Two-Dimensional Quantum Materials

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By

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PREFACE

The realm of material science has witnessed only a handful of discoveries and technological advancements with the potential to revolutionize our world, and the emergence of two-dimensional (2D) materials stands prominently among them. Originating from the isolation of graphene from graphite in 2004, this class of materials, characterized by their atomically thin nature and dominated by surface effects, has opened up a new frontier in material science. Research on 2D materials, including graphene and its counterparts like silicene, germanene, phosphorene, as well as transition metal dichalcogenides (TMDs), MXenes, and other layered semiconductors, has burgeoned into a global effort involving thousands of researchers across diverse fields such as physics, chemistry, engineering, and biology. The distinctive feature of 2D materials lies in their layered structure, comprising strong in-plane chemical bonds juxtaposed with weak out-of-plane coupling between layers. This structural arrangement allows for the cleavage of individual atomic layers, giving rise to extraordinary variations in electronic properties when the material's thickness is reduced to a single or few layers. This phenomenon, known as quantum confinement, imparts unique and often unexpected properties to 2D materials, fuelling exploration into novel applications and innovative avenues in various domains. As researchers delve deeper into the intricacies of these layered materials, it becomes increasingly evident that they hold the promise of unlocking unprecedented possibilities and paving the way for ground-breaking advancements in science and technology.

Welcome to "Two-Dimensional Quantum Materials," a comprehensive exploration of the fascinating world of 2D materials and their implications in the realm of quantum phenomena and applications. This book delves into the multifaceted aspects of 2D materials, from their fundamental properties to cutting-edge applications, promising to provide valuable insights into the forefront of nanoscience and technology.

In the introductory chapters, readers will embark on a journey through the classification of materials based on confinement, tracing the historical milestones leading to the discovery of graphene, and uncovering the vast landscape of other 2D materials such as transition metal dichalcogenides (TMDs), black phosphorus, and boron nitride. The significance and diverse applications of these materials across various fields will also be elucidated, setting the stage for a deeper exploration.

Subsequent sections delve into the crystal structure and properties of 2D materials, unravelling the atomic intricacies of their stacking configurations and polymerization phenomena. Readers will gain insights into the electronic band structure, as well as optical, electrical, and mechanical properties that underpin the unique characteristics of 2D materials.

Synthesis and fabrication techniques, ranging from top-down to bottom-up approaches, are meticulously elucidated, providing readers with a comprehensive understanding of the methods employed in the production of 2D materials. Characterization methods such as Raman spectroscopy, photoluminescence (PL) spectroscopy, and transmission electron microscopy (TEM) are also explored, shedding light on the techniques used to unravel the structural and optical properties of these materials at the nanoscale.

The book further delves into quantum phenomena exhibited by 2D materials, including quantum conductance, the quantum Hall Effect, and the emergence of Dirac and Weyl fermions. Exciton and multibody physics in 2D materials are also investigated, offering valuable insights into the quantum behavior of these materials.

The applications of 2D materials in nanoelectronics, optoelectronic devices, and energy storage and conversion are thoroughly examined, highlighting their potential to revolutionize various technological domains. Furthermore, the book explores emerging topics such as spintronics, valleytronics, twistronics, and the interplay between charge density waves (CDW) and superconductivity in 2D materials.

Finally, the challenges, future directions, and conclusions drawn from the collective insights presented in this book offer valuable reflections on the scalability, integration challenges, environmental considerations, and potential breakthroughs in the field of 2D quantum materials.

We hope this book serves as a valuable resource for researchers, students, and enthusiasts alike, fostering a deeper understanding of the intricate world of two-dimensional quantum materials and inspiring further exploration and innovation in this burgeoning field.

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CHAPTER 1

INTRODUCTION TO QUANTUM MATERIALS

Quantum materials are substances that exhibit novel and exotic physical properties below the quantum confinement limit, where the behavior of particles is governed by the principles of quantum mechanics. These materials are characterized by unique electronic structures, such as the arrangement of electrons in energy bands or levels that lead to intriguing phenomena. On the microscopic level, four fundamental degrees of freedom *i.e.,* charge, spin, orbit and lattice become intertwined, resulting in complex electronic states.[1] Quantum materials often display emergent properties that arise from the collective behavior of electrons or other quantum particles. These properties can be very different from what one would expect based on the individual components of the material. In quantum materials, electron-electron interactions play a major role and these interactions can lead to phenomena like superconductivity, magnetic ordering, and fractional quantum Hall effect and so on.[2] These materials can undergo quantum phase transitions at very low temperatures, where small changes in external conditions lead to abrupt changes in the material's properties. They also exhibit unusual physical anomalies, such as non-Fermi liquid behavior, that challenge conventional theories of condensed matter physics. These distinctive physical properties are dictated by quantum mechanical effects, particularly when studied at length scales comparable to or smaller than the de Broglie wavelength of the constituent particles and the exciton Bohr radius.

1.1 De Broglie Wavelength

The de Broglie wavelength is a fundamental concept in quantum mechanics, and it relates the momentum of a particle to its wavelength, $\lambda = \frac{h}{mv}$ where λ is the wavelength of the particle, m and v are the mass and velocity of the particle respectively, and h is the Planck constant.[3]

In quantum materials, when the characteristic length scale of the material approaches or falls below the de Broglie wavelength of the particles involved, quantum effects become increasingly prominent. This can lead to phenomena such as wave-particle duality, quantum confinement, and quantization of energy levels.

1.2 Exciton Bohr Radius

Excitons are bound electron-hole pairs that exist in certain materials, including quantum materials. The exciton Bohr radius is a crucial parameter that defines the typical spatial extent of these excitonic states within the material. In quantum materials, when the size of the material becomes comparable to or smaller than the exciton Bohr radius, the behavior of excitons can significantly impact the material's optical and electronic properties.

Bohr radius

The equation for the Bohr radius of an electron is given by,[4]

$$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{mq^2} \tag{1}$$

Where ε_0= 8.85×10^{-12} F/m (permittivity), $\hbar$ =1.054× 10^{-34} J.s (Planck's constant over 2π), m_e = 9.11× 10^{-31} kg (mass of a free electron) and q = 1.602× 10^{-19} C (charge). If you plug all the numbers in and do the math you come up with result

$$a_0 = 5.28\times 10^{-11} \text{ meters} = 0.528 \text{ Å}$$

This is the standard Bohr radius one sees all the time.

Derivation

Basically we need to balance the centrifugal (outward) force of a carrier with the Coulomb attractive (inward) force.

$$\frac{mv^2}{r} = \frac{q^2}{4\pi\varepsilon_0 r^2} \tag{2}$$

Here we make use of the relation

$$2\pi r = n\lambda \tag{3}$$

Where, n is an integer. The de Broglie relation comes in by the wavelength $\lambda = \frac{h}{p}$, where h is Planck's constant and p is the momentum of the particle ($p = mv$). Starting with the above equation we rearrange it to get

$$\lambda = \frac{2\pi r}{n} = \frac{h}{p} = \frac{h}{mv} \tag{4}$$

Solve v for to get

$$v = \frac{nh}{2\pi mr} = \frac{n\hbar}{mr} \tag{5}$$

Replace this into the main equation

$$\frac{n^2\hbar^2}{mr} = \frac{q^2}{4\pi\varepsilon_0} \tag{6}$$

Rearrange this to get

$$r = \frac{4\pi\varepsilon_0\, n^2\hbar^2}{mq^2} \tag{7}$$

If $n = 1$ (the lowest orbit) this gives us the Bohr radius

$$a_0 = \frac{4\pi\varepsilon_0\, \hbar^2}{mq^2} \tag{8}$$

Which is the standard textbook equation we showed earlier.

At this point we note that if the electron or carrier is not in vacuum the equation should be modified to take into account the dielectric constant of the medium. (Instead of ε, replacing it with $\varepsilon\, \varepsilon_0$)

$$a_0 = \frac{4\pi\varepsilon_0\, \varepsilon\, \hbar^2}{mq^2} \tag{9}$$

Furthermore, for the case of an exciton (electron hole pair) in a semiconductor just replace the mass of the electron with the effective mass of the exciton.

$$\frac{1}{m_{eff}} = \frac{1}{m_e} + \frac{1}{m_h} \tag{10}$$

Where m_e and m_h are the effective masses of electron and hole in the material.

This equation gives the relation between the de Broglie wavelength and the exciton Bohr radius. So, in effect, our initial statements about confinement dealing with either the exciton Bohr radius or de Broglie wavelength are essentially one and the same. The de Broglie wavelength or exciton Bohr radius are therefore natural length scales by which to compare the physical size of a nanomaterial. In general objects with dimensions smaller than these natural length scales will exhibit quantum confinement effects.

1.3 Quantum Confinement

Quantum confinement is a fundamental concept in condensed matter physics that refers to the confinement of electrons or charge carriers within a space so small that their quantum mechanical properties dominate their behavior. This phenomenon becomes significant when the physical dimensions of a material, such as its thickness or particle size, become comparable to the de Broglie wavelength associated with quantum mechanics.[5] The concept of quantum confinement arises from size reduction in materials, leading to tighter confinement of electronic wave functions and resulting in changes in electronic and optical properties in nanomaterials. A smaller (or bigger) particle size results in a stronger (or weaker) confinement which gives rise to enhancement (or decrease) of the band gap and modifies the band structure of the material. These changes affect electron mobility, effective mass, relative dielectric constant, and optical properties, among others. Quantum confinement effects give rise to intriguing properties in metallic nanoparticles, such as color variations in colloidal suspensions with changing particle size, UV photoemission, and enhanced photoluminescence.

1.4 Density of States

Density of States (DOS) is a concept in condensed matter physics that describes the distribution of energy states available to particles, typically electrons, within a material. Quantum confinement, especially in nanoscale materials like quantum dots or nanowires, has a significant impact on the DOS, leading to discrete energy levels rather than a continuous band structure, as seen in bulk materials. Here's an explanation of DOS in the context of quantum confinement:

Bulk vs. Nanostructured Materials

Bulk Materials: In a bulk material (e.g., a large piece of semiconductor), electrons occupy energy states forming continuous energy bands. There is a continuous range of energy levels available for electrons to occupy, and this band structure is a fundamental concept in solid-state physics.

Nanostructured Materials: When the dimensions of a material become comparable to or smaller than the de Broglie wavelength of its electrons (quantum confinement regime), the DOS changes dramatically. In nanomaterials like quantum dots, quantum wires, or thin films, electrons are confined in three, two and one dimensions. In quantum dots, the electrons are confined in all three dimensions. This confinement results in the quantization of energy levels. Electrons can only occupy discrete energy states or energy levels. These discrete energy levels are often referred to as "energy shells" or "quantum levels." In the case of quantum wells (confinement in one dimension) or quantum wires (confinement in two dimensions), there is still quantization of energy levels, but the quantization occurs in fewer dimensions.

Effect on DOS:

Bulk DOS: In bulk materials, the DOS is continuous, forming energy bands. The number of energy states per unit energy interval is relatively constant within a band.

Nanostructure DOS: In nanostructured materials with quantum confinement, the DOS exhibits distinct peaks or steps corresponding to the quantized energy levels. These energy levels are determined by the size and shape of the nanostructure and are often referred to as "quantum energy levels" or "quantum states."

DOS also helps us understand the electronic structure of materials based on their dimensionality. Here's an explanation of 0D, 1D, 2D, and 3D materials in terms of DOS.

1.5 Classification of the Materials [0D, 1D, 2D and 3D] based on DOS

0D Materials (Zero-Dimensional)

0D materials are quantum dots or nanoparticles that have zero dimensions in space, meaning they are extremely small in all three dimensions. In 0D materials, DOS exhibits discrete energy levels due to quantum confinement. These discrete energy levels are often referred to as "energy states" or "quantum levels." The energy spacing between these levels is determined by the size of the quantum dot, with larger dots having wider energy spacings.

1D Materials (One-Dimensional)

1D materials are nanowires, nanotubes, or nanorods that have one dimension significantly larger than the other two. In 1D materials, DOS shows continuous energy bands along one direction (the dimension along which the material is extended). These energy bands are quantized along the other two dimensions, resulting in a 1D electronic structure with energy states that vary with wave vector along the extended direction.

2D Materials (Two-Dimensional)

2D materials, like graphene, transition metal dichalcogenides (TMDs), and black phosphorus, are composed of atomic layers with strong in-plane covalent bonds but weak van der Waals bonds between layers. In 2D materials, DOS displays two-dimensional behavior. There is a continuous band of energy states within the atomic layers (in-plane) and a quantization of energy states perpendicular to the layers. This quantization leads to the formation of discrete Landau levels in the presence of a magnetic field.

3D Materials (Three-Dimensional)

3D materials include conventional bulk materials like metals, semiconductors, and insulators, where all three dimensions are extended and of comparable size. In 3D materials, DOS exhibits the typical behavior seen in bulk materials. There are continuous energy bands in all three dimensions, resulting in a three-dimensional electronic structure with a high density of energy states. The DOS curve is smoother and denser compared to lower-dimensional materials.

In summary, the dimensionality of a material strongly influences its DOS behavior. 0D materials show discrete energy levels, 1D materials have continuous energy bands along one direction, 2D materials exhibit two-dimensional electronic behavior, and 3D materials have a bulk-like DOS with continuous energy bands in all three dimensions as depicted in Figure 1.

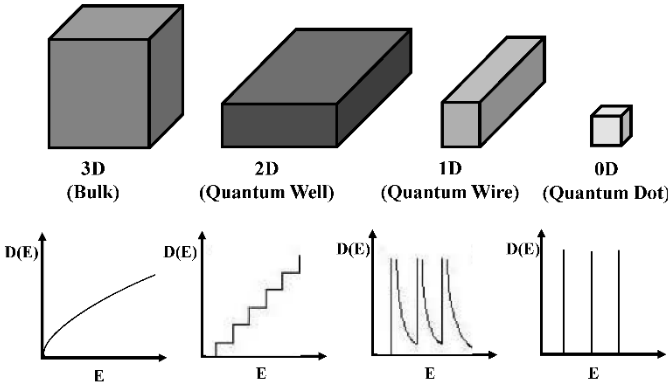

Figure 1. Schematic diagram of density of states for 3D, 2D, 1D and 0D systems. Reproduced with permission.[6]

Since this book is concentrating on 2D quantum materials, the following chapters and their constituent sections will mostly talk about 2D materials and related quantum phenomena responsible for those. Although there exists a plethora of 2D materials now a days, we must start with Graphene, the earliest discovered 2D quantum material which revolutionized the scientific community for its indigenous design and multifaceted applications.

1.6 Historical Overview and Discovery of Graphene

Graphene is a two-dimensional (2D) structure consisting of sp^2 hybridized carbon atoms covalently bonded in a hexagonal honeycomb lattice. It has the capability to form zero-dimensional (0D) fullerenes when wrapped, one-dimensional (1D) nanotubes when rolled, or three-dimensional (3D) graphite when stacked. Figure 2 displays the schematic of graphene and its unit cell. P.R. Wallace, a Canadian physicist, made significant theoretical contributions by conducting calculations on graphene.[7] Prior attempts to isolate graphene predominantly centered on chemical exfoliation. In this methodology, bulk graphite underwent an initial process of intercalation, whereby graphene layers were separated by intermediate layers of atoms or molecules. Brodie altered graphite through chemical treatment with strong acids and oxidants, resulting in the oxidation of graphite.[8] Brodie's approach was subsequently refined for the production of graphite oxide (GO) by Hummer and Staudenmaier. [9,10] In 1962, Boehm *et al.*[11] produced graphene by chemical reduction of GO.

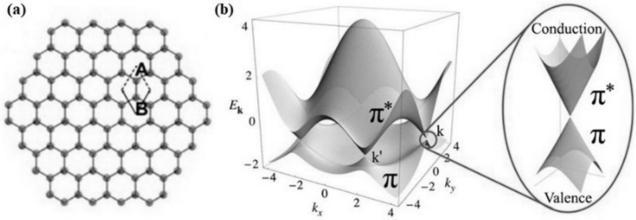

Figure 2. (a) Hexagonal honeycomb lattice of graphene including two atoms (A and B) in a unit cell;[12] (b) Electronic dispersion in the honeycomb lattice, in which the conduction band minima and valence band maxima meet at six Dirac points (left), and close view of the energy bands at one of the Dirac points (right). Reproduced with permission.[13]

Epitaxial growth of graphene has been achieved through chemical vapor deposition of hydrocarbons on metal substrates. In 1966,[14] hot single crystals of nickel was exposed to methane at a temperature of 900°C, resulting in the formation of thin crystalline films of graphite. Moving forward, in 1975, Lang *et al.* [15] successfully demonstrated the deposition of a monolayer graphitic structure on platinum using ethylene. Eizenberg *et al.*[16] in 1979 reported the formation of graphitic layer on Ni (111). A significant milestone occurred in 1992 when Land *et al.* [17] synthesized single layer graphite structures on platinum by decomposition of hydrocarbons. Additionally, thermal decomposition of silicon carbide has been another method yielding single layer and few layer graphene. [18,19].

In 1999, Ruoff *et al.*[20] achieved the production of graphite islands with a thickness of approximately 200 nm using oxygen plasma etching. However, the year 2004 marked a significant breakthrough when physicists from the University of Manchester and the Institute for Microelectronics Technology in Chernogolovka, Russia, led by Novoselov *et al.*, successfully isolated graphene films from highly oriented pyrolytic graphite HOPG using a technique known as mechanical exfoliation.[21] This ground-breaking work represented a pivotal moment in the extraction and identification of both few-layer and single-layer graphene from graphite. The process involved the repetitive cleaving of a graphite crystal using adhesive tape until it reached its maximum limit. Subsequently, the thinned-down graphite was transferred onto an oxidized silicon wafer (figure 3.). This achievement brought to fruition the long-standing goal of creating a two-dimensional carbon material. In recognition of their remarkable contribution to this advancement, A. Geim and K. Novoselov were jointly awarded the Nobel Prize in Physics in 2010. The extraordinary electronic, mechanical, and thermal properties of graphene, including its high electrical conductivity [20-23] and exceptional mechanical strength,[22,23] immediately, captivated the scientific community. These remarkable attributes can be attributed to the unique arrangement of carbon atoms in a honeycomb lattice. This pivotal discovery ignited widespread interest in exploring other two-dimensional carbon allotropes and materials with similarly exceptional properties.

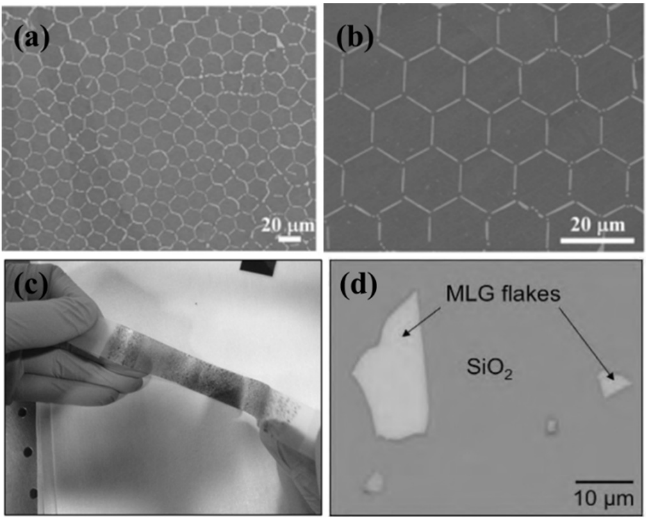

Figure 3. (a) SEM image of CVD grown hexagonal graphene flakes (b) the magnified image showing honeycomb lattice structure. Reproduced with permission.[24] (c) Mechanically exfoliated Graphene flakes and (d) optical microscope image for the exfoliated Multi-Layer Graphene flakes. Reproduced with permission.[25]

1.7 Other 2D Materials

There are a plethora of 2D materials apart from graphene that have garnered significant attention due to their unique properties and potential applications. Some of the notable examples are mentioned below.

1.7.1 Transition Metal Dichalcogenides (TMD)

TMDs with chemical formula MX_2 (M = transition metal and X = chalcogen) are a class of 2D quantum materials that have garnered significant attention in recent years due to their unique properties and versatile applications. These compounds consist of transition metal atoms, like molybdenum (Mo), tungsten (W), or tantalum (Ta), bonded to chalcogen atoms, typically sulfur (S), selenium (Se), or tellurium (Te).[26] They have a layered crystal structure where one metallic layer is sandwiched between two chalcogen layers. The resulting structures exhibit remarkable electronic, mechanical, and optical features.

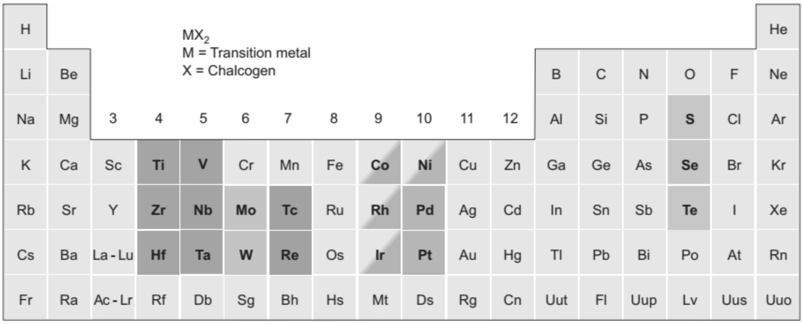

Figure 4. The transitional metals and three chalcogen elements compounds which crystallize in layered structure. The half-highlighted elements means only some of the dichalcogenides with these elements are in layered structures. Reproduced with permission.[26]

One of the key features of TMDs is their tunable bandgap. In the bulk form, these materials are indirect bandgap semiconductors, but when exfoliated down to monolayers, they become direct bandgap semiconductors. This property makes them suitable for optoelectronic applications. For instance, monolayer MoS_2, a widely studied TMD, has a direct bandgap around 1.9 eV, making it ideal for light-emitting diodes (LEDs), solar cells, and photodetectors.[27] The family of TMD materials also exhibits exceptional mechanical strength and flexibility. MoS_2, for example, is known for its robust intralayer covalent bonds and weak interlayer van der Waals interactions, resulting in extraordinary mechanical properties. This mechanical flexibility makes TMDs suitable for applications in flexible electronics and strain-sensitive devices.[28] Furthermore, TMDs are promising candidates for field-effect transistors (FETs). Due to their 2D nature, they can be easily integrated into semiconductor devices, offering excellent electrical performance. The 2D structure of TMDs enables gatetunable carrier transport, allowing for efficient control of current flow.[29] In addition to their electrical and mechanical properties, TMDs exhibit unique optical characteristics. The direct bandgap transition leads to strong photoluminescence, which is crucial for LED applications. Their quantum confinement effects also enable efficient light-matter interactions.[30] They also display strong spin-orbit coupling, which is useful in spintronics.[31] The field of TMD research is rapidly evolving, with an increasing number of applications emerging, such as quantum dots, catalysts, and sensors. Their exceptional properties and tunable bandgaps position TMDs as a versatile class of materials with wide-ranging practical implications.

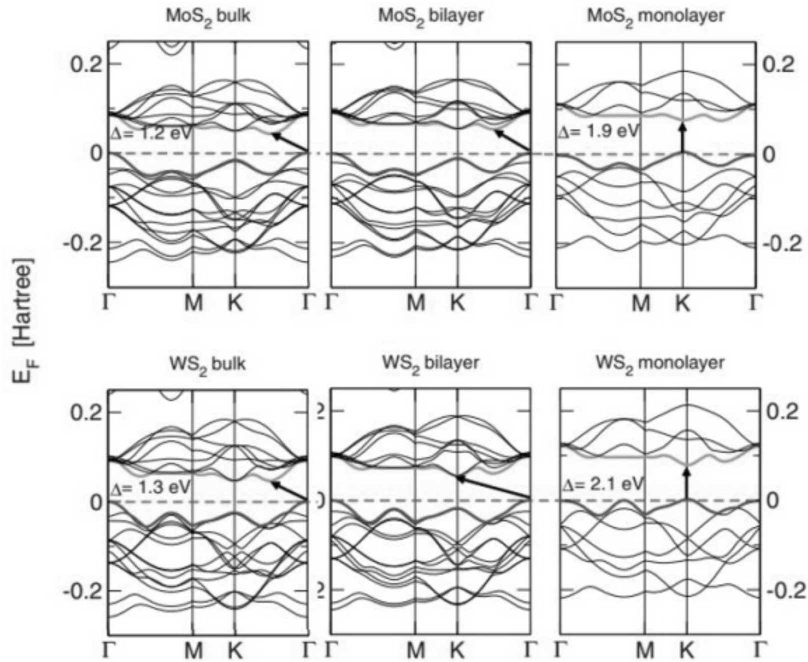

Figure 5. Band structures for bulk, bilayer, and monolayer MoS_2 and WS_2 suggesting transformation from indirect (bulk) to direct band (monolayer) gap. Reproduced with permission.[32]

1.7.2 Black Phosphorus (BP)

Black phosphorus or Phosphorene, is a unique 2D quantum material that has gained significant attention in the field of nanoscience and materials research. This material is distinct from its more common allotropic forms of white phosphorus and red phosphorus. BP was first isolated and characterized by the Scottish chemist Hugh Marshall in 1914. It naturally occurs in certain minerals like lazurite and Hapsburgite, but its isolation in pure form was a significant development. BP has a layered structure consisting of covalently bonded phosphorus atoms. These layers are held together by van der Waals forces. Each layer is made up of a puckered honeycomb lattice similar to graphene, but with each phosphorus atom covalently bonded to three neighbouring atoms. This puckered structure gives black phosphorus its anisotropic properties, making it a promising material for electronic and optoelectronic applications. BP exhibits anisotropic properties, with varying electronic and optical characteristics along different crystallographic directions. This anisotropy is advantageous for designing electronic devices and sensors. In contrast to graphene, black phosphorus has a direct band gap, making it suitable for optoelectronic applications such as photodetectors and LEDs. The band gap of BP is tunable through the number of layers, strain, and electrical gating, allowing for versatile device design. It has high carrier mobility, which is crucial for fast and efficient charge transport in electronic devices. It has strong light-matter interaction, making it promising for applications in photonics and optoelectronics. BP based FETs have shown promising results due to their high carrier mobility, making them suitable for next-generation electronic devices.[33] Its direct band gap and high carrier mobility make black phosphorus an ideal material for photodetectors, enabling efficient light absorption and charge separation.[34] BP based LEDs have the potential for use in displays and optical communications. Its anisotropic properties and strong light-matter interaction make black phosphorus sensors highly sensitive and suitable for various sensing applications.[35]

1.7.3 Hexagonal Boron Nitride (*h*-BN)

h-BN also known as white graphene, is a 2D material that has gained substantial attention in recent years due to its remarkable properties and versatile applications. Here, we provide an overview of *h*-BN, covering its origin, structure, properties, and applications. The existence of hexagonal boron nitride was first theorized by Hermann in 1910, but it was not until the 1940s that the compound was synthesized. The high-temperature, high-pressure synthesis of *h*-BN was independently reported by H. R. Verma and Robert N. Hall in 1945. Hexagonal boron nitride has a hexagonal lattice structure, similar to graphene. In this structure, boron and nitrogen atoms alternate in a two-dimensional honeycomb lattice. The arrangement of B and N atoms leads to the formation of strong covalent bonds within the layers. These layers are held together by weak van der Waals forces, allowing them to be easily exfoliated into single- or few-layer sheets.

h-BN is an excellent insulator with a wide band gap, making it ideal for use in electronic devices as an insulating layer. It exhibits exceptional thermal conductivity, even at the nanoscale, making it a valuable material for applications like thermal management in electronics.[36] It is chemically inert and thermally stable, even at high temperatures, making it a suitable material for extreme environments. In its bulk form, *h*-BN has been used as a dry lubricant due to its low friction properties. *h*-BN is used as a dielectric in electronic devices.

It is employed as an insulating material in various electronic devices, such as transistors, to prevent electrical leakage.[37] Its high thermal conductivity makes *h*-BN a promising material for thermal management in electronics, including heat sinks and thermal interface materials. In bulk form, *h*-BN serves as a solid lubricant in various mechanical applications to reduce friction and wear.[38] *h*-BN hosts color centres, such as the nitrogen-vacancy center, that are used in quantum optics and quantum information applications. It is utilized in photonics and nanophotonics for applications like the generation of single photons and as a platform for integrated photonic devices. The unique combination of electrical insulating properties, exceptional thermal conductivity, and chemical stability makes *h*-BN an attractive material for a wide range of applications in electronics, photonics, and quantum technologies. Researchers continue to explore and develop new applications for this versatile 2D material.

2D materials exhibit a diverse range of electronic properties, spanning from semimetals to insulators. Graphene is a semimetal, characterized by a remarkable electronic conductivity. It features a single Dirac cone-like electronic band structure where electrons behave as massless relativistic particles.[39] In contrast, materials like *h*-BN are insulators where the electronic structure is defined by a wide bandgap, which means it doesn't conduct electricity effectively.[40] This property makes *h*-BN a valuable insulating layer or substrate in 2D material-based electronic devices. Between these extremes, there are 2D materials with varying properties. TMDs like MoS_2 and WSe_2, are semiconductors with tunable bandgaps, making them ideal for electronic applications.[41] BP is a semiconductor with a moderate bandgap of 0.3 to 2 eV, allowing for versatile use in electronics and optoelectronics.[42] A schematic illustration of these materials' properties and band structures is depicted in figure 6. These diverse electronic properties enable engineers and scientists to design a wide array of 2D material-based devices, from high-conductivity graphene transistors to insulating layers of *h*-BN in heterostructures. The ability to fine-tune the electronic characteristics of 2D materials offers tremendous litheness for applications in nanoelectronics, photonics, and beyond.

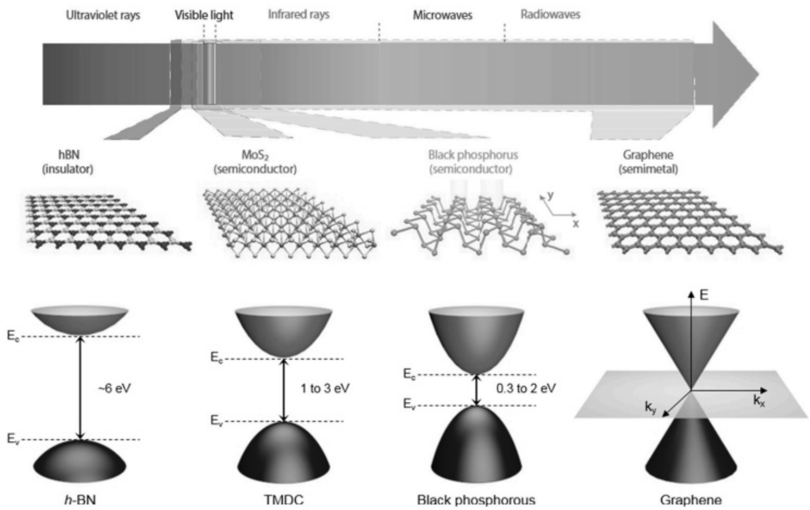

Figure 6. Energy spectrum of various 2D materials and their atomic crystal structures; Electronic band structures of hexagonal boron nitride (*h*-BN), transition metal dichalcogenides (TMDCs), black phosphorous, and graphene. Reproduced with permission.[43]

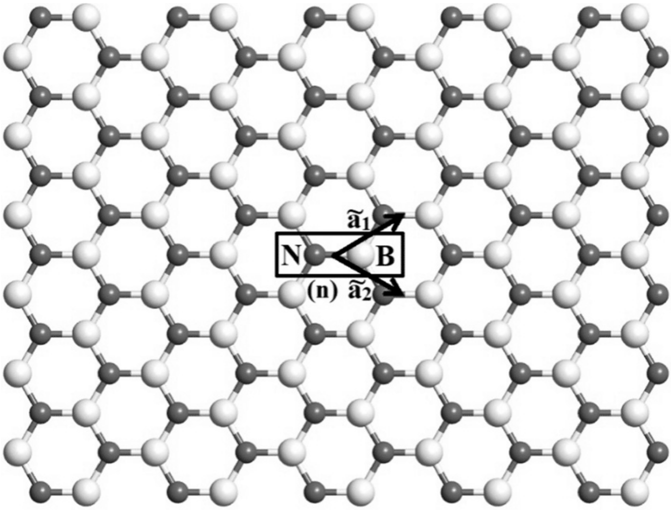

Figure 7. Schematic of a hexagonal boron-nitride nanosheet; $\tilde{a}_1$ and $\tilde{a}_2$ are primitive lattice vectors. Reproduced with permission.[44]

1.7.4 Stanene

Stanene is a fascinating two-dimensional material that has attracted significant attention in the field of condensed matter physics. Also known as 2D tin, it belongs to the family of 2D materials alongside graphene, phosphorene, and others. Stanene's remarkable properties and potential applications make it an exciting material for scientific probe and technological advancements. The concept of stanene was first proposed theoretically in 2013 by Shou-Cheng Zhang and his research team.[45] Stanene consists of a single layer of tin (Sn) atoms arranged in a hexagonal lattice, similar to graphene. The unique characteristic of stanene is its buckled structure, where the tin atoms form a honeycomb pattern, with every other atom slightly elevated above the plane. This buckling imparts distinctive electronic properties to stanene.

Stanene is a topological insulator, meaning it acts as an insulator in its interior but conducts electricity along its edges or surfaces.[46] This property has implications for the development of low-power electronics. It exhibits exceptionally high carrier mobility, which makes it promising for ultrafast electronic devices. Stanene is known for its potential to exhibit the quantum spin Hall Effect, a phenomenon crucial in the development of spintronic devices.[47] Stanene holds enormous promise for various applications, like low-power electronics, quantum computing, and high-temperature superconductors.[48] It could play a pivotal role in advancing next-generation electronic devices and quantum technologies. Researchers are continually investigating stanene's properties and potential applications, and while it remains challenging to synthesize in its purest form due to its extreme reactivity, the future of this 2D material looks promising. It may lead to ground-breaking developments in the world of materials science and technology.

1.7.5 Layered Double Hydroxides (LDHs)

LDHs, also known as hydrotalcite-like compounds or anionic clays, are a class of synthetic materials that belong to the larger family of layered materials. They are structurally similar to naturally occurring minerals and have a wide range of applications due to their distinctive properties. LDHs have a layered structure composed of positively charged brucite-like layers and interlayer anions, water molecules, or organic molecules. LDHs possess several noteworthy characteristics, including high anion exchange capacity, good thermal stability, and excellent reactivity. The tunability of their composition allows for control over various properties, making them versatile materials. LDHs find applications in diverse fields, such as catalysis,[49] drug delivery,[50] flame retardants,[51] and environmental remediation. They are excellent anion exchangers,[52] which is particularly useful in water purification[53] and wastewater treatment. In the pharmaceutical industry, LDHs are utilized for controlled drug release due to their ability to intercalate drug molecules in the interlayer space. Additionally, LDHs serve as efficient catalysts in various chemical reactions.

1.7.6 MXenes

MXenes are a novel class of 2D materials that have garnered significant attention in the field of materials science and engineering due to their exceptional properties and a wide range of potential applications. MXenes belong to the larger family of transition metal carbides and nitrides and have a general formula of $M_xM'_{2-x}T_x$, where M represents transition metals, M' stands for carbon and/or nitrogen, and T_x denotes surface terminations, such as hydroxyl, oxygen, or fluorine groups. The discovery of MXenes can be traced back to 2011 when Yury Gogotsi and his team established a selective etching method to generate 2D nano-crystals through exfoliation of Ti_3AlC_2.[54] The resulting material consists of 2D layers with excellent electrical conductivity and mechanical properties. MXenes have a unique structure with strong in-plane metallic conductivity. They possess several remarkable properties like excellent electrical conductivity, high mechanical strength, and good thermal stability. They also exhibit good environmental stability and can withstand exposure to air and moisture. Furthermore, MXenes demonstrate tunable surface chemistry and can be modified to have different functional groups, making them versatile for various applications.

MXenes have a rapidly growing list of applications. They are considered promising candidates for energy storage and conversion devices, such as supercapacitors, lithium-ion batteries, and hydrogen evolution catalysts.[55,56] Additionally, their high conductivity and surface functionalization make them suitable for sensors,[57] electromagnetic interference shielding,[58] and water purification.[59] In the field of catalysis, MXenes exhibit potential for various reactions due to their active surface chemistry. Overall, the unique properties and versatile applications of MXenes have made them a subject of intense research, and their impact on various industries, including electronics, energy, and environmental technologies, is continually expanding. Researchers are exploring novel synthesis methods and functionalization techniques to unlock the full potential of MXenes for future applications.

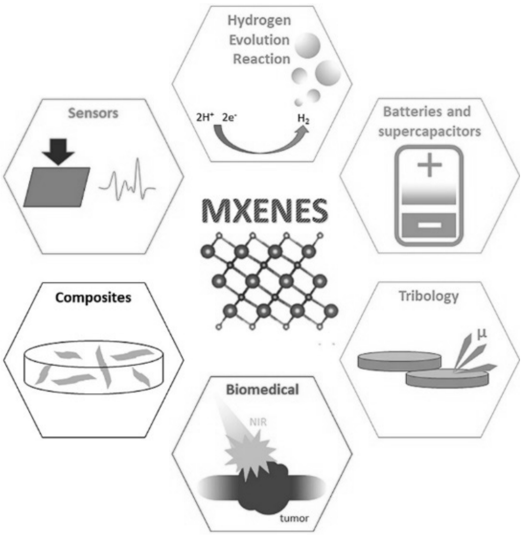

Figure 8. Schematics of crystal structure and multifunctional applications of Mxene. Reproduced with permission.[60]

1.7.7 Silicene and Germanene

Silicene is a 2D allotrope of silicon, akin to graphene, but with silicon atoms arranged in a honeycomb lattice. Theoretical predictions of silicene date back to the 1990s, but it wasn't until 2012 that it was first synthesized on a silver substrate through a process known as molecular beam epitaxy.[61] Silicene has unique electronic properties that arise from its buckled structure, where silicon atoms form a hexagonal lattice with one sub-layer slightly above the other. This buckling leads to a bandgap in the electronic structure of silicene, making it a potential candidate for semiconductor applications.[62]

Germanene is a 2D material composed of germanium atoms arranged in a hexagonal lattice, similar to graphene. Just like silicene, germanene also exhibits a buckled structure. While theoretical predictions for germanene existed for some time, it was successfully synthesized on gold substrates through molecular beam epitaxy in 2014.[63] Germanene's unique electronic structure and inherent semiconducting properties have led to its exploration for use in electronic devices, particularly FETs.[64]

Both silicene and germanene have characteristics that make them attractive for electronic applications. Their structural and electronic properties are tunable, and they exhibit good thermal stability. The buckled structure provides an intrinsic bandgap, allowing for the development of 2D transistors. Additionally, their compatibility with existing silicon-based electronics makes them viable candidates for future semiconductor technology. Further-more, these materials have potential applications in optoelectronics, where their 2D nature could be harnessed for photodetectors and light-emitting devices.[65] Their versatile properties and ongoing research into synthesis and functionalization make silicene and germanene exciting prospects in the field of 2D materials and nanoelectronics.

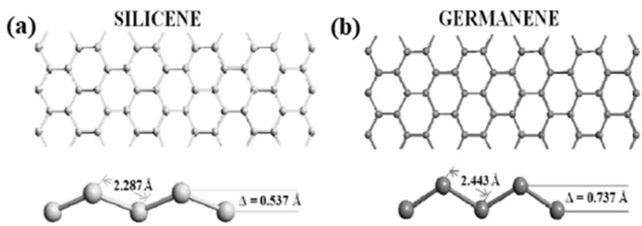

Figure 9. Crystal Structure of 2D materials (a) Silicene and (b) Germanene depicting their planar structure. Reproduced with permission.[66]

1.7.8 Phosphorene-like Materials

The group V elements Arsenic (As), Antimony (Sb), Bismuth (Bi) can form 2D materials with properties similar to phosphorene. For example, bismuthene (2D bismuth) has recently gained attention for its unique electronic properties and potential applications in topological insulators,[67] quantum computing,[68] and spintronics.[69]

These 2D materials have expanded the landscape of materials science and nanotechnology, offering a wide range of properties and applications. Researchers continue to investigate their synthesis methods, fundamental properties, and practical uses in various technological fields, shaping the future of materials science and electronics.

1.8 Importance and Applications in Various Fields

2D materials have sparked significant interest in the field of nano-electronics due to their exceptional electronic properties and the potential to revolutionize existing technologies. Here's an overview of their applications in key areas like Nanoelectronics, Optoelectronics, Energy storage and conversion as well as Quantum Computing.

1.8.1 Nanoelectronics

High-Performance Transistors: 2D materials, such as graphene and TMDs like MoS_2 and WSe_2, are being explored to create high-performance FETs.[70] Monolayer TMDs have a direct bandgap, making them suitable for FETs with excellent on-off current ratios.[71]

Flexible Electronics: The mechanical flexibility of 2D materials allows for the development of flexible and wearable electronics. Graphene-based FETs can be integrated into flexible substrates, enabling bendable and stretchable electronic devices.[72]

Low-Power Electronics: 2D materials enable the fabrication of low-power transistors. Their ultra-thin nature and excellent charge carrier mobility make them promising for energy-efficient electronics, which is crucial for portable devices and Internet of things (IoT) applications.[73]

1.8.2 Optoelectronics

2D materials have made significant strides in the field of optoelectronics, offering unique advantages for various devices. Here are their applications in key areas like photodetectors, light-emitting diodes (LEDs), and solar cells.

High-Performance Photodetectors: 2D materials such as graphene, MoS_2, and black phosphorus have been utilized to create high-performance photodetectors. These materials exhibit excellent electrical conductivity and light absorption properties, making them ideal for detecting light across a broad spectrum. [74,75,76]

Broadband Sensing: The tunable bandgap of 2D materials allows for the development of broadband photodetectors. By stacking different 2D materials or combining them with traditional semiconductors, engineers can design detectors capable of sensing light from ultraviolet (UV) to infrared (IR) wavelengths.[77]

Ultrafast Response Times: 2D material-based photodetectors offer ultrafast response times in the picosecond or even femtosecond range. This rapid response makes them suitable for high-speed communication systems and imaging applications.[78]

1.8.3 Light-Emitting Diodes (LEDs)

Efficient Light Emission: 2D materials like TMDs exhibit efficient light emission due to their direct bandgap nature. Monolayer TMDs, such as MoS_2 and WS_2, can emit light in the visible spectrum, making them promising for LEDs.[79]

Flexible and Transparent LEDs: The mechanical flexibility and transparency of 2D materials allow for the fabrication of flexible and transparent LEDs. These characteristics are vital for emerging technologies like flexible displays, wearable electronics, and smart windows.[80]

Color Tunability: By using different 2D materials or heterostructures, LED emission colours can be tuned precisely. This tunability is crucial for display technologies and RGB (red, green, blue) lighting applications.[81]