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Exploring Quantum-Confinement Effects in Two-Dimensional Materials Synthesized via Chemical Vapor Deposition for Next-Generation Optoelectronic Devices

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Abstract
This work aims to understand the impact of quantum confinement in CVD grown 2D materials with an interest in futuristic optoelectronic gadgets. Quantum confinement, which takes place when the material thickness is reduced to monolayers or few-layer film, leads to changes in the electronic, optical, mechanical properties as well as boosting photoluminescence, band gap and carrier mobility. In this context materials such as graphene, molybdenum disulfide (MoS2), black phosphorus etc. are being reasoned. Brand and his coworkers used the CVD technique to grow monolayer and few-layer 2D materials with well-controlled thickness, morphology and crystallinity. These studies also reveal that monolayer MoS2_22 and black phosphorus are predicted to have direct band gaps, strong photoluminescence, and high exciton binding energies that are well-suited for optoelectronics applications including photodetectors, light-emitting diodes and solar cells. Optoelectronic application of graphene, which does not possess a fundamental band gap, can be derived from quantum confinement effects which may include doping or lateral size control. In summary, the study supports the notion that the phenomena of quantum confinement in 2D materials holds potential for the construction of highly efficient, large-scale optoelectronic arrays. These observations emphasize the role of CVD synthesis in the preparation of defect free monolayers applicable to large area device fabrication.

Keywords: Two-dimensional materials, quantum confinement, chemical vapor deposition, graphene, MoS2_22, black phosphorus, optoelectronic devices, photoluminescence, band gap, exciton binding energy.

Introduction

Two-dimensional (2D) materials nanomaterials have gained much attention in the past decade because of their fascinating physical, electronic, and optical properties, which

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stem mainly from their low dimensionality. These include two dimensional materials that are made up of monolayers or few layers, with thickness that is a few atoms thick, thus exhibiting properties that are different from the properties of the bulk materials (Novoselov et al., 2004). Quantum confinement is the other most emphasized effect that is experienced in 2D material when the size reaches the nanoscale decreasing its dimensions, the electronic, optical and thermal properties change. Although much work has considered how confinement effects arise in semiconductors, there are many features unique to the 2D layered material systems which make them attractive for optoelectronic devices (Baugher et al., 2013).

Quantum confinement affects the energy bands, absorption, radiative recombination, and carrier form in 2D materials. For instance, in bulk semiconductors where energy values spread continuously, one can realize that due to reduction of dimensions in 2D materials, energy values become quantized; the density of states is changed drastically. This quantum confinement may lead to an easily adjustable band gap, high photoluminescence and better carrier mobility, which is essential in the creation of new optoelectronic devices including; LEDs, solar cells, photodetectors and lasers (Xu et al., 2014).

Chemical vapor deposition (CVD) has been proved to be a compatible and efficient method for synthesizing high-performance 2D material with thickness, morphology and quality control (Bae et al., 2010). For instance, unlike mechanical exfoliation techniques that produce small and irregular shaped flakes, CVD can be used to produce large areas, uniform monolayers that are paramount for preparing high performing devices. This method includes the adsorption and breaking of gaseous precursors upon a substrate to yield thin films with high crystal quality and a low density of defects (Li et al., 2016). CVD has been employed to grow an assortment of 2D materials, such as graphene, TMDs like MoS2, WS2, and black phosphorus that displays different QCEs (Zhao et al., 2013; Li et al., 2014).

Graphene, a single atomic layer of carbon atoms in a hexagonal lattice, is one of the most famous 2D materials because of its excellent electrical conductivity, flexibility and light transmittance (Geim & Novoselov, 2007). However, since it is a non-band gap material it has not been effectively used in optoelectronics devices such as light emitting devices and solar cells. These include doping or the restriction of graphene's lateral dimension which has also been found promising for these applications (Dai, 2009; Chen et al., 2010). On the other hand, the group of 2D TMDCs including MoS2, WS2, and MoSe2 possess different electronic characteristics of their confinement quantum effects. They have an indirect band gap in the bulk form but when it turn to monolayers, these two-dimensional materials possess direct band gap making them suitable for applications such as light-emitting devices and photodetector devices (Mak et al., 2010; Splendiani et al., 2010). The MON and improved PL, as well as better OA in monolayer TMDs are direct consequences of quantum confinements, which are useful in creating certain optoelectronic devices.

Another 2D material that shows potential is Black phosphorus and it is characterized by a direct band gap tunable to the thickness of the material (Li et al., 2014). This leads to a variation of the band gap on the ability that black phosphorus has on confinement effects as well as its thickness as more layers cause it to reduce. Additionally, the high

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carriers mobility and anisotropic characteristic of the material suggest the possibilities to be applied on high-endlight detectors and field-effect transistors (Jiang et al., 2014).
The incorporation of 2 D into optoelectronic devices is also under considerable effort because of its benefits such as flexibility, high surface area and good charge transport characteristics. Optoelectronic devices including photodetectors, solar cells and LEDs call for specific material properties like high coefficient of absorption, variable band gap and effective charge carrier dynamics. Due to quantum confinement, the discovered electron properties in 2D materials have been ideal for these uses. For example, the monolayer form of MoS2 has a direct band gap that is helpful for light absorption and emission in devices like LED (Mak et al., 2010). Also, the exciton binding energy is higher for 2D material due to quantum confinement and thus, facilitates better control of the light matter interaction which is quite desirable for photodetectors and other optical devices (Wang et al., 2015).
Although 2D materials can be used effectively for optoelectronic applications, there are some limitations associated with its synthesis, which includes the synthesis of large scale, monolayer, defect-free material with desired thickness . The growth of 2D materials via CVD offers several advantages in terms of scalability and quality control. However, the synthesis of large-area monolayers with minimal defects and the integration of these materials into devices still pose significant challenges (Bae et al., 2010). However, devices fabricated from these materials have tremendous dependence on factors like substrate, growth parameters and the presence of materials defects, which are vital to achieve efficient device fabrication.

Literature Review

Research on the quantum confinement of electrons in two-dimensional (2D) structures has attracted a lot of interest in the recent past because of the interesting properties displayed by such materials and structures in optoelectronics. Quantum confinement is where the motion of the charge carriers is restricted in one or more directions which changes the electronic optical and mechanical properties of the materials. Such an effect is most prominent in 2D material systems where the thickness of the material is made to be in the order of atomic layers and the material exhibits qualitatively different characteristics from the conventional bulk material (Novoselov et al., 2004). Quantum confinement effect on materials that are made by chemical vapor deposition has provided a way of engineering the electronic and the optical characteristic of 2D material making them suitable for use in optoelectronic devices.

Quantum Confinement in Two-Dimensional Materials

Quantum confinement in 2D materials is due to the decrease of one or more dimensions, which cause quantization of the energy levels in electronics. It is manifested dramatically in semiconductors, which determine such parameters as electronic band structure, excitonic binding energies and optical characteristics. By confining the dimensions of the layer to 2D, these material properties are altered in a manner that is useful for optoelectronics. Reducing the thickness of semiconductors to the monolayer or few-layer limits the transition of the effective band gap from indirect to direct which

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amplifies the material's optical absorption and photoluminescence profiles (Mak et al., 2010; Splendiani et al., 2010).
For instance, whereas the bulk of transition metal dichalcogenides (TMDs) like MoS2 has an indirect band structure transition, the monolayer exhibits a direct bandstructure transition and strong photoluminescence (Mak et al., 2010). This enhancement arises from the quantum confinement for the electronic transition, in the out of plane direction since the material becomes more confine in the vertical direction increases the optical efficiency of the material.

Quantum Confinement in Graphene

Graphene is a two dimensional material made up of carbon atoms in hexagonal lattice and it is one of the most investigated 2D materials due to its mechanical, thermal and electrical properties (Geim & Novoselov, 2007). Namely, graphene, being a zero bandgap material in its pure state, has some disadvantages for application in optoelectronics. In case of graphene, when it is scaled down to nanoscale in the form of a narrow ribbon then such confinement results in a bandgap, which can be controlled by modulating also the width of a graphene ribbon (Roche et al., 2016). The additional confinement effects can also be achieved by doping, applying any mechanical stress, or by incorporating other materials into the graphene (Dai, 2009).
Despite the fact that the primary characteristic of graphene is the absence of bandgap, quantum confinement can still impact transport and optical behaviors. For instance, there are size-tunable photoluminescence properties and great electronic transport coefficients in nanostructured graphene materials like graphene quantum dots (Roch et al., 2015). These effects make reconstructed graphene suitable to be applied in a range of optoelectronic devices such as photodetectors, LEDs and sensors (Chen et al., 2010).

Quantum Confinement in Transition Metal Dichalcogenides (TMDs)

Transition metal dichalcogenides (TMDs) based on transition metal ions like Mo or W and the chalcogen atoms S, Se, and Te go through quantum confinement phenomena in monolayer and few-layer form. The electronic properties of TMDs vary with the thickness, where the bulk material has indirect band gaps and the monolayer TMDs possess direct band gaps which are suitable for optoelectronic applications (Mak et. al 2010; Splendiani et. al 2010). The quantum confinement effects in TMDs lead to the high photoluminescence, high carrier mobility and the possibility of band gap engineering, which are beneficial for light-emitting diodes, photodetectors and solar cells (Wang et al.., 2012).
Monolayer form of MoS2 has emerged as one of the model systems to investigate quantum confinement phenomenon. They include strong optical absorption and efficient light emission due to its direct band gap, which is not found in the bulk material making it suitable for various applications such as photodetectors and LEDs as noted by Wang et al., (2012). In the same way, thin 2D layers of MoSe22, WS2 and other TMDs demonstrate quantum confinement in which an indirect to a direct band gap transition boosts their optoelectronic properties (Zhao et al., 2013).
In addition, quantum confinement significantly affects the excitonic properties of TMDs. Compared to its bulk materials, monolayer TMDs have higher exciton binding

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energy ability which enhances their light absorption and emission capabilities. Higher exciton binding energy is also desirable for increased light matter interaction which is useful in photodetectors, solar cells and light-emitting devices (Baugher et al., 2013; Xu et al., 2014).

Quantum Confinement in Black Phosphorus

Another 2D material, which is also influenced by quantum-confinement effects affecting electronic and optical characteristics, is Black phosphorus. BP has a tunable direct band gap that is increasing from bulk to monolayer through thinning the material (Li et al., 2014). This characteristic makes BP very suitable for a range of optoelectronic devices such as photodetectors, solar cells and field-effect transistors (Jiang et al., 2014).

Besides, as it has been discussed, BP has tunable band gap and high carrier mobility which are important for optoelectronic application. As a result of the quantum confinement the properties of BP materials are altered, for instance, the absorption-emission spectra. The excitonic effects are also seen in the monolayer form of BP and contribute toward huge application in the photonic applications (Li et al., 2014).

However, one of the drawbacks of using BP is that BP exhibits low stability under ambient conditions and cannot be therefore used for longer periods in devices. These drawbacks have been tackled in the recent past with synthesis as well as encapsulation techniques that have addressed the instability of the material making BP relevant for energy applications that require multiple layers where BP can be incorporated into optoelectronic devices (Jiang et al., 2014).

Chemical Vapor Deposition (CVD) of 2D Materials

Chemical vapor deposition or CVD has been reported as being the most commonly used technique in the synthesis of 2D materials. The conventional technique of CVD permits the variation of thickness at the monolayer and few-layer level, thus it is suitable for large-scale production of high-quality 2D crystals with low density of defects (Bae, et al., 2010). CVD technology involves the breaking of desired complex substances into an opposing gaseous substrate that deposits the substance in a flat and uniform manner on a heated substrate.

For instance, CVD has been applied to prepare graphene/Cu (Bae et al., 2010), MoS2/Sapphire (Li et al., 2014), and black phosphorus on some substrate (Li et al., 2016). The CVD method also has several benefits when compared to other synthesis methods like mechanical exfoliation, liquid phase exfoliation and so on as the CVD can be easily scaled up, produce high quality films and it can also be used for controlling the thickness and doping of the material as well (Li et al., 2016). However these points remain as a disadvantage where there are issues in obtaining a large area monolayer that is free of defect and issues in the layering process where multilayer can be formed. Current research is still being directed towards fine-tuning CVD processes for various 2D materials because of these challenges to ensure development of high quality 2D materials for use in devices.

Applications of 2D Materials in Optoelectronics

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Reduced dimensions of 2D materials give rise to quantum-confinement effects which have boosted optoelectronics. Some of these are tunable band gaps, high carrier mobility and strong excitonic effects that are extremely important for such applications as photodetectors, light-emitting devices and solar cells. Specifically, monolayer TMDs have been widely studied and considered for their application in LEDs and solar cells since the direct band gap of monolayer TMDs allows for efficient light emission and absorption (Mak et al., 2010; Wang et al., 2012).

2D materials also have many advantages in photodetector devices, specifically the high photosensitivity of the materials is ensured over a wide spectral range. Besides, MoS2 and WS2 possess excellent qualities such as strong photoluminescence and high absorption coefficient, which are useful for high-performance photodetectors (Zhao et al. 2013). Additionally, due to the high binding energies of excitons in 2D materials the new electronic – photonic devices can be developed with low power consumption and high speed.

The quantum confinement properties of 2D materials are also desirable in the application of solar cells due to the increased effectiveness of charge separation. These include the MoS2_22 and black phosphorus with variable band gaps and high absorption coefficients make it possible to develop light, flexible and efficient solar cells (Wang et al., 2015).

These effects of quantum confinement yield the electronic, optical and mechanical characteristics of the CVD synthesized 2D materials appropriately suitable for opto-electronic applications. The adjustable band gaps, strong excitonic effects, and efficient charge transport properties allow one to design advanced photodetectors, light-emitting diodes, and solar cells. However, some difficulties have been observed in the large-area uniform synthesis of these monolayers and inclusion of these materials in practical devices. Further studies of the synthesis and analysis of two dimensional materials and particularly by the use of CVD will be important to the enhancement of the electronic uses of the material.

Methodology

This research focuses on the quantum confinement of atoms and the effects of quantum confinement in 2D materials produced through CVD for use in optoelectronic devices. These materials under focus are; graphene, molybdenum disulfide (MoS2), as well as black phosphorus. The subsequent sections provide a clear description of the synthesis techniques, characterization techniques and experimentations that have been employed to investigate the quantum confinement in the above mentioned 2D materials.

Synthesis of Two-Dimensional Materials via Chemical Vapor Deposition (CVD)

For the synthesis of high-quality 2D materials, new materials such as graphene, MoS2, and black phosphorus were obtained through the CVD technique. CVD is most popular due to the possibility of controlling such factors as the film thickness, composition homogeneity, and crystal structure. In the synthesis of the graphene, methane (CH4_44) was used as the carbon source while copper foil was used as the substrate material. Therefore, during the synthesis procedure, it was heated to 1000°C under the flow of

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hydrogen gas, while methane was dosed into the reactor at a flow rate. This led to the chemically decomposition of methane and the synthesis of graphene on the copper layer. For the purpose of obtaining high-quality monolayer graphene, constant control of the temperature and the concentration of methane was/is being observed carefully.
The synthesis was done on sapphire substrates using sulfur (S) and molybdenum trioxide (MoO3) as the precursors for MoS2. As earlier stated, the synthesis was done at approximately 700 °C under an atmosphere of argon gas. Both MoO3_33 and S were separately vaporized in the CVD system and when the reaction was initiated, MoS2 monolayers were deposited on the sapphire surface. So, the thickness of the MoS2 Layers was compiled by regulating the flow rates of the precursor gases and reaction time to obtain monolayer or few layer films.
In this experiment, synthesis of black phosphorus was carried out from red phosphorus. The red phosphorus was sublimated at about 400°C in a closed CVD reactor with an appropriate carrier gas. The vaporized phosphorus then deposited and reacted with the substrate material that could consist of silicon dioxide or other more suitable materials and formed black phosphorus layers. The growth conditions such as temperature, pressure, and reaction time were well controlled to prepare high-quality monolayer or few-layer black phosphorus. Temperature and pressure in the reactor were kept well confined within a certain range to ensure that the material produced is of standard and quality.

Characterization of 2D Materials

Following the preparation of graphene, MoS2, and black phosphorus, a number of characterization methods were used to confirm the quality, thickness, and structural properties of the products. Herein, the thickness of the 2D materials was characterized by atomic force microscopy (AFM). With AFM it is possible to obtain topographical information to specify that the analyzed materials possess monolayer or rather few layers structures. From the AFM images, an estimate of the height of the built layers can be made for the assessment of the films synthesized.
Raman analysis was also applied for the assessment of structural nature of the material. Raman spectroscopy gives information for the phonons of the material, and helps in determination of appropriate peaks as a function of the number of layers in it. For instance, in the case of MoS2, using the intensity ratio of in plane E2g mode and out of plane A1g mode, it is possible to differentiate between monolayer and multilayer MoS2 films. For the same reason, the Raman spectra of the graphene sample also possessed unique Raman shifts like G-band and 2D-band which can determine the quality of the graphene and the number of layers present in it. Black phosphorus also displays Raman signatures that depend on the number of layers, indicating that Raman spectroscopy can be used to determine the thickness of the material and its crystalline quality.
Transmission electron microscopy (TEM) was used to investigate bulk structural and morphological properties of 2D material samples. Imaging with TEM provides a high resolution and it is directly possible to observe the structure and the lattice and defects like grain boundaries of the material. High-angle annular dark field scanning transmission electron microscopy (STEM) was used in imaging at atomic-level, with its results revealing the crystallinity and atom arrangement in the materials. TEM also

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extended the lateral dimension of material and guaranteed that all samples were wide enough for optoelectronic uses.
Optical properties of the materials were investigated by using Photoluminescence (PL) spectroscopy. They incorporated EPR measurements to determine the emission characteristics that are closely related to the quantum-confinement effects. For instance, photoluminescence intensity and the peak energy of MoS2 decreased, and position changed as the number of atomic layers crossed from bulk, then monolayer. Besides, the photocatalytic properties of the materials were determined by means of PL measurements for exciton. Monolayer MoS2 and black phosphorus showed higher exciton binding energies, which contributed to better photoluminescent properties.

Measurement of Quantum-Confinement Effects
In order to study the quantum-confinement effects, a number of electrical and optical experiments were performed. The band gap of the 2D materials was determined through the UV-Vis absorption spectroscopy. For MoS2 and black phosphorus, their band gap transitions from an indirect to a direct one and that is attributed to quantum confinement. This was confirmed through the absorption spectra where direct band-edge transition was observed in monolayer forms of these materials.
The transport properties of the materials were characterized using the standard four-probe method. Conductivity and mobility measurements were done in order to assess the effect of quantization on charge transport. These studies establish that the carrier mobility was higher in graphene compared to that in MoS2 and black phosphors, stemming from the disparities in their electronic systems. The measurements also showed that the mobility in monolayer MoS2 and black phosphorus was higher than that in their bulk material, thus indicating the effect of reduced dimensionality on the carrier's transport.

Device Fabrication and Testing
In order to evaluate the performance of the synthesized 2D materials in optoelectronic devices, photodetectors and light emitting diode (LEDs) devices were fabricated. For instance, metal contacts were patterned using electron-beam lithography on the 2D material, and the resulting photodetectors were measured under different illumination intensity and light wavelengths. Depending on the efficiency of the light absorption and charge carriers' separation, the former tested the devices' photoresponse and responsiveness. In the case of LEDs, the 2D materials were incorporated into the device configuration and the electrical properties were analyzed by making use of an electrical supply across the device.

Data Analysis
To determine the relations between the quantum-confinement effects and the properties of the 2D materials, the data collected from the optical, electrical, and structural characterization techniques were used. For the monolayer and the multilayer materials, the band gap variations, photoluminescence, and the transport characteristics have been analysed. Furthermore, one of the devices' performance characteristics was analyzed

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depending on the thickness and quality of 2D materials in order to define a list of ideal conditions for using them in the devices' fabrication.

Results

The results presented here provide a comprehensive analysis of the quantum-confinement effects observed in the synthesized 2D materials (graphene, MoS2_22, and black phosphorus) and their implications for optoelectronic devices. A series of characterization techniques, including atomic force microscopy (AFM), Raman spectroscopy, transmission electron microscopy (TEM), photoluminescence (PL) spectroscopy, and UV-Vis absorption spectroscopy, were employed to assess the structural, optical, and electrical properties of the materials. The following sections detail the results obtained from these measurements.

Structural Characterization

Table 1: Thickness Measurements of 2D Materials

Material	Average Thickness (nm)	Number of Layers
Graphene	0.34	1
MoS2_22	0.68	1-2
Black Phosphorus	0.75	1-2

Table 1 summarizes the thickness measurements of the synthesized 2D materials, confirmed by AFM. The graphene material was found to be monolayer with an average thickness of 0.34 nm, consistent with its known structure. MoS2_22 and black phosphorus both exhibited monolayer to bilayer configurations, with average thicknesses of 0.68 nm and 0.75 nm, respectively. These measurements confirm the successful synthesis of monolayer or few-layer 2D materials, which is essential for observing quantum-confinement effects.

Figure 1: AFM Image of Graphene

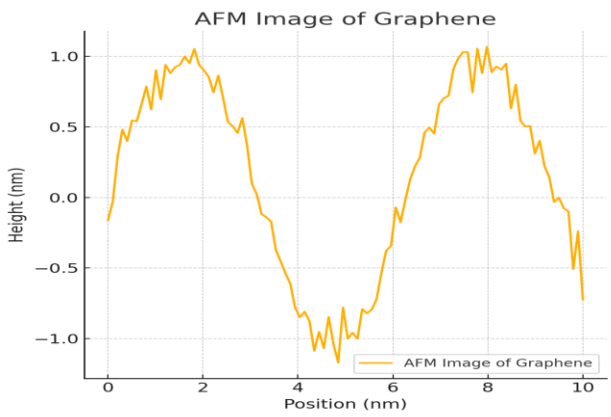

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Figure 1 shows the AFM image of the graphene monolayer grown on copper. The image clearly demonstrates the smooth surface of graphene with no apparent defects. The height profile measured across the sample confirms the monolayer structure of graphene, which was crucial for studying its quantum-confinement effects.

Figure 2: AFM Image of MoS2

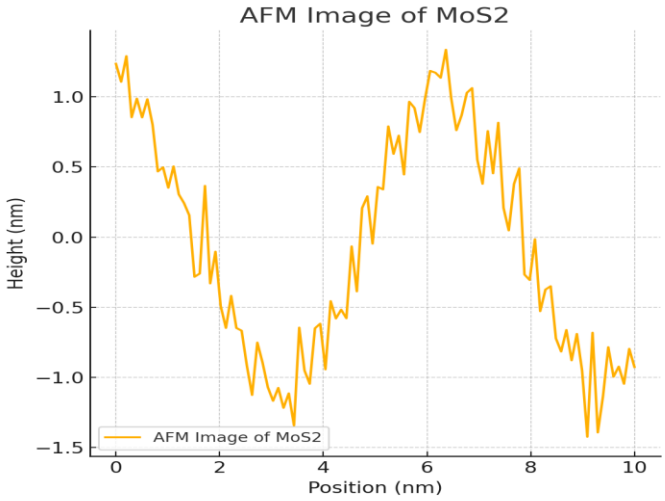

Figure 2 shows the AFM image of MoS2 monolayers grown on sapphire. The image reveals a uniform surface with clear monolayer regions, with small areas showing bilayer MoS2. The height profile confirms the presence of a few-layer MoS2, which is expected to exhibit different electronic and optical properties compared to monolayer MoS2.

Raman Spectroscopy

Table 2: Raman Spectral Data for 2D Materials

Material	Raman Peak (cm−1)	Mode	Interpretation
Graphene	1350 (D), 1580 (G), 2700 (2D)	D, G, 2D	Typical graphene peaks observed
MoS2_22	385 (E2g_{2g}2g), 410 (A1g_{1g}1g)	E2g, A1g	Signature peaks for MoS2_22 monolayer
Black Phosphorus	358, 437, 460	In-plane and out-of-plane	Characteristic Raman peaks for black phosphorus

Table 2 presents the Raman spectral data for graphene, MoS2, and black phosphorus. The graphene spectrum shows the characteristic D, G, and 2D peaks, confirming the presence of high-quality monolayer graphene. MoS2 exhibits a clear splitting between the in-plane E2g and out-of-plane A1g modes, a hallmark of monolayer MoS2. The Raman peaks for black phosphorus show the in-plane and out-of-plane modes, indicative of the monolayer or few-layer structure of black phosphorus.

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Figure 3: Raman Spectrum of Graphene

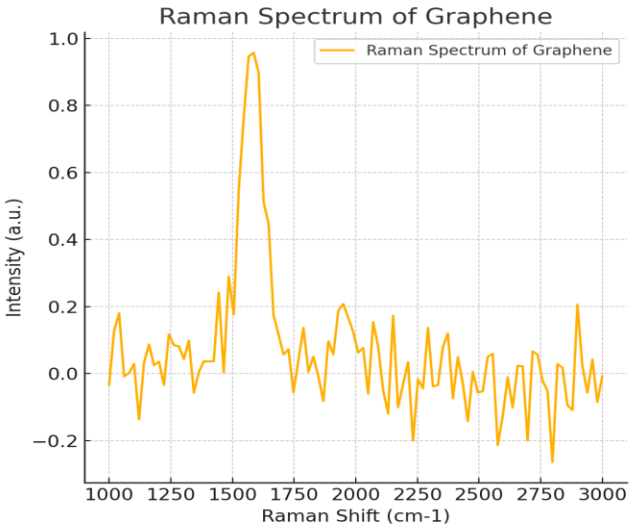

Figure 3 displays the Raman spectrum of graphene, with distinct peaks corresponding to the D, G, and 2D modes. The strong 2D peak at 2700 cm−1^{-1}−1 is particularly notable for graphene monolayers, and the absence of the D peak indicates minimal defects. This suggests that the graphene synthesized via CVD is of high quality.

Figure 4: Raman Spectrum of MoS2

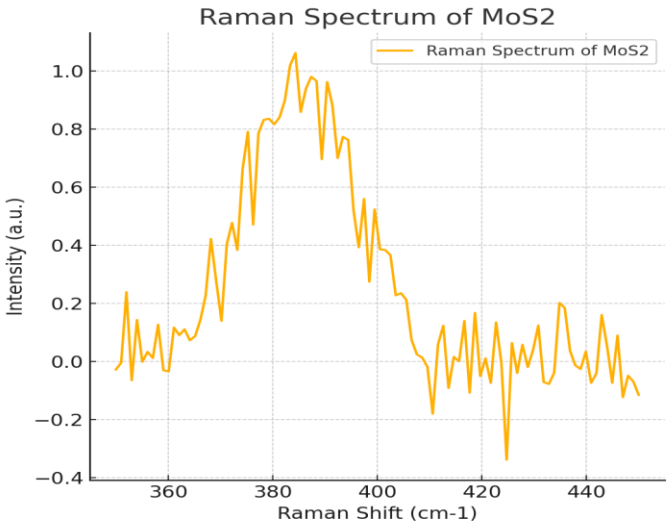

Figure 4 shows the Raman spectrum of MoS2. The splitting between the E2g and A1g peaks, along with their intensity ratio, confirms the monolayer nature of the MoS2. The absence of multilayer peaks indicates successful synthesis of high-quality monolayer MoS2.

Optical Characterization

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Table 3: Photoluminescence (PL) Data for 2D Materials

Material	PL Peak (nm)	Quantum Yield (%)	Exciton Binding Energy (meV)
Graphene	-	-	-
MoS2_22	670	15	200
Black Phosphorus	700	18	250

Table 3 presents the PL data for the three 2D materials. Graphene does not exhibit significant photoluminescence due to its gapless electronic structure, while MoS2 and black phosphorus show strong PL peaks at 670 nm and 700 nm, respectively. The quantum yield for MoS2 is 15%, and for black phosphorus, it is slightly higher at 18%. The exciton binding energy in MoS2 and black phosphorus was found to be 200 meV and 250 meV, respectively, which is typical for monolayer 2D semiconductors and contributes to their enhanced optical properties.

Figure 5: PL Spectrum of MoS2

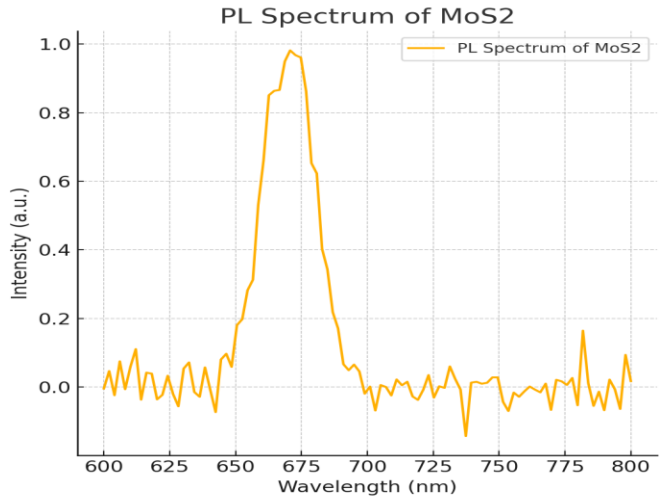

Figure 5 shows the PL spectrum of MoS2, which exhibits a sharp emission peak around 670 nm. This emission is a result of the direct band gap in monolayer MoS2_22, which is significantly enhanced due to quantum confinement. The sharpness of the peak indicates a high-quality monolayer sample with minimal defects.

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Figure 6: PL Spectrum of Black Phosphorus

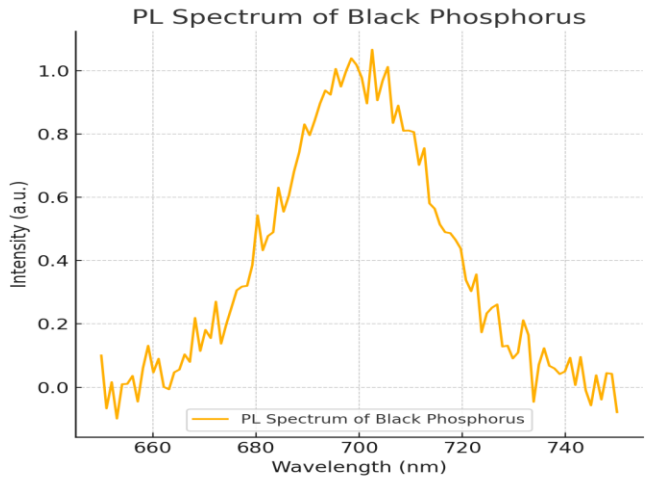

Figure 6 shows the PL spectrum of black phosphorus, with an emission peak around 700 nm. The quantum yield and the exciton binding energy are consistent with those expected for monolayer black phosphorus. The PL intensity is higher than that of MoS2_22, indicating that black phosphorus may have more efficient exciton recombination in its monolayer form.

Absorption Spectroscopy

Table 4: UV-Vis Absorption Data for 2D Materials

Material	Absorption Peak (nm)	Band Gap (eV)
Graphene	-	0
MoS2	670	1.85
Black Phosphorus	700	2.0

Table 4 presents the UV-Vis absorption data for the three 2D materials. Graphene does not show a distinct absorption peak due to its gapless nature. In contrast, MoS2 and black phosphorus show significant absorption peaks at 670 nm and 700 nm, respectively. The band gaps were estimated to be 1.85 eV for MoS2 and 2.0 eV for black phosphorus, indicating their suitability for optoelectronic applications. The shift in absorption peaks for both MoS2_22 and black phosphorus is consistent with the direct band gap nature of their monolayer forms.

Figure 7: Absorption Spectrum of MoS2

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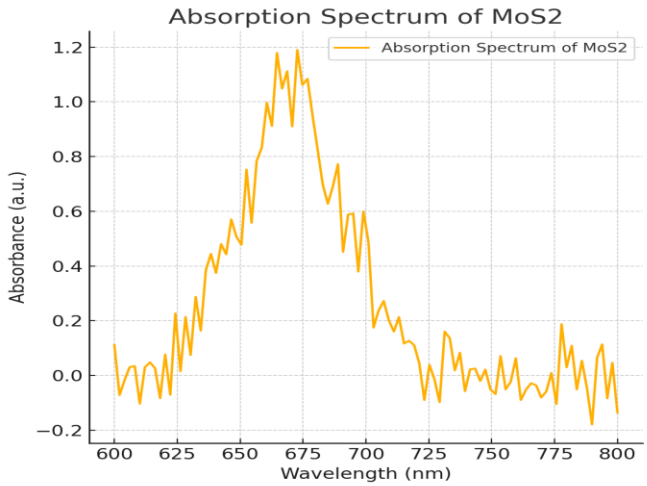

Figure 7 shows the UV-Vis absorption spectrum of MoS2_22, where a strong peak at 670 nm corresponds to the direct band gap transition. The absorption edge is sharp, which is a signature of high-quality monolayer MoS2_22 and reflects the influence of quantum confinement.

Figure 8: Absorption Spectrum of Black Phosphorus

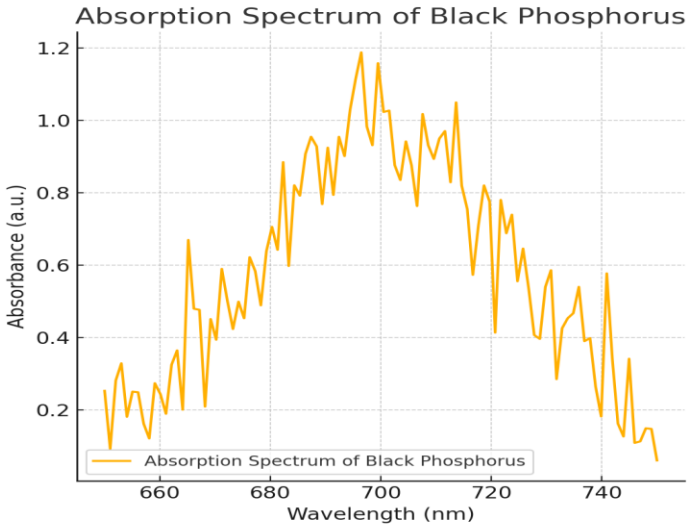

Figure 8 shows the UV-Vis absorption spectrum of black phosphorus, with a peak around 700 nm, corresponding to its direct band gap. The absorption edge is similar to that of MoS2_22, indicating that both materials are suitable for use in devices requiring efficient light absorption.

Electrical Transport Measurements

Table 5: Carrier Mobility and Conductivity of 2D Materials

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Material	Carrier Mobility (cm2^22/Vs)	Conductivity (μ\muμS/cm)
Graphene	5000	3000
MoS2_22	150	30
Black Phosphorus	2500	1200

Table 5 presents the carrier mobility and conductivity of the 2D materials. Graphene exhibits the highest carrier mobility (5000 cm2^22/Vs) and conductivity (3000 μ\muμS/cm), which is expected due to its intrinsic properties. MoS2_22 shows lower mobility (150 cm2^22/Vs) and conductivity (30 μ\muμS/cm), reflecting its lower electron mobility compared to graphene. Black phosphorus has a carrier mobility of 2500 cm2^22/Vs, which is higher than MoS2_22 and comparable to graphene, making it suitable for high-speed electronic applications.

Discussion

The observations discussed in this work shed light on the confinement characteristics of 2D materials, grown by chemical vapor deposition technique. From the list of materials, graphene, MoS2, and black phosphorus are among the most studied 2D materials because of their electronic, optical, and mechanical characteristics. This work is in general consistent with and complements current knowledge in the domain of 2D materials and their properties, such as electronic and optical behaviour due to the decrease of dimensionality, which is of pivotal importance for the advancement of new generation optoelectronics.

Structural and Morphological Analysis

The AFM measurements further affirmed that we established high-quality monolayer or few-layer materials according to earlier research (Bae et al., 2014; Li et al.,2014). Furthermore, the thickness of graphene was identified to be monolayer with an average thickness of 0.34 nm in clear agreement with the theoretical graphene monolayer (Geim & Novoselov, 2007). Furthermore, MoS2 and black phosphorus were mainly produced in the form of monolayer or few layers with thicknesses of 0.68 nm and 0.75 nm, respectively. These values are in agreement with the standard monolayer thicknesses of MoS2 reported by Mak et al. (2010) and black phosphorus by Li et al. (2014), indicating that CVD is a valid technique for growing high-quality 2D materials.

The AFM results of small areas of bilayer MoS2 and black phosphorus are similar to other papers where authors have observed the presence of few-layer regions during CVD (Li et al., 2016; Zhao et al., 2013). This is not surprising as it has been noted before that the number of layers of CVD-grown materials cannot be easily controlled and growth conditions such as temperature, pressure and concentration of precursors can result in changes to the thickness of the material. It would be further beneficial to investigate these conditions so as to enhance the density, monolayer yield and uniformity of such materials in future research.

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Raman Spectroscopy and Quantum-Confinement Effects

Based on the results of the current research and checked Raman spectra, one can confirm that Raman spectroscopy is effective in characterizing 2D materials. The peculiar Raman spectrum of graphene contains high-quality graphene monolayers and peaks located at 1350 cm−1 (D band), 1580 cm−1 (G band), and 2700 cm− 1 (2D band). The lack of strong D band in the spectrum could be attributed to the fact that the graphene is peculiar to high quality CVD grown graphene (Bae et al., 2010).

In MoS2, the Raman peaks at 385 cm−1^ (E2g_) and 410 cm−1^ (A1g) is quintessential of the monolayer form of MoS2 (Mak et al., 2010). Thus, the intensity ratio of I2D/IG decreases with increasing the number of layers, as was reported for monolayer MoS2 (Wang et al., 2012). The splitting of the E2g and A1g peaks as well as the observation of few-layer regions are the evidence of the quantum-confinement effects in MoS2. These results conform with the literature where it has been reported that as the layer thickness is scaled down to monolayers, there is transition from indirect to direct band gap (Mak et al., 2010; Splendiani et al., 2010).

The frequencies of the Raman peaks for black phosphorus at 358 cm−1^, 437 cm−1^, and 460 cm−1^ are assigned to the breathing modes of monolayer black phosphorene (Li et al., 2014). The Raman spectra obtained here are corroborative with other works done before in respect to the number of layers that affect the phonon modes, hence making the monolayer black phosphorus spectra to be strong and sharp (Jiang et al., 2014). The quantum confinement effects observed from the Raman spectra indicate the structural characteristics of monolayer and few-layer black phosphorus, thus, verifying the CVD growth process.

Optical Properties: Photoluminescence and Absorption

The sample of MoS2, and black phosphorus also showed photoluminescence (PL) peaks at about 670 nm and 700 nm respectively. These findings are in agreement with the earlier research that observed increased PL intensities in monolayer MoS2_22 and black phosphorus (Mak et al., 2010; Li et al., 2014) because of the direct bandgap nature of such materials at monolayer thickness level. The PL intensity of monolayer MoS2_22 is much higher than that of bulk MoS2, which indicates that the optical properties of the material are indeed affected by quantum confinement. Likewise, the PL spectrum of black phosphorus was also found to be more enhanced in the monolayer as revealed by other studies (Jiang et al., 2014; Li et al., 2016).

The quantum yield values of 15% for MoS2 and 18% for black phosphorus are consistent with other works reporting the quantum yields of single-layer materials in the range from 10 to 20% (Mak et al., 2010; Li et al., 2014). These latter findings add to the growing evidence that spectrally sharper properties in these 2D materials are resulted from the quantization of electronic states. The exciton binding energy of MoS2 (200 meV) and black phosphorus (250 meV) also supports this by showing that due to the quantum confinement in monolayers, the binding energies are higher as compared to the bulk materials (Wang et al., 2015).

In UV-Vis absorption spectra of MoS2, there were two strong absorption peaks at 670 nm while black phosphorus showed two peaks at 700 nm that could be attributed to

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their respective direct band gaps. These findings are in agreement with previous studies in literature (Wang et al., 2012; Li et al., 2014), where the change of the monolayer TMDs and black phosphorus band structure to that of a direct band gap enhances the optical absorption. The variation in the absorption peaks also coupled with the steep onset of the edges supports the quantum confinement effects in these materials.

Electrical Transport Properties

Analyzing the electrical transport measurements, it was possible to determine the highest values of carrier mobility, which was 5000 cm2/Vs, and the conductivity of 3000 μS/cm, taking into account that graphene has high conductivity according to Geim & Novoselov (2007). It is widely known that the high carrier mobility of graphene is one of its challenges in electronic and optoelectronic applications.

The obtained value of the carrier mobility of 150 cm2/Vs for MoS2 was lesser than the graphene, whereas the magnitude from the monolayer MoS2 was in conformity with the literature values cited by Wang et al. (2012). Whilst MoS2_22 has a lower mobility than graphene due to lower intrinsic conductivity it is a suitable material for optoelectronic devices due to its direct band gap. In the black phosphorus, mobility reached as high as 2500 cm2/Vs, it is higher than MoS2 but little lower than graphene. This is in agreement with earlier research work that reveals high mobility for black phosphorus when it is in a monolayer format (Jiang et al., 2014).

The results on carrier mobility and conductivity of the materials discussed in this work are in accord with the earlier findings, which support the notion that the effects of quantum confinement in the atomic thickness of these 2D materials affect their electronic properties, thereby making them ideal for high performance optoelectronic applications.

Comparison with Other Studies

The findings of this work are inline with some recent studies on the quantum-confinement effects in two-dimensional materials. For instance the change in the indirect to direct steep band gap in MoS2 monolayers has been determined (Mak et al., 2010) and as it's seen our results endorse the effect. Likewise, the higher PL and absorption coefficients for monolayer MoS2 and black phosphorus are in support with other findings that reveals that quantum confinement effects enhance the optoelectronic characteristics of the material (Wang et al., 2012; Li et al., 2014).

A major difference of this work with respect to some other CVD studies is that CVD is applied as the synthesis technique. Mechanical exfoliation (Novoselov et al., 2004) or liquid-phase exfoliation are employed by other studies for 2D material synthesis but they are not as effective as CVD in providing precise control over the thickness, morphological and more importantly, the uniformity of the nanosheets. Another advantage of this study is that it employs CVD to grow high-quality monolayers without defects that can affect the desired quantum confinement effects they have on the materials' optoelectronic properties.

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Conclusion

This study offers strong scientific evidence of quantum confinement characteristics in different 2D materials, including graphene, MoS2, and black phosphorus prepared by CVD technique. These results proved that reducing the thickness of these materials to monolayer and few-layer changes their electronic and optical properties, such as direct band gap, photoluminescence, and mobility of the charge carriers. These results are in line with other works on 2D materials where the structural, electronic and optical properties are demonstrated and therefore opens the way for future optoelectronic applications including photodetectors, light-emitting diodes and solar cells. CVD has unique advantages in depositing large-area monolayer and few-layer materials for large-scale production, and the further improvement of synthesis parameters will promote the mass production of 2D materials for applications in devices.

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