1
Introduction

Nanotechnology is one of the most emerging fields in the last two decades due to its usefulness and importance in the industry. Scientists are putting continuous efforts and developing the expertise to bring nanotechnology from a research lab with an affordable price in the market. Nanomaterials showed unusual properties compare to their bulk materials. The nanotechnology market is exponentially increasing worldwide. Silicon-based electronics industries face a physical and technological limitation that's why substantial research efforts are going on to search for new materials that can be coupled with present technology. Recently, the research is mainly focusing on the incorporation of nanomaterials that exhibit the extraordinary properties on the commonly used substrates to get improved device performance.

1.1 Two-Dimensional Materials

Two-dimensional (2D) materials consist of mono or a few atomic layers. Before the isolation of graphene from the graphite, the perception for 2D materials was that these are unstable in reality due to thermal fluctuations. Within this context, the ignition in 2D materials research came after the successful isolation of graphene from the graphite by Geim and Novoselov in 2004 (K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, 2004). Graphene is the thinnest material to date, made of carbon atoms arranged into the honeycomb lattice, and having sp^2 hybridization in C-C bonding. The demonstration of ultrahigh electrical, thermal conductivity, and mechanical properties led to attracting graphene 2D material from different research fields (C. Zhang, Li, Zhao, Bai, & Zhang, 2018). Due to the massless charge carrier, it has very high carrier mobility. Researchers from different fields are attracted to this "miracle material" due to its excellent physical/chemical and optoelectronic properties compared to the bulk graphite. These materials are having in-plane strong covalent bonding and weak coupling van der Waals (vdW) interaction between the layers. Figure 1 shows the graphene and corresponding band structure, which illustrates the semi-metallic behavior.

After discovering graphene, scientists initially believed that graphene could replace silicon in the 21st century. However, due to semi-metallic behavior, graphene can't be used in modern electronics. The group-IV based 2D materials, such as silicene and germanene, have emerged as strong contenders to the graphene. There are various theoretical studies available related to the fundamental properties of such 2D materials (Balendhran, Walia, Nili, Sriram, & Bhaskaran, 2015). Moreover, practical synthesis methods are being explored to establish fabrication techniques and growth parameters (Bianco et al., 2013). The initial studies also suggest the semi-metallic nature of silicene and germanene systems. Thus, these materials can't be used in their pristine form for electronic devices due to the well-known switch-off problem (Z. Ni et al., 2012). Various experimental and theoretical modifications are investigated and explored, such as multilayer, nanoribbons, external strain, and electric field are used to open the bandgap. The small bandgap can be opened; however, that may not be sufficient for semiconductor device applications.

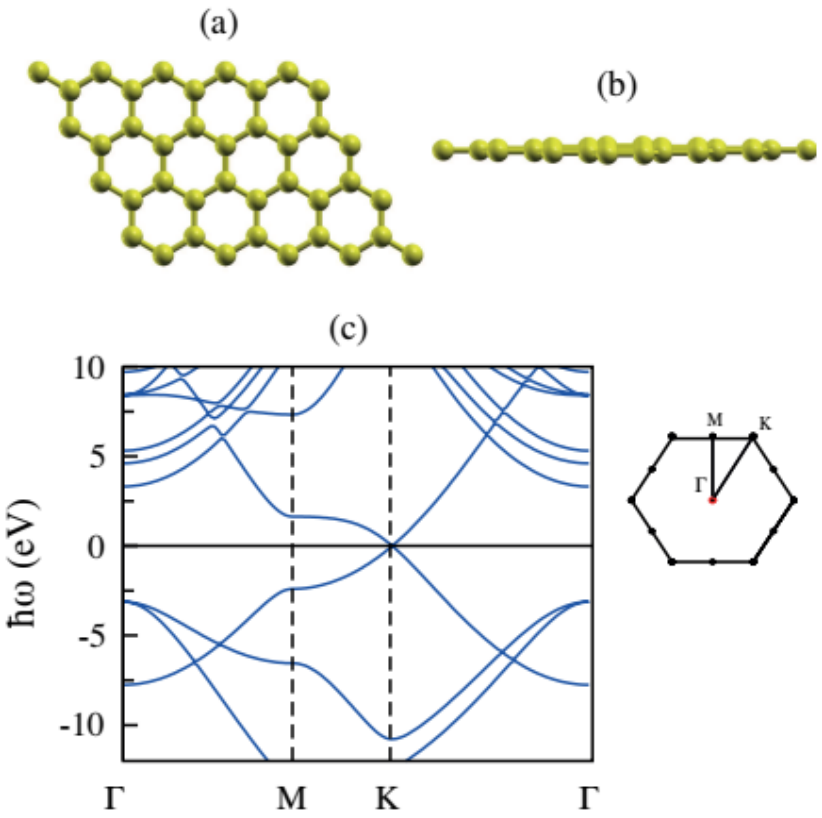

Figure 1.1 (a) top view, (b) side view, and (c) band structure along with high symmetry of BZ of graphene (Torbatian & Asgari, 2018).

The other category of 2D materials is the compound hexagonal boron nitride (h-BN) monolayer analog to the sister graphene system, where carbon atom replaced by boron and nitrogen atom (Torbatian & Asgari, 2018). This h-BN monolayer forms the hexagon honeycomb planar structure similar to graphene together with sp^2 hybridization. This insulator material may be the ideal support for 2D materials like graphene for transport measurement, which demonstrates the significant improvement in the charge carrier mobility of graphene (Torbatian & Asgari, 2018). Due to excellent properties, h-BN monolayers may be used as gate dielectric materials for the field-effect transistor, sensor, photonic devices, and buffer material for materials growth.

Another 2D material of interest is phosphorene, made of a single layer of black phosphorus. It is considered as a strong candidate against graphene due to its semiconducting characteristics. Phosphorene was first isolated from bulk material in 2014 by mechanical exfoliation, which has a reasonable bandgap with very high mobility (L. Li et al., 2014). The phosphorus atom has five valence electrons forming the sp^3 hybridization of a phosphorus atom in the phosphorene. The 2D materials have a strong tuning capability of electronic properties, depending on the number of layers. It has excellent potential for optoelectronics and semiconductor industries. In phosphorene, three electrons of phosphorus atom covalently bonded with the other three phosphorus atoms and leave one lone pair (Woomer et al., 2015). Phosphorene based various electronic devices are demonstrated with unusual electronic properties. The main worry for phosphorene monolayer is its air sensitivity, so an inert atmosphere is required for fabricating materials and devices (Wood et al., 2014). Due to the presence of the lone pairs in the phosphorene, it will react quickly with the water molecule and oxygen assisted by visible light.

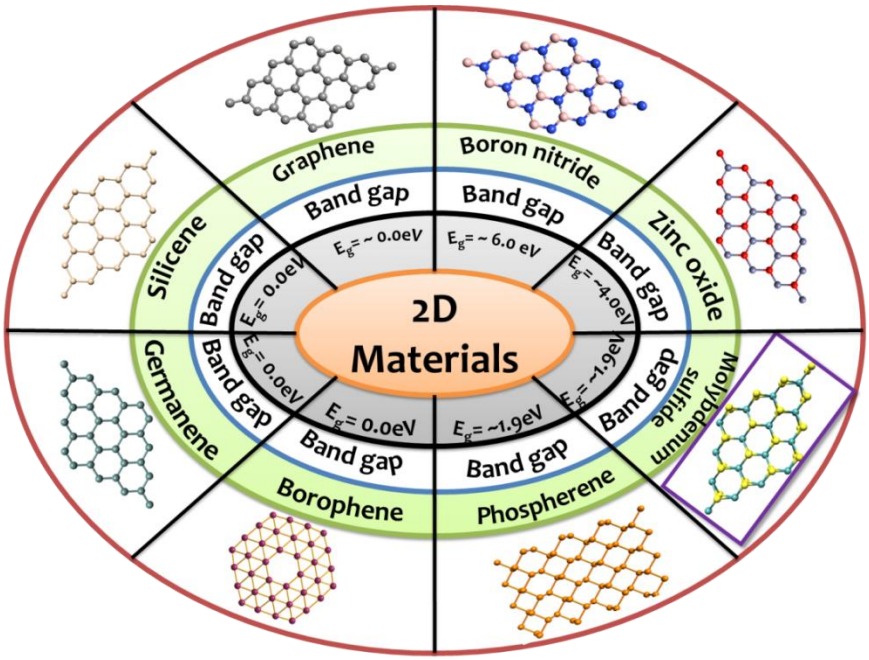

Figure 1.2 Schematic representations of few selected 2D monolayers and corresponding electronic band gap

1.2 Motivation

The Transition metal dichalcogenides (TMDs) are one the most studied 2D materials because of their wide range of electronic properties from metal to semiconductor to semi-metal depending on the types of transition metal and chalcogen atoms (Manzeli, Ovchinnikov, Pasquier, Yazyev, & Kis, 2017). Group VI transition metal based materials have good optoelectronic properties for nano device application (Q. H. Wang, Kalantar-Zadeh, Kis, Coleman, & Strano, 2012). Mo/W(S/Se)$_2$ monolayers having reasonable band gap, high mobility, and stability motivated researchers to explore their unusual properties and the underlying physics. WS_2 and WSe_2 materials have very high absorption coefficient and thus, can be used as the absorber materials for solar cell application. Recently Lou and co-workers (Jing Zhang et al., 2017) and Li and Zhang co-workers (Lu et al., 2017) synthesized the noble kind of structure, in which the top or bottom layer consists of different chalcogen atom, called the Janus MoSSe layer. These kinds of Janus structure provide additional degree of flexibility in designing novel materials, consisting of functional properties of both the chalcogen atoms. The crystal structure of a Janus monolayer is similar to the traditional TMDs, but the crystal symmetry is reduced from D_{3h} to C_{3v}, and broken out-of-plane symmetry and induced the vertical dipoles. Since, Janus is the newly synthesized monolayer, whose chemistry and basic properties are still unexplored. This motivates me to explore more about the properties of Janus monolayers and based on that predict the possible application for real life applications.

1.3 Objective

This work is mainly focused on the investigation of materials' characteristics of Janus transition metal dichalcogenides (JTMDs) and predicting their possible applications. The silent objectives covered in this thesis include

1) Strain engineering of WS_2, WSSe and WSe_2 monolayers
2) Pristine and defect included WSSe and MoSSe monolayers for gas sensing application
3) Janus WSSe and WSeTe buffer layer for WS_2 and WSe_2 based absorber materials solar cell
4) Thermoelectric properties of pristine and strained WSSe monolayer

1.4 Outline of the Thesis

The thesis presented here is the investigation of the stability and materials properties of TMDs based on Janus monolayer together with their possible applications. **Chapter 1** of the thesis describes the introduction of two-dimensional materials. It also briefly describes the properties of graphene, silicene, germanene, h-BN, and phosphorene 2D materials. The motivation and objectives of the current research work are also briefly covered in this chapter. **Chapter 2** explains the basic properties of TMDs and applications. This chapter also discusses the synthesis approach of Janus MoSSe monolayer, experimental and computational study on group VI based JTMDs monolayers. **Chapter 3** presents the introduction of Density Functional Theory (DFT) and one-dimensional (1D) solar capacitance simulator. It is also explaining the BoltzTrap package used for predicting the thermoelectric properties. **Chapter 4** of the thesis describes the introduction and importance of TMDs based on 2D materials. It also describes the dynamic stability of pristine and strained monolayers. Biaxial strain mediated electronic properties also studied. **Chapter 5** covers the stability of possible point defects in MoSSe and WSSe monolayers. It is also explaining the electronic and magnetic properties of defect included monolayers. The gas sensing mechanism of toxic gases e.g., H_2S, NH_3, NO_2, and NO molecules on Janus MoSSe and WSSe monolayers are tested. It also deals with the effect of most stable point defects on gas sensing performance. **Chapter 6** discusses the optoelectronic properties of bulk WS_2 and WSe_2 for absorber materials and WSSe and WSeTe materials as buffer materials. Photovoltaic (PV) performance of the solar cell is also investigated using SCAPS-1D simulator. **Chapter 7** describing the thermoelectric properties of pristine WSSe monolayer. In this chapter, the strain effect also considered improving the thermoelectric performance of WSSe monolayer.