC heterostructures.

In figure 4.9, it is observed from the graph that most of the values for spin orbit coupling are taken in room temperature. Some of the spin orbit coupling of Graphene + TMDC materials are taken in different temperatures. We can see that at a temperature of 4.2 K, the spin orbit coupling of Graphene + WS_2 is 5 meV and at 1.5 K, the spin orbit coupling value increases to 17 meV (both are experimental values). For that particular case, we can see that as temperature decreases, the spin orbit coupling increases. However, decreasing the temperature to such a low value for just a slight increase in spin orbit coupling is very impractical.

The graphical data of figure 4.9 are tabulated in table 4.5 below.

Table 4.5: A graph of spin orbit coupling versus temperature of Graphene and TMDC heterostructures.

Compound	Spin orbit coupling (meV)	Reference
Graphene+WS_2 at 1.5K	17	[17]
Graphene+WS_2 at 4.2K	5	[28],[46]
Graphene+MoS_2 at 4.2K	0.5	[46], [43]
Graphene+WSe_2 at 4.2K	10	[46]
WSe_2 at 160K	466	[37], [44]
Graphene at 298K	0.024	[43], [27]
0.05% hydrogenated Graphene at 298K	2.5	[16]
0.006% fluorographene at 298K	5.1	[47]
0.06% fluorographene at 298K	9.1	[47]
MoS_2 at 298K	148	[37], [45]
WS_2 at 298K	430	[37], [43]
$MoSe_2$ at 298K	184	[37], [45]
$MoTe_2$ at 298K	215	[37], [45]

4.4 Graphical Representation of a Future Possibility

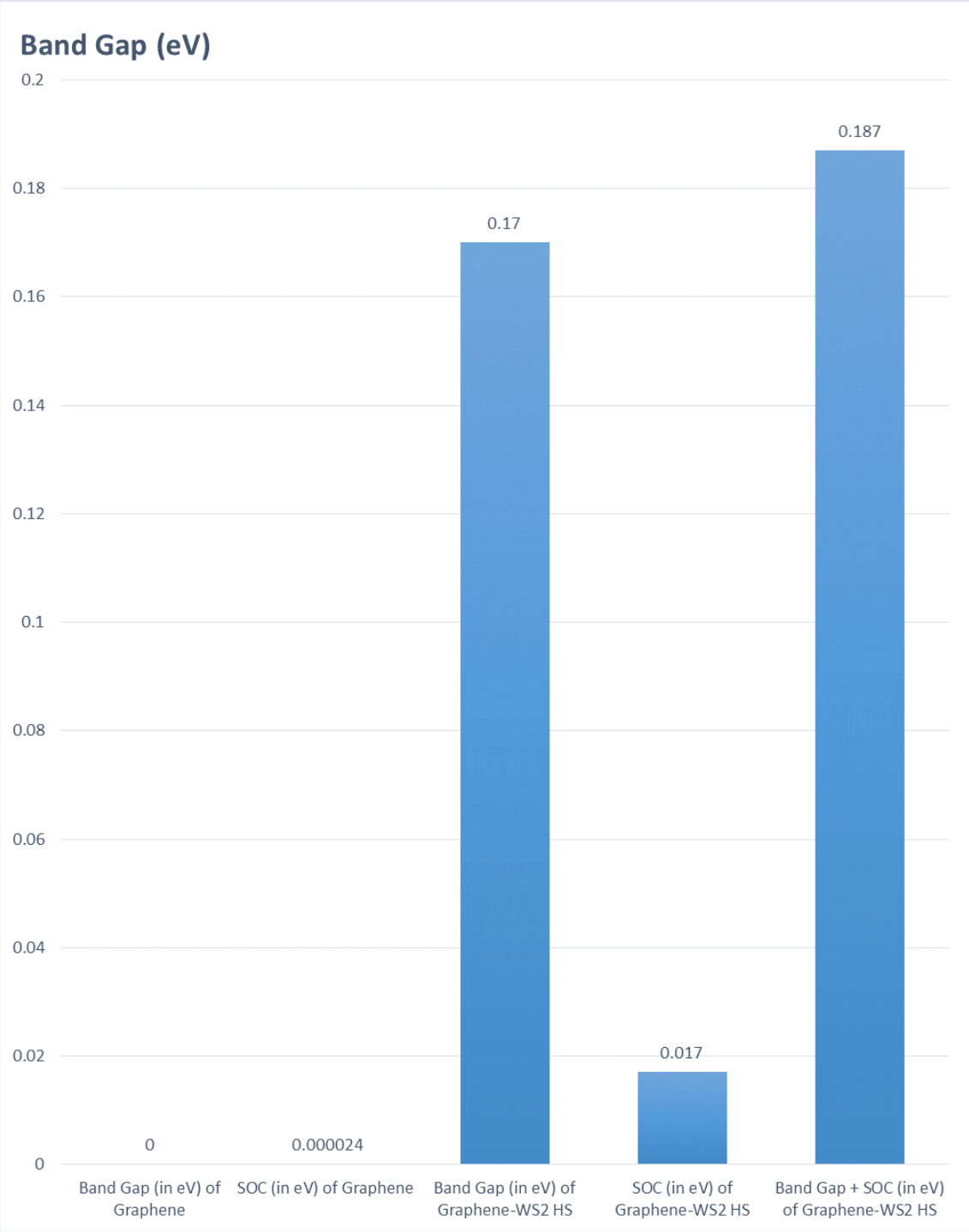


Figure 4.10: Graphical representation of spin orbit coupling, band gap and spin orbit coupling + band gap of Graphene + WS_2 heterostructure and sandwiched heterostructure as a future possibility

In the future, we may be able to simultaneously control the electronic band gap and the spin orbit coupling of a Graphene + TMDC heterostructure. Here, we have graphed MoS_2 as an example to show what the effects would look like.

In the graph, in figure 4.10, we can see a relatively small but clear improvement if the band gap and spin orbit coupling of a Graphene + TMDC heterostructure is combined by a possible simultaneous control of the both.

The graphical data are tabulated in table 4.6 below.

Table 4.6: Tabular representation of spin orbit coupling, band gap and spin orbit coupling + band gap of Graphene + WS_2 heterostructure and sandwiched heterostructure as a future possibility

Band Gap (in eV) of Graphene	0.000
SOC (in eV) of Graphene	0.000024
Band Gap (in eV) of Graphene + WS_2 HS	0.170
SOC (in eV) of Graphene + WS_2 HS	0.017
Band Gap + SOC (in eV) of Graphene + WS_2 HS	0.187

5

Conclusion

This chapter gives us a summary of the thesis, discussion regarding the process of conducting our research along with considerable mentions of what sort of limitations we have in our current level of work. This chapter not only provides a conclusion to our research but also gives an insight about the future use of this study and how it could be beneficial for manufacturing next generation transistors driven by the combination of band gap and spin orbit coupling of Graphene paired with various TMDCs.The chapter is divided into sections starting from 5.1 (Summary of the thesis), 5.2 (Discussion), 5.3 (Limitation of Current work), 5.4 (Future Work) and 5.5 (Conclusion).

5.1 Summary of the Thesis

Chapter one of our thesis informs our reader about what, how and why we chose this particular area of study. It delivers to make any personnel, even if not from the scientific community, to try to imagine what sort of research scientists have conducted over the past year. We introduce the reader with well written explanations of what Graphene and TMDCs are, what is a semi conductor, what is Moore's law and how it is related to our interest in this subject area. This chapters goes on to describe the two key factors, band gap and spin orbit coupling of individual, sandwiched and interfaced materials, and how they contribute to our hypothesis of combining these values and creating more efficient transistors for the next generation.

Chapter two of our thesis makes relevant comparisons with the most used transistor, i.e. Silicon based MOSFETs that the semiconductor industry depends on. In this chapter, the reader can relate and understand what sort of substitution could be done. Later on, it introduces us to various other terms as spin injection and detection, spin modulation, spin transportation etc. to make the picture clearer. Thus, we incorporated some concepts of spintronics, which are required to be understood for our research work.

Chapter three gives us a more thorough knowledge of Graphene and its characteristics. A proper understanding of the advantages and disadvantages of this material is crucial since it is one of the key materials used for all the simulations and comparisons. Apart from having a full comprehension of the properties of this wonder material, we also concentrated on TMDCs, which have turned out to be the perfect fit to be used with Graphene. Thus, chapter three goes on to make similar comparisons regarding TMDCs also, thereby letting us conclude why these materials, no matter in whichever way they are used, prove to give more efficient results in terms of performance.

Chapter four deals with the data values, simulations, graph plots, band structures generated and band gaps calculated. We have used a software to calculate the band gaps, while various renowned and reliable scientific papers have helped us gain values of spin orbit coupling of these materials. We have given captions and proper explanations of the graphs generated for mobility, spin orbit coupling and so on. Relevant figures for atomic structures, orbital structures and band structures have been added for clarity and to make our research validated.

Chapter five gives us the opportunity to share our experience while working on this thesis. We have included information regarding the software used, limitations of our current work, predictions for future use and so on. Hence, this chapter gives us an abridged version of our entire research work.

References and an appendix section have been added at the end of the thesis for an understanding of what type of information we choose to base our thesis on. These have helped us to confirm our hypothesis to certain extents and we would want to conclude by mentioning that this study requires further effort and time to discover the full potential in this particular arena of study.

5.2 Discussion

Our thesis has been all about exploring various materials and their combinations, either Graphene-TMDC interface or Graphene being sandwiched between TMDCs. Initially when we started, our focus was towards the understanding of spin orbit coupling of materials and about learning more about spin driven field effect transistors, replacing our traditional Silicon based ones for higher efficiency, i.e. needing a lower voltage to turn on a device. We have been able to come up with a decent number of compelling data regarding the spin orbit coupling of these materials from various

scientific journals and papers. Moreover, we realized that, to validate our thesis, simulations were necessary, which was when we started to work on generating band structures in order to calculate the band gap of these materials. For a thorough comparison, we worked on simulations through a software named, VNL ATK 2016.4, for individual materials (such as Graphene, MoS_2 etc.), sandwiched compounds (such as MoS_2 + Graphene + MoS_2) and interfaced materials, i.e. one material upon another one (such as Graphene on MoS_2). Our data includes comparisons of spin orbit coupling with materials and their mobility and temperature. Moreover, to summarize all the information gathered, we have incorporated the data obtained from spin orbit coupling and band gap for interfaced materials into one single bar graph for the ease to compare and portray the trends of Graphene with TMDCs in such conditions. This has allowed us to envision a next generation transistor that could come into play if these values are combined, leading to an increase of the on/off current ratio in the device, thus creating better and more efficient transistors, requiring a lower voltage to start a device. After our simulation, we have focused on writing our thesis paper fully, giving details wherever required with references to show our thorough academic research. On another note, we decided to make use of Share Latex to write our thesis as it takes the most dynamic and effective approach for writing scientific research papers around the world, to be well formatted and structured in comparison with the standard worldwide in today's time.

5.3 Limitation of Current Work

Our research has dealt with new emerging concepts which made it very difficult to gather information about all the respective areas being covered in our thesis. One of the most initial and biggest challenges we had to overcome was to obtain the data for spin orbit coupling with their individual corresponding temperatures. The incorporation of temperature into our research was extremely difficult since all these figures that we gained were experimental values, which were the output of particular experiments in the scientific papers used as guidelines. We believe that these temperatures obtained from these well renowned papers stand to justify our conclusion; however, the percentage of error still does stand, as we were unable to confirm that under all conditions, these materials would give these same spin orbit coupling values at these specific temperatures. We propose further research to be conducted in this arena. To validate our claims, we have mentioned the values obtained in our generated plots with their respective temperatures along with proper references. The second challenge that we faced was with the use of the software for simulating band structures in order to find out the band gap in materials individually, such as Graphene and TMDCs (MoS_2, MoT_2 etc.). We were also focused on generating band structures for sand-

wiched materials with Graphene and various TMDCs and by interfacing these materials too. In this process, we struggled to build all types of interfaces and sandwiched materials along with the inability to incorporate temperature variables in generating these plots. The values of band gaps were difficult to find considering that they are in the meV range mostly but we later on we learned to zoom in the pictures of our simulated band structures. However obtaining the best fit ones was a taxing job. We marked the Fermi levels in each of these plots to make the understanding better for the readers.

5.4 Future Work

The importance of this research and its new perspective on combining the band gap and spin orbit coupling are still in the primary phase and thus require more effort and time to be able to discover its full potential. For future use, we can definitely envision that sandwiched materials of Graphene and various TMDCs would increase the efficiency of the transistors and a new generation of field effect transistors would be in use in integrated circuits. A thorough knowledge of the software we used, VNL ATK 2016.4, is mandatory for making any further progress in this research. We were able to generate simulations of individual materials (such as Graphene, MoS_2, $MoTe_2$ etc.), interfaced combinations (such as Graphene and MoS_2, Graphene and MoTe2 etc.) and sandwiched combinations (such as MoS_2 + Graphene + MoS_2, $MoTe_2$ + Graphene + $MoTe_2$ and etc.) by using the software. The readings obtained from the band gaps of these materials have helped us predict how new materials can serve the purpose of switching on a device, but at a much lower supply voltage to develop an almost similar current turn on/off ratio as that of MOSFETs for advanced transistors. For future work, more studies should be conducted and combinations such as Graphene + MoS_2 + Graphene, Graphene + $MoTe_2$ + Graphene etc. can be made. Various combinations can be simulated through this software and we hope to see more work done on the manipulation of spin for a fully functioning next generation field effect transistors and we believe that our research data would serve as a primary help for such kinds of research activities.

5.5 Conclusion

We believe our research conducted by combining the data obtained for band gap and spin orbit coupling for various combinations of materials (Graphene and TMDCs) will shed more light in this subject area. In the beginning of our thesis, we started to broaden our knowledge on the effect of

spin orbit coupling in a material for next generation transistors in the semiconductor industry. We have been successful in obtaining theoretical data of the spin orbit coupling and also in calculating the band gaps of various materials, both individually and with interfaces. This progress made us believe that it could lead us to propose a newer and better model of transistors for future use in integrated circuits. If the band gap and spin values can be simultaneously controlled, in the future, we may be able to create a Graphene/TMDC based device with a better on/off current ratio than existing one. As we all know, ideally, for MOSFETS, we gain an on/off ratio of around 10^6 to 10^9 and this new incorporation will possibly help us reach closer to our goal of creating better transistors for the future generation. We hope our research was compelling enough to make the readers believe in the potential of this proposal and hence, will be encouraged to explore the capability of the combinations of Graphene with various TMDCs.

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A

Appendix

The software used for our simulation is "VNL-ATK 2016.4," downloaded from quantumwise.com. It is a very user friendly software. To calculate the band structure, the following steps need to be followed.

Step 1: Launch the software and click on "Builder" on the top left of the window. A new pop up window will appear.

Step 2: On the new pop up window, go to "File" -> "Add" -> "From Database."

Step 3: Choose the material of your choice. For example, type Graphene in the search box and double click. Also type MoS_2 in the search box and double click. You will now see that figures of Graphene and MoS_2 appear in the bottom of the page

Step 5: For instance, if you want to find the band structure of Graphene-MoS_2 interface (calculating the band structure of only MoS_2 or Graphene is much easier. Go to step 6 from here). On the right side of the window, Click "Builder" -> "Interface." Then two small spaces will appear asking for the material that you want to interface. Drag Graphene and MoS_2 and click "Create."

Step 6: On the bottom right of the window, there is a blue arrow sign, click it and select "Script Generator." Another new pop up window will appear.

Step 7: Double click new calculator on the top left. Then double click "Analysis" and select "Bandstructure" from the top of the list that will appear.

Step 8: Under the script section you will see that "Bandstructure is listed." Double click. In "Brillouin zone route," erase the default and type "G, Z, Y, G. And click okay.

Step 9: Click the blue arrow on the bottom right of the "Script Generator" window and select "Job Manager."

Step 10: Save the .py file in your computer and tick to start job manager automatically.

Step 10: Wait for about half and hour to one hour as the software performs its calculations. Once done, go to the initial window that appeared during the launching of the software. Click "File" and add your file directory. You will see a list of default names and also your file name as saved.

Click there. As it expands, two logos shall appear. Select the second one. And from the right side of the window click "Bandstrucutre Analysis."

Step 11: In a new window, bandstructure will appear for the material(s) of your choice. You will see a set of tool on the bottom left of that screen. You can zoom the image by using the tool and also measure the bandstrucutre using the measurement tool. Finally, save your images using the save logo on the bottom of the page.