CHAPTER 1
Introduction

1.1 Graphene: The rise of two-dimensional materials

The solid materials in their bulk phase are referred as three-dimensional (3D) materials while with reduced dimensions they are known as low dimension materials. These low dimensional materials are classified as two-dimensional (2D), one-dimensional (1D) and zero-dimensional (0D) materials depending upon their dimensional confinement. These low dimensional materials exhibit diverse and unique properties as compared to their bulk counterpart subjected to two factors, that are respectively quantum confinement effect and increase in relative surface area. The carbon based nanostructures such as fullerene and carbon nanotubes were existing even before the realization of graphene, as it was considered only a theoretical concept at that time.[1] Besides this, the synthesis of two-dimensional materials was assumed to be a difficult task from a thermodynamics point of view, due to the occurrence of thermal fluctuations in low-dimensional crystal lattice.[2–4] The era of two-dimensional (2D) materials begun just over a decade after the isolation of graphene.[5] During that period of time, the 2D materials were considered as integral of the 3D structures.[6,7] Thereafter, the experimental discovery of graphene became as a blueprint for all newly predicted and synthesized 2D materials, not only due to its incredible existence with mono-layered geometry but also due to its unique physicochemical properties that arise due to confinement effect as compared to its bulk counterpart.[8–11]

Graphene was earlier known as layered graphite or carbon layers as it is the derivative of graphite. Later, the International Union of Pure and Applied Chemistry (IUPAC) defined a single carbon layer of the graphite as graphene. Graphene is one atomic layer of graphite with

sp^2 hybridization and possesses semi-conducting properties despite of having zero-band gap. Owing to many advantages of graphene applicable to wide range of cutting-edge fields, its semi-metal nature is a major challenge for its utilization in optical devices and field effect transistors.[12] Graphene is the first 2D material which does not require any other 3D base material for synthesis as it is mechanically exfoliated from pyrolytic graphite through scotch tapes method [8,13] and, later, the same trend was followed for other 2D materials namely, BN, MoS_2, $NbSe_2$ and $Bi_2Sr_2CaCu_2O_x$.[8] Among these free standing 2D atomic crystals, BN and $Bi_2Sr_2CaCu_2Ox$ exhibit insulating nature[8]. The graphene amongst remaining 2D materials, has attained huge attraction from researchers and material scientists due to its unique properties besides its semi-metal nature, which again set a new goal of bandgap engineering for opening the band gap. The opening of band gap and search of suitable substrate for the fabrication of graphene-based devices was initiated with SiO_2 substrate; however, it resulted in highly disordered graphene that made it less suitable for device applications.[14,15] Theoretically, hexagonal boron nitride (h-BN) has been predicted to be suitable for opening the band gap[16] with hetero-structured configuration as graphene/h-BN. h-BN is the most stable form of bulk boron nitride, where boron and nitrogen atoms are bound through strong covalent bonds and the layers are held together by weak van der Waals force similar to graphene. It possesses wide band gap with magnitude 3.5 eV, which makes it a suitable substrate that provides dielectric environment and reduces sensitivity of charge point defects originating due to SiO_2 substrate.

Experimentally, these hetero-structures were shown to provide high electron mobility[17] and now have been used for the production of 2D hetero-structures composed of various types of 2D semi-conducting transition metal dichalcogenides possessing ultrahigh mobility. Transition metal dichalcogenide (TMDs) and many other such as, Graphitic Carbon Nitride (g-C_3N_4), Black Phosphorus (BP), transition metal oxides (TMOs) and Layered Double Hydroxides (LDHs)[18–24] are also layered structures held by Van der Waals force as depicted in Fig. 1.1. These 2D materials cover a wide range of band gap (1-3 eV) which inspire scientific community to explore novel 2D materials beyond graphene. Recently, many 2D materials from group III-V binaries are predicted theoretically and synthesized successfully.[25,26] The issue with some of these materials like, hexagonal aluminium nitride (h-AlN), is that they exhibit a wide electronic band gap similar to the hexagonal boron nitride (h-BN). Therefore, these binary compounds are

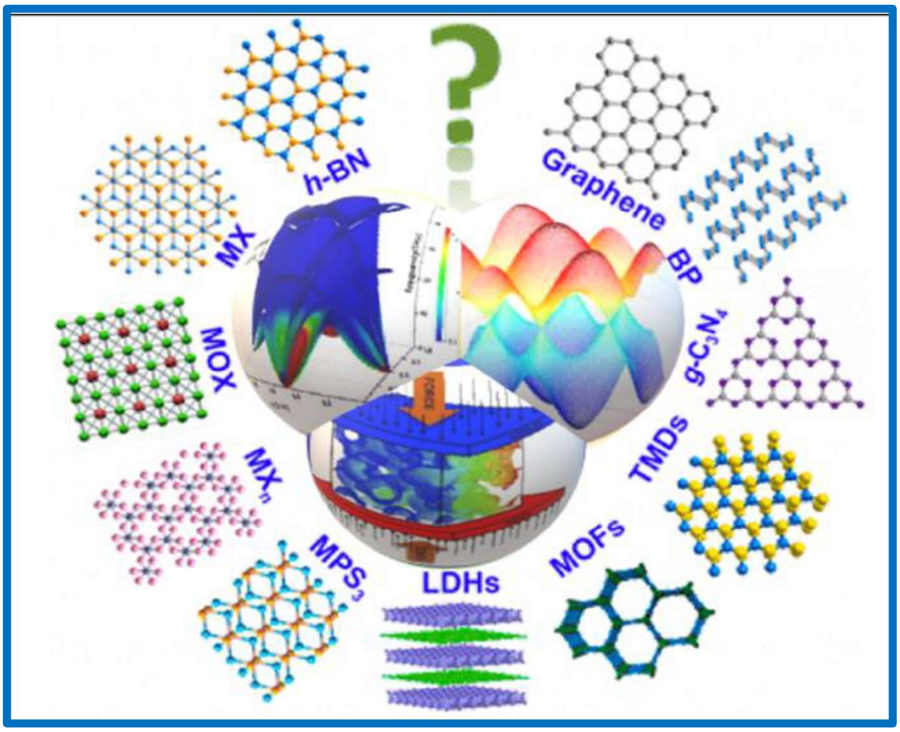

Figure 1.1: Schematic depicts the different classes of ultrathin 2D materials along with electronic, mechanical and dynamical properties of graphene at centre. Reproduced from Ref.23.

not well suited for electronic application. From this point of view, the TMDs are one of the most useful 2D materials for the electronic applications owing to their desired electronic profiles. However, some of the TMDs exhibit indirect nature of electronic band gap and hence are not suitable for optoelectronic applications. Despite of above mentioned limitations, these materials have been utilized in various energy application fields such as hydrogen storage, water splitting, ionic batteries etc. [27–33] Interestingly, the graphene is still considered as the thinnest and strongest material among the class of 2D materials.[34] Therefore, there is less probability of replacing graphene with certain type of material until the new discovery is made. Moreover, most of the graphene like other 2D materials such as silicene, germanene, stanene etc. do not occur naturally and they need to be synthesized on a substrate. Therefore, the choice of suitable substrate is also an important factor for the growth of these 2D materials as they can alter the properties of these 2D materials. Although, the selection of substrate is quite crucial as in some cases they offer mechanical support while in the other cases, they promote disordered growth.[35]

The search of 2D materials beyond graphene has given rise to new era of 2D materials. The newly predicted 2D materials do not only overcome the limitations of graphene but also provide a pathway for enhancing the material properties for their applicability in the wide range of energy applications. This class of 2D materials includes hexagonal boron nitride, mono elemental 2D materials such as borophene, arsenene, bismuthene and many more including MXenes.[36–39] The 2D monoelemental materials such as silicene, germanene and stanene exhibit similar electronic nature like graphene.[36,40] This new era of fascinating 2D materials also provoked scientists to search the 2D perovskites that can be exfoliated from the layered perovskite materials as cleaving a single layer of perovskite material is easy due to less required exfoliation energy.[41] The perovskites have shown their great utility in solar cells and opto-electronics and hence are receiving significant attention from researchers.[42–44] The 2D perovskites compared to their bulk counterpart are found highly efficient in the fabrication of photovoltaic devices like solar cells owing to their unique layered geometry. It is found that the efficiency and stability of solar cell increase with the introduction of 2D materials as an absorber layer due to their tunable structural and electronic properties.[45] Graphene, TMDs and 2D perovskites have been utilized in solar cell devices for better results that enhance by combining the 2D and 3D materials compared to only bulk counterparts based device.[46–48] This process of

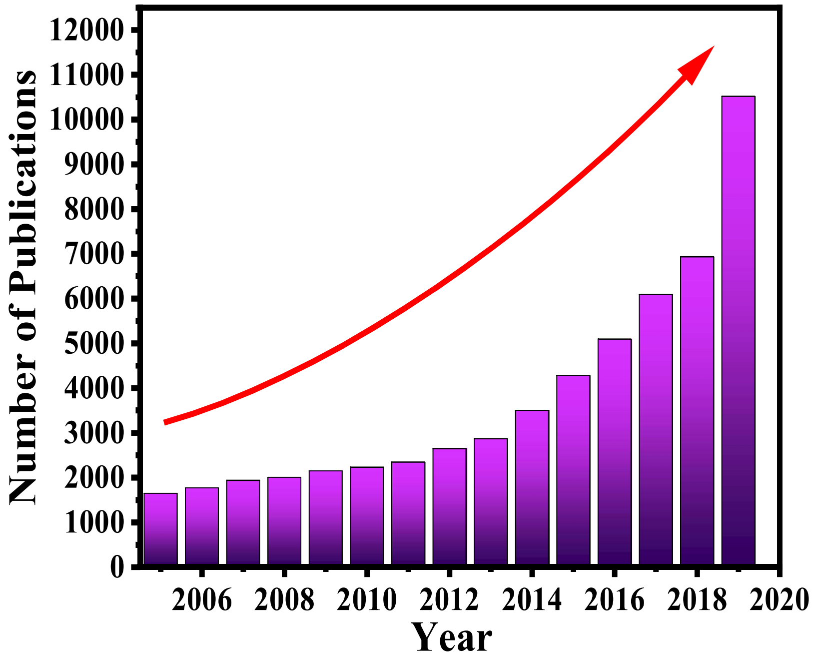

Figure 1.2: Growth of research papers based on two-dimensional materials. (From web of science data www.webofknowledge.com).

development and exploration of new 2D materials is still progressing, as entire periodic table contains the possibility of creating single-atom thin layer or few atoms polyhedral thick 2D layer made-up of element/s evident from the data of publications reported on 2D materials in recent decades (see Fig. 1.2).

Discovery of these 2D materials are of utmost importance because they are capable of fulfilling the demand of energy in today's scenario. Further, many graphene allotropes such as graphyne, graphdiyne, penta-graphene etc. are predicted using density functional theory (DFT) based *first-principles* calculations and experimentally synthesized which exhibit semi-conducting nature as compared to graphene that leads to their utilization in various applications in the field of nanotechnology as nano-fillers, transistors, sensors, anisotropic conductors, and desalinates.[49,50] Recently, these allotropes have attracted a lot of interest and inspired researchers to predict/synthesize allotropes of TMDs that may show their applicability in various fields.[51] There are many possibilities of tuning properties of these 2D materials and allotropes like by tuning dimensionality/imposing quantum confinement, or by applying strain/electric field/pressure, or by introducing defect or adding dopants, or constructing hetero-structure and intercalation of foreign atoms/molecules,[23,24,27,28] which are discussed briefly in the following sections.

1.2 Approaches for tuning the properties of two-dimensional materials

Two-dimensional materials are popular for their tunable properties due to their unique crystal structure and highly anisotropic nature.[52]

Following approaches are generally used for tuning the electronic, mechanical, dynamical and optical properties of 2D materials.

1.2.1 Dimensional Tuning

Layered structures such as graphene, TMDs are best example of dimensional tailoring agent as one or more of the dimensions of these materials (See Fig. 1.3) reduce their physicochemical properties such as electrical, mechanical and optical properties compared to bulk counter parts'

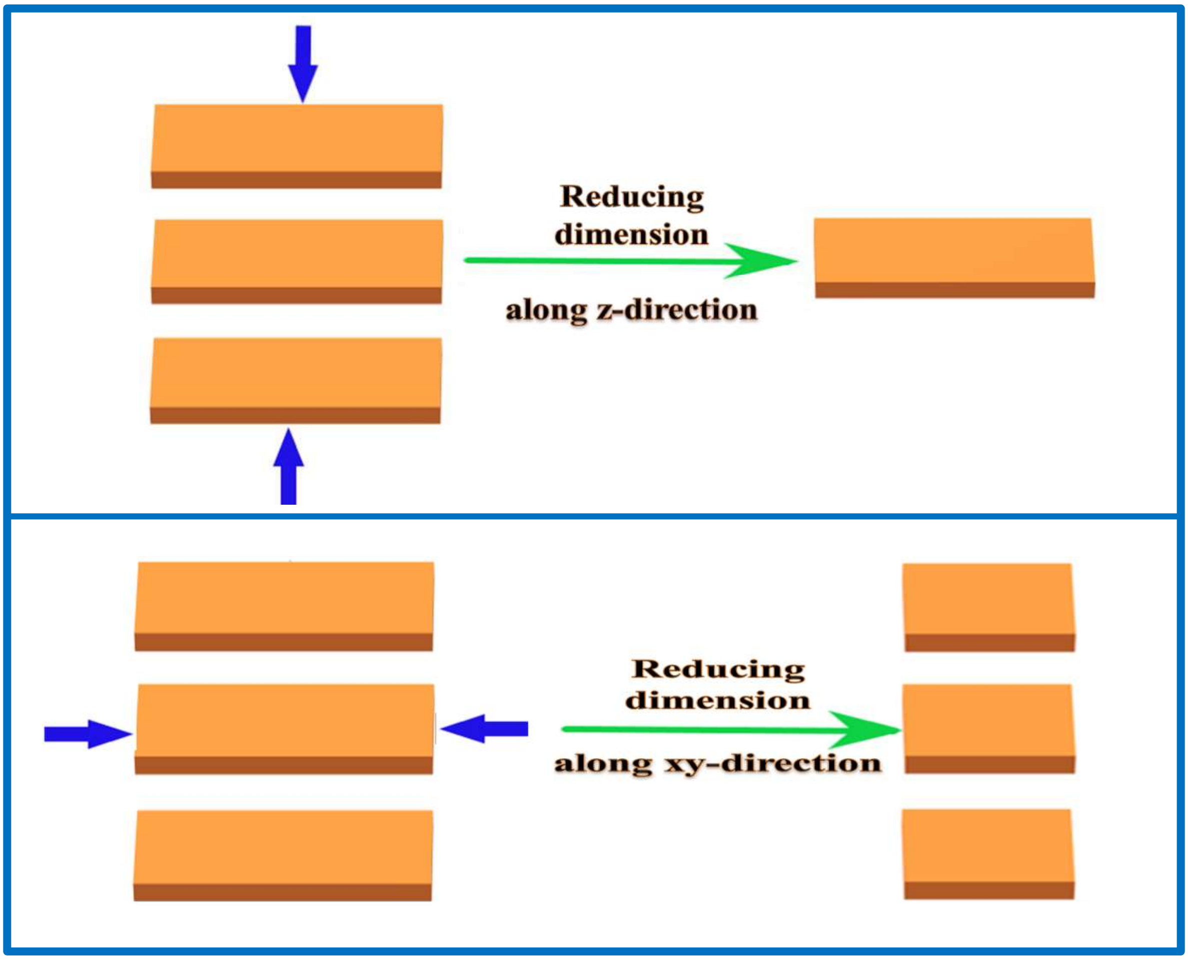

Figure 1.3: Schematic diagram of constructing 2D materials by reducing dimension along the z-direction and xy-directions.

in-plane stiffness.[53] These systems are referred to as low-dimensional structures. Graphene, TMDs and many other layered structures are thinned through confining their z-direction leading to 2D materials that are periodic in xy-directions. The confinement of electrons or holes in z-direction results in enhancement of electronic band gap and might change band nature from indirect to direct, as observed in case of MoS_2, whereas, reducing dimension along xy-plane changes its electronic and catalytic properties at edges.[54]

1.2.2 Elastic strain

2D materials are not only well-known for their highly anisotropic nature but also for their high stretchability.[55] Therefore, electronic, mechanical and dynamical properties of these materials can be controlled with the help of external strain. During experimental synthesis, these materials experience strain due to lattice mismatch between the material to be synthesized and the bottom substrate which also helps in tuning its properties. The strain is a powerful tool for understanding the carrier transport mechanism between substrate and host 2D material and even between hetero-structures. The bending of substrates also exerts external strain on host 2D material. The external strain also helps in determining the flexibility and ductility of materials through evaluation of elastic constants. The strain can be defined as $\varepsilon = (a-a_0)/a_0$; where, a is the lattice constant under strained condition and a_0 is the equilibrium lattice constant. The mechanical properties of these materials can be obtained from strain energy which is defined as, $E_s = E(\varepsilon) - E(0)$; namely, the energy difference between systems under a given strain ε and equilibrium. The in-plane stiffness constant is defined as, $C = 1/A_0(\partial^2 E_S/\partial\varepsilon^2)$, where, A_0 is the equilibrium area of the super-cell which is an important parameter to measure the strength. The in-plane stiffness constant C and Poisson's ratio can be used to know the homogeneous and isotropic nature of 2D materials. The Poisson's ratio can be defined as $\upsilon = \varepsilon_{trans}/\varepsilon_{axial}$, where, ε_{trans} and ε_{axial} are the transverse and axial strain, respectively. It is found that applying uni-axial or bi-axial strain on two-dimensional materials does not only tune their electronic properties, but also modulates their dynamical and mechanical properties.[56]

1.2.3 Doping and defect

The most common technique to overcome the limitations of a conventional 2D semi-conductor is chemically doping of the material. Dopant is an addition of foreign atomic species with desired concentration in the host 2D material. Doping of foreign atoms depends on the nature of chemical dopant and its size and charge. Dopant can be of two type: n-type and p-type. The dopant donates (accepts) electrons to (from) the host. Alkali metals are considered as n-type dopants, whereas, the non-metal such boron, chlorine etc., are considered as the p-type dopants. Moreover, doping can be classified as interstitial, substitutional and chemical.[57] Interstitial doping means that the dopant atom is not incorporated in the crystal lattice, whereas, it resides between the crystal atoms on an interstitial site, and the substitutional doping is referred to the incorporation of the dopant atom into the lattice that perturbs the pristine geometry of the 2D materials. Experimentally, the chemical doping can be done by adsorption of dopant atoms or molecules on the surface of the 2D materials. Due to interaction between atoms or molecules over adsorbate, there is a surface charge transfer which depends on the nature of atoms or molecules which further alters the electronic structure of 2D materials. Similarly, if one of the host atoms are removed or missing from its original location, it is considered as a defect creation in the host system. Defects also play a vital role in tuning the properties of 2D materials such as structural and electronic properties[58] due to modifications in lattice constant and crystal geometry. The change in lattice constant can be attributed to the strain that is experienced by the host material due to introduction of defects and the modulation in the over-all charge of the system.

1.2.4 Two-dimensional hetero-structures

The term 2D hetero-structure can be referred to the merger of two or more than two layers of different 2D materials in vertical or lateral direction. Hetero-structuring is the advanced technique for precisely controlling the carrier dynamics within the materials through transport engineering. The properties of these hetero-structured 2D materials depend on the structural configuration, lattice mismatch and interaction between substrate and 2D host material/s. If the interaction between the two layers is governed by weak van der Waals force, then it would allow the layer to get cleaved very easily, otherwise, it would lead to the formation of hetero-structure. The best example is free standing layer of graphene that exhibits semi-metal nature, whereas, graphene on h-BN substrate results in opening of bandgap subjected to varying interlayer distance.[16] Graphene/h-BN hetero-structure has been an area of a great interest for both theoretical and experimental point of view to investigate the role of the carrier dynamics at graphene/h-BN interface. Similar to the graphene/h-BN hetero-structure, it is shown that the growth of silicene on TMDs such as MoS_2, WS_2 and $PtSe_2$ tunes the electronic properties of silicene.[59,60] The electronic properties of 2D materials basically depend on the lattice mismatch between substrate and material itself that leads to the generation of strain within the material

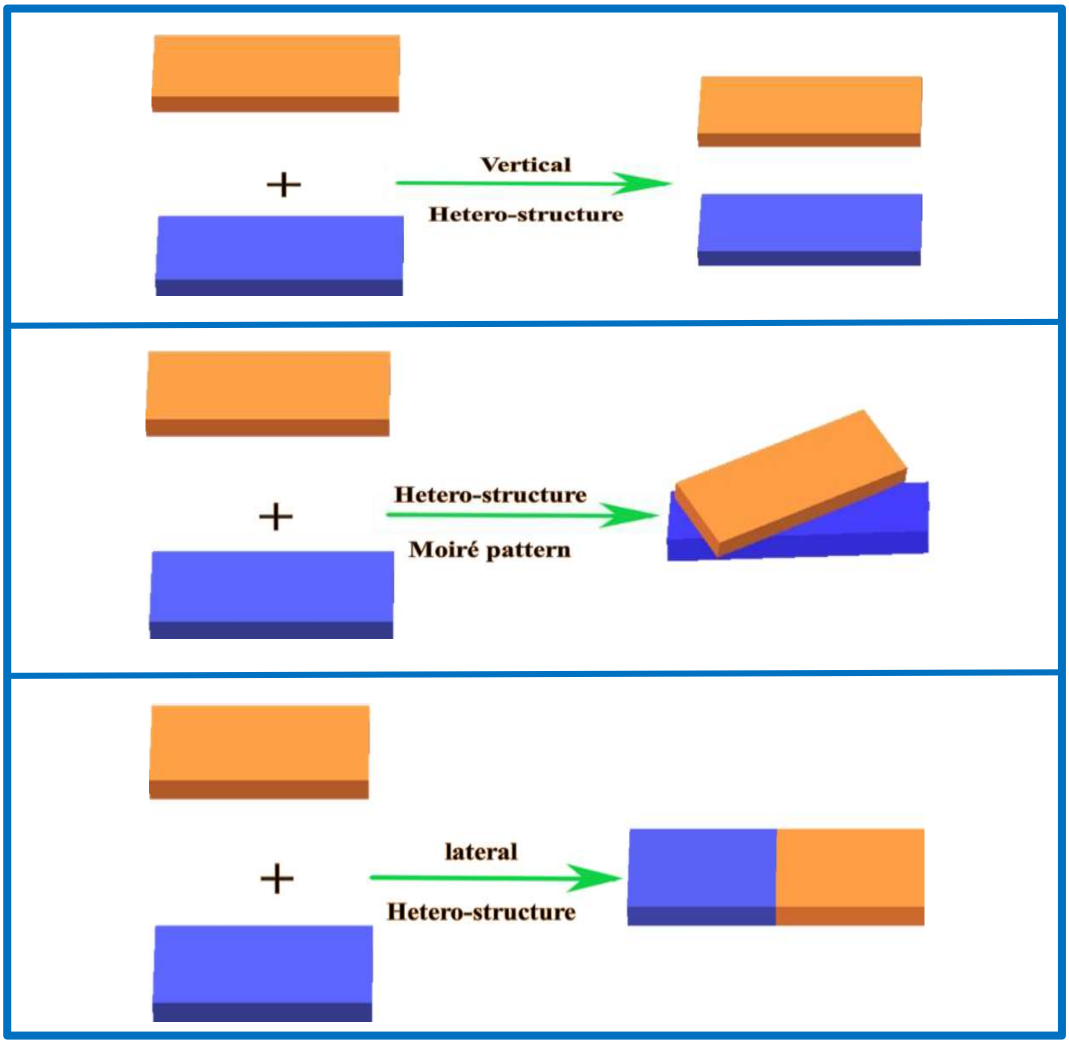

Figure 1.4: Schematic diagram of tuning properties of 2D TMD by constructing hetero-structure.

during the growth process. There are mainly two types of hetero-structures: (a) vertical and (b) lateral as show in Fig. 1.4. Fig. 1.4 represents a schematic diagram of vertical hetero-structure which follows two models, the topmost panel is for lattice match model, where lattice match is between the layers is less than 1.8 %, and the other is for lattice mismatch model, where one of the layer of 2D material is rotated to certain angle so as to minimize the lattice mismatch, and termed as so called formation of Moiré pattern.[61] When two 2D monolayers are grown side by side on a substrate, the 2D configuration is thus referred as lateral hetero-structure, for example WSe_2@MoS_2.[62]

1.2.5 Intercalation

The process of intercalating the foreign atom/s or molecule/s between the layers of vertical hetero-structure is known as intercalation. In one of the study, the intercalation of different

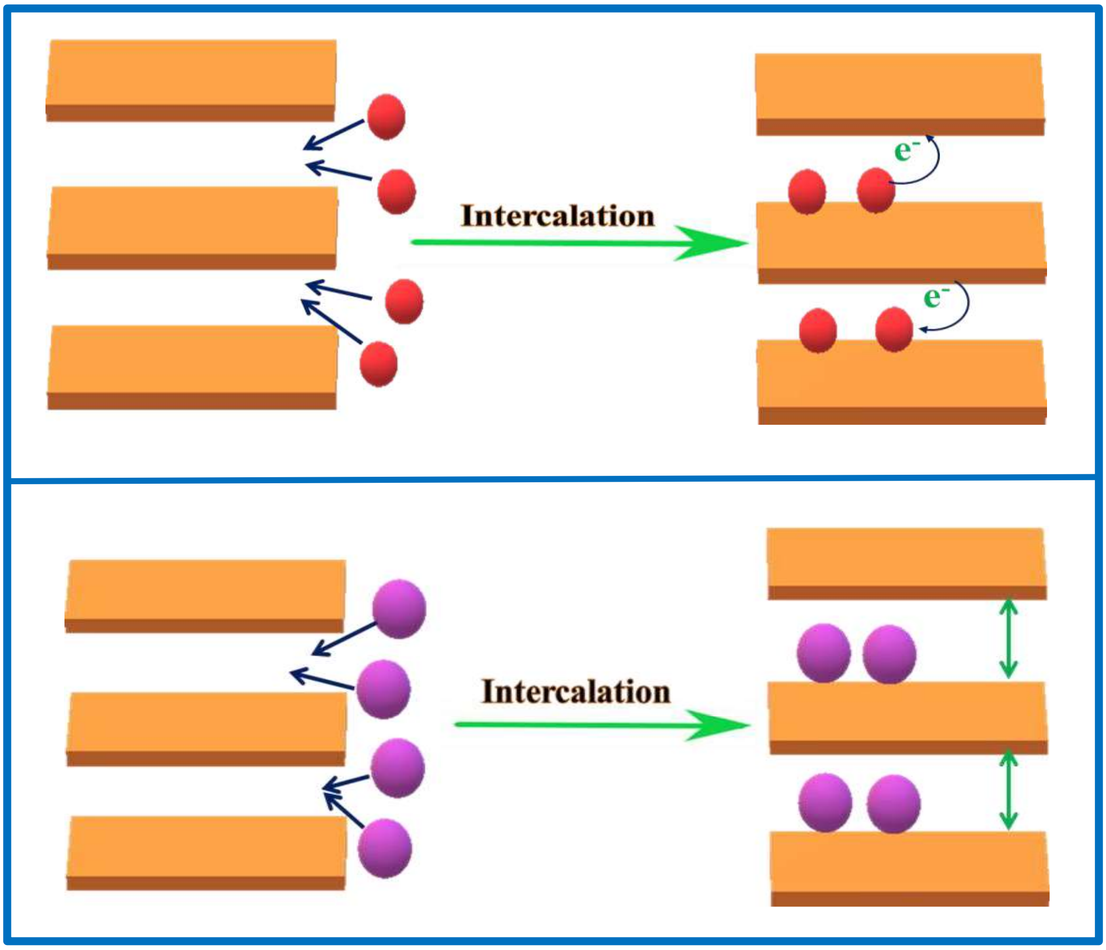

Figure 1.5: Schematic diagram of 2D hetero-structure with ion or molecules intercalation.

atoms/molecules such as, alkali atoms (Li, Na and K), halogen atoms (Cl, Br and I) and other impurity atoms (Cu, Si and Ni) have been done to study graphene/h-BN hetero-structure.[63] This process changes the electronic properties of hetero-structure and makes it suitable for device applications. Alkali atoms generally donate electron to host materials whereas, other types of impurity atoms (Ni, Cu, Br) induce magnetic nature into hetero-structure[63] and increase the spacing between the layers of hetero-structure. The hetero-structures are held tightly with each other via Van der Waals force, which makes them difficult to be exfoliated. Furthermore, the van der Waals interaction weakens with inclusion of gas molecules like CO_2, NO_2 and NH_3.[64]

In present research work, the unique 2D materials such as arsenene, silicene, TMDs and hybrid organic-inorganic perovskites are investigated using DFT based on *first-principles* calculations with a prime objective of tuning their ground state properties for making them suitable for energy applications such as optoelectronics, hydrogen production and photovoltaics.

1.3 Research objectives

The present work aims to investigate the electronic, mechanical and dynamical properties of few selected 2D materials under different conditions for tuning different parameters of the considered systems and to understand the underlying mechanism. The increased importance of 2D materials in various fields urges to explore their properties and stability before directly synthesizing the materials and using them for device applications. Hybrid organic-inorganic perovskites have also gained a lot of attention due to their significantly high efficiency for solar cells beside its poor stability against moisture and phase modifications with difference in ambient temperature. The specific objectives of the present work are as under:

1. To obtain better understanding of the confinement effect on the properties of the bulk materials like Methylammonium lead iodide, silicon (Si), arsenic (As), bismuth (Bi), zirconium di-chalcogenides ($ZrSe_2$, ZrS_2 and ZrSSe) and tin di-selenide ($SnSe_2$).
2. To understand the effect of strain on the electronic, mechanical and dynamical properties of selected two-dimensional materials.
3. To study the catalytic behavior of arsenene, ZrS_2, $ZrSe_2$ and ZrSSe for their utilization in the hydrogen generation applications.
4. To understand the structure stability of selected layered structures.
5. To computationally design the 2D perovskites based solar cell devices.

1.4 Structure of the present thesis

The present thesis is organized in the following manner.

Chapter 1 is about the progress and development of two-dimensional (2D) materials, their unique properties and applications in the novel fields such as electronics, optical, hydrogen storage, nano catalysis for hydrogen evolution reaction (HER) and photovoltaic solar cells. Further, the prediction of new 2D materials provides a novel pathway to have better technology and applications for betterment of the society. To fulfill the need of required energy demands, the eco-friendly production of renewable sources has become a mandatory task. One of the cleanest forms of energy is the pure hydrogen, which can be produced by the process known as water-splitting in which the water molecules are broken for liberation of hydrogen and oxygen so as to further utilize the free hydrogen for generating energy. Moreover, many 2D materials such as TMDs, borophene, graphene etc., have gained attention as a potential catalyst for HER (hydrogen evolution reaction) to reduce the cost as compared to the noble metal platinum-based catalysts. In addition, studies show that the catalytic activity of the materials can be enhanced with chemically doping the material, creating defect, applying electric field, strain and substrate engineering. The crystal structure of arsenene, antimonene and bismuthene shares buckled honeycomb geometry similar to those of buckled silicene, that is helpful to stabilize the crystal structures. Besides this, it is observed that these materials overcome the drawback of silicene which is semi-metallic in nature whereas, the arsenene, antimonene and bismuthene exhibit semi-conducting nature that make them suitable for opto-electronic devices, catalysts and photo detectors.

Theoretical description of the computational methodology used throughout the research work is presented in **Chapter 2**. In this chapter, theoretical concepts which form the basis of density functional theory (DFT) are presented and discussed. In particular, all quantities which help to calculate the electronic, dynamical and mechanical properties of 2D materials on the basis of DFT are discussed. We present all basic ideas of many body problem, Born-Oppenheimer approximation, Hartree and Hartree-Fock approximations followed by density-based method and Kohn-Sham equation. Moreover, the use of plane-waves to represent electron wave-functions and density needed to deal with valance and core electrons as implemented in Quantum Espresso simulation package are discussed. We also discuss in detail the Grimme's dispersion correction which is of most importance not only to predict correct cohesive and adsorption energies but also essential to consider the Van der Waals interaction that dominates in layered systems. Finally, we discuss the determination of elastic properties of the proposed 2D materials.

In **Chapter 3**, we summarize and discuss the results of systematically investigated, stability and electronic properties of two-dimensional honeycomb structures of arsenic known as arsenene, and zirconium chalcogenides (ZrX; X=S_2, SSe and Se_2). We have analyzed their catalytic activity for water-splitting process utilizing DFT based *first-principles* calculations. We have included dispersion correction in all calculations, to get accurate adsorption energy and for understanding their catalytic activity towards hydrogen evolution reaction. From the DFT based calculations, it is found that the arsenene, ZrS_2 and Janus ZrSSe exhibit semi-conducting nature with band gap magnitude of 1.62 eV, 1.58 eV and 1.08 eV, respectively and hence acquire potential as HER photocatalyst, whereas $ZrSe_2$ monolayer is well-suited as an electrocatalyst. Furthermore, we sieved different dopants for enhancing the catalytic activity through electronic band gap modulation, as the band gap is one of the important parameters for tuning the catalytic activity of any material. The fundamental band gap of arsenene could be altered by introducing B, N, O, Ga, Ge and Se dopants and ZrX monolayers with Nb, Pt and W dopants. We found that B, N and Ga-doped arsenene shows a p-type semi-conducting nature, as the Fermi level is located close to valence band maximum (VBM) with band gap of 0.74, 0.65 and 0.57 eV respectively, while Ge-doped arsenene shows n-type semi-conducting nature as minimum of conduction band is nearer to Fermi level. However, O and Se doped arsenene show metallic nature. The O doped arsenene is found to be the most promising candidate for HER, as its adsorption energy is 0.24 eV, whereas, B doped arsenene is most promising candidate for OER catalyst amongst all other doped monolayers, as its adsorption energy is found to be 0.37 eV that is very close to the ideal magnitude 0.33 eV. In a nut-shell, the HER activity gets enhanced by 82% for O-doped arsenene and OER activity by 87% for B-doped arsenene as compared to the pristine counterpart. The Zirconium based doped systems exhibit metallic nature and it is found that all three dopants increase the catalytic activity of basal planes as compared to pristine ZrX. The functionalization of systems with dopants improves the basal activity of systems, as the Gibbs free energy of $ZrSe_2$ is positive among all three systems leading to desorption process feasible. We conclude that the Nb-$ZrSe_2$ is well-suited for HER catalyst as Gibb's free energy is closer to zero following the sequence Nb-$ZrSe_2$ > Pt-ZrS_2 >Nb-ZrSSe > Nb-ZrS_2 > ZrSSe. We observed that dopants play an important role in the enhancement of the catalytic activity of materials.

Chapter 4 presents the results on strain dependent electronic and lattice dynamical investigation for 2D monolayers of Bi, BiAs and BiSb. The DFT based calculations show that the band gap of these materials can withstand for large range of tensile strain and, the direct-indirect-metal electronic phase transition occurs for compressive strain in all three materials. Absence of imaginary vibrational frequencies in the calculated phonon dispersion curves validates the dynamical stability of Bi, BiAs and BiSb monolayer. We predict that monolayer structure of Bi, BiAs and BiSb is stable and compressive strain induces direct-indirect metallic transition whereas tensile strain reduces the direct band gap. Under the effect of strain, the phonon dispersion curves of Bi, BiAs and BiSb show remarkable changes as the out of plane ZA mode turns quadratic in nature from its linear relationship with **k** whereas, the two acoustic modes LA and TA preserve their linear behavior. The overall results suggest that owing to high stability even at large strain magnitudes, the BiAs and BiSb can be a potential candidate for nano electronic devices.

In **Chapter 5**, the investigation on the structural and electronic properties of silicene, $SnSe_2$ monolayer, and silicene/$SnSe_2$ hetero-structure is performed using dispersion corrected density-functional theory and respective results are discussed. To know the energetically favorable configuration of hetero-structure and possibility of growing silicene over $SnSe_2$, we have calculated the formation and cohesive energies of these systems. Moreover, the lattice match model[15] is utilized for the construction of hetero-structure, as the lattice mismatch between $SnSe_2$ and silicene is about 0.48 %. After optimization of individual structures, it is observed that the buckling height of free standing silicene monolayer is 0.47 Å which increases by 5.4 % in hetero-structured configuration due to strong interaction between both Si and $SnSe_2$ monolayers. The silicene exhibits semi-metallic nature, while the $SnSe_2$ shows semi-conducting nature with band gap of 0.84 eV and most-importantly, their hetero-structure shows metallic characteristic. The calculated formation energy of hetero-structure is -0.54 eV which suggests that the formation of hetero-structure occurs under exothermic process and is energetically favorable compared to the reported values of the semi-conducting substrates (−0.12 eV over MoS_2, −0.13 eV over GaS and −0.28 eV over $PtSe_2$).[51, 52] It is shown that the strong interaction between the hetero-layers can be weakened by intercalation of different atoms such as alkali, halogen atoms and molecules (CO_2, NO_2 and NH_3) that also help to tune the electronic properties of the systems.[51,52] It has been proved good enough to recover the Dirac cone which disappears/distorts due to the strong interaction between the silicene and metal substrate together with the opening of the electronic band gap. We have investigated the structural and electronic properties of Si/$SnSe_2$ with intercalation of phosphorous (P) and chlorine (Cl) atoms and NH_3 molecule. We observed that P and Cl atoms due to their high electronegativity/electron withdrawing nature binds strongly with silicene sheet instead of $SnSe_2$ substrate leading to metallic nature of system. The NH_3 molecule shows interesting nature, as it depends on intercalation configuration within the hetero-structure. The nitrogen atom prefers to bind with silicene atoms leading to metallic nature whereas, it remains inert in case the of nitrogen facing towards $SnSe_2$ monolayer. The interaction between both monolayers weakens van der Waals interaction between them and charge distribution is also found to be lesser, that consequences to band opening of 0.23 eV. We also sensed CO molecule over all considered systems to know the reactivity of CO towards it and, we observed that the intercalation of atoms and molecules enhances the sensing properties of the hetero-structure.

In **Chapter 6**, we have analyzed the effect of quantum confinement; biaxial and uniaxial strains on electronic properties of 2D, 1D and few layers of methylammonium lead iodide (MAPI) with cubic phase under the framework of DFT, and its implications to photovoltaic solar cells. As the solar cell performance parameters can be tuned by varying electronic band gap of materials, we have tuned the electronic properties of MAPI by applying bi-axial and uni-axial strains, respectively to 2D and 1D MAPI. The strain in the present calculations is imposed within the range from −6% to 6% uni-axial strain for 1D MAPI, and bi-axial strain for 2D MAPI, respectively. From our calculations, we found that the band gap of 2D MAPI increases on imposing tensile strain (positive strain) and reduces under compressive strain (negative strain). Moreover, there is a direct to indirect band gap transition beyond 4% of compressive strain. However, in case of 1D MAPI, the band gap increases in both tensile and compressive strains and shows parabolic behavior with strain. Our studies show that the solar cell parameters of MAPI are highly influenced by confinement, strain and number of layers in the case of 2D MAPI. The 2D MAPI is found to be better for solar cell applications due to the lower effective mass of electron and hole, arising from the strong s-p anti-bonding coupling and enhanced solar cell parameters. The highest theoretical efficiency of 23.6% is obtained for 2D MAPI with mesoporous (mp)-TiO_2 electrode.

The detailed systematic investigation and the results on electronic, dynamical and mechanical properties of 2D materials using DFT have been summarized in **Chapter 7**. The unique properties of 2D materials particularly under the influence of external parameters have been discussed in the light of their potential applications such as optoelectronic, hydrogen production and solar cell. Finally, we have concluded the thesis with a brief discussion on scope of future research work.

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