IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 18, Issue 5 Ser. 1 (Sep. – Oct. 2026), PP 49-58
www.iosrjournals.org

Theoretical Investigation of Quantum-Mechanical Properties in Low-Dimensional Materials: A First-Principles Study of Electronic Structure, Defect Engineering, Strain Effects, and Structure–Property Relationships

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Abstract
Low-dimensional materials have attracted considerable scientific interest because spatial confinement at the nanoscale can produce quantum-mechanical properties that differ substantially from those observed in conventional bulk materials. Their reduced dimensionality, large surface-to-volume ratio, modified electronic interactions, and sensitivity to structural perturbations provide opportunities for tailoring electronic, magnetic, optical, and other functional properties. However, the relationship between atomic-scale structure and quantum-mechanical response remains complex, particularly when defects, chemical modifications, mechanical strain, and dimensionality are considered simultaneously. The proposed research aims to theoretically investigate the quantum-mechanical properties of selected low-dimensional materials using first-principles computational approaches, with Density Functional Theory serving as the principal theoretical framework. Atomic models of selected two-dimensional and one-dimensional systems will be constructed and subjected to geometry optimization and systematic convergence testing. Structural stability will be evaluated through total, formation, and cohesive energies, while electronic characteristics will be examined using band structures, band gaps, density of states, projected density of states, and Fermi-level analysis. The effects of vacancies, substitutional atoms, chemical functionalization, and controlled mechanical strain will be investigated to determine their influence on electronic states and charge distribution. Charge-density-difference calculations will be used to understand electron redistribution, while spin-polarized calculations will be employed for systems exhibiting potentially significant magnetic behaviour. Selected optical properties may also be evaluated where computationally appropriate. Comparative and quantitative analyses will be performed to establish relationships among dimensionality, structural parameters, defects, strain, charge redistribution, and quantum-mechanical properties. The study is expected to identify important structure–property relationships and theoretically promising low-dimensional configurations with tunable electronic, magnetic, or optical characteristics. The resulting framework may contribute to the fundamental understanding of quantum phenomena in confined systems and provide theoretical guidance for future investigations in nanoelectronics, optoelectronics, sensing, spintronics, energy-related technologies, and quantum-material applications.

Keywords: *Low-dimensional materials; Quantum mechanics; Density Functional Theory; Electronic structure; Defect engineering; Strain engineering; First-principles calculations*

I. Introduction

Low-dimensional materials have emerged as an important area of contemporary condensed-matter physics because their electronic, optical, magnetic, and structural properties can differ substantially from those of their bulk counterparts. When the dimensionality of a material is reduced from three dimensions to two-dimensional (2D), one-dimensional (1D), or zero-dimensional (0D) systems, quantum confinement, reduced dielectric screening, enhanced surface effects, and altered electron–electron interactions become increasingly significant. These effects can produce distinctive physical phenomena and provide opportunities for developing advanced materials for nanoelectronics, optoelectronics, quantum technologies, sensing, energy conversion, and spin-based applications. The quantum mechanical behaviour of low-dimensional systems is strongly influenced by their atomic structure, chemical composition, dimensionality, defects, strain, external fields, and interfacial interactions. In two-dimensional materials such as graphene, transition-metal dichalcogenides, hexagonal boron nitride, and other layered compounds, the confinement of charge carriers within atomically thin structures can substantially modify the band structure and density of electronic states. Similarly, one-dimensional nanoribbons,

nanowires, and atomic chains may exhibit quantum confinement and edge-dependent electronic states that are absent in their corresponding bulk materials. Understanding these properties at the microscopic level is therefore essential for establishing relationships between material structure and quantum-mechanical behaviour.

Theoretical and computational approaches provide powerful means for investigating these phenomena without relying exclusively on experimental measurements. Quantum-mechanical calculations based on density functional theory (DFT), tight-binding methods, Hartree–Fock approaches, many-body techniques, and related computational frameworks can be employed to examine electronic structures, energy levels, charge distributions, band gaps, density of states, magnetic properties, optical transitions, and response to external perturbations. Such approaches are particularly useful for predicting material behaviour and identifying promising systems before experimental synthesis and characterization. However, the quantum properties of low-dimensional materials are not governed by a single factor. Changes in dimensionality may interact with defects, chemical functionalization, lattice deformation, substrate effects, and external electric or magnetic fields. Consequently, a systematic theoretical investigation is required to distinguish intrinsic quantum effects from those introduced by structural or environmental modifications. The present study therefore focuses on the theoretical investigation of selected low-dimensional materials using appropriate quantum-mechanical and computational approaches. Particular emphasis is placed on understanding their electronic structure, quantum confinement effects, stability, and the influence of selected structural or external parameters. The study seeks to establish a theoretical framework connecting atomic-scale structural characteristics with observable quantum-mechanical properties. Such an investigation can contribute to the fundamental understanding of low-dimensional matter while also providing computational insights relevant to the design and optimization of materials for future technological applications.

Research Questions

The proposed study is guided by the following research questions:

1. How does dimensional reduction influence the quantum-mechanical and electronic properties of selected low-dimensional materials?
2. What changes occur in the electronic band structure, band gap, density of states, and charge distribution when the dimensionality or structural configuration of a material is modified?
3. How do structural parameters such as bond length, lattice arrangement, thickness, edge configuration, and atomic coordination affect the quantum-mechanical stability of low-dimensional materials?
4. What is the influence of defects, vacancies, substitutional atoms, or controlled chemical modifications on the electronic and magnetic properties of the investigated systems?
5. How do external factors such as strain and electric or magnetic fields modify the electronic structure and quantum states of low-dimensional materials?
6. Which computational and quantum-mechanical parameters are most significant for accurately predicting the properties of the selected materials?
7. Can theoretical calculations identify low-dimensional material configurations with desirable electronic, optical, or magnetic characteristics for potential technological applications?
8. What structure–property relationships can be established from the calculated quantum-mechanical parameters?

Research Objectives

The primary objective of the study is to **theoretically investigate the quantum-mechanical properties of selected low-dimensional materials and establish the relationship between their structural characteristics, dimensionality, and electronic behaviour using appropriate computational methods.** The study aims to:

1. **Select and construct suitable atomic models** of representative low-dimensional materials for theoretical investigation.
2. **Optimize the geometrical structures** of the selected systems and evaluate their structural stability using quantum-mechanical calculations.
3. **Investigate the electronic structure** of the materials through analysis of band structures, electronic energy levels, density of states, and related parameters.
4. **Examine quantum confinement effects** associated with dimensional reduction and determine their influence on electronic properties.
5. **Evaluate the effects of structural modifications**, including defects, vacancies, edge configurations, or selected atomic substitutions, on the properties of the investigated systems.
6. **Study the influence of strain and external fields**, where applicable, on band structure, electronic states, and other quantum-mechanical properties.
7. **Analyze charge redistribution and chemical bonding** to understand the microscopic origin of changes in material properties.
8. **Investigate selected magnetic and optical properties** of the materials where these properties are theoretically relevant.

9. **Compare the calculated properties of different low-dimensional configurations** to identify important structure–property relationships.
10. **Identify theoretically promising material configurations** that may possess desirable properties for potential applications in nanoelectronics, optoelectronics, sensing, energy-related technologies, or quantum devices.
11. **Assess the reliability and limitations of the adopted theoretical models** by comparing selected calculated results with established theoretical or experimental findings available in the literature.

Significance of the Study

The proposed research is significant from both **fundamental and applied perspectives**. From a fundamental viewpoint, low-dimensional materials provide an important platform for studying quantum phenomena that become particularly pronounced when spatial dimensions are restricted. Investigating their electronic structures and quantum states can improve understanding of quantum confinement, reduced screening, charge localization, defect-induced states, and dimensionality-dependent behaviour. The theoretical approach is also significant because computational investigations can provide detailed atomic-level information that may be difficult to obtain directly through experimental techniques. Parameters such as charge density, electronic wave functions, density of states, energy levels, and atomic-scale structural changes can be examined systematically through simulations. This enables the mechanisms responsible for observed or predicted material properties to be explored in greater detail.

From an applied perspective, understanding and controlling the quantum properties of low-dimensional materials is relevant to the development of **miniaturized electronic and optoelectronic devices, nanosensors, quantum information technologies, flexible devices, energy-conversion systems, and spintronic components**. Theoretical predictions can help identify material compositions and structural configurations with desirable characteristics before significant experimental resources are invested in their fabrication. The study may also contribute to materials-by-design strategies by demonstrating how specific structural modifications influence electronic and quantum properties. In particular, identifying controllable parameters such as dimensionality, defects, strain, and chemical functionalization can provide useful guidelines for tailoring material behaviour. The resulting computational data and structure–property relationships may therefore serve as a theoretical reference for subsequent experimental investigations.

Need of the Study

Although substantial research has been conducted on low-dimensional materials, several important issues remain unresolved. Existing studies have frequently concentrated on individual material classes or isolated physical properties, while a systematic understanding of the relationship between **dimensionality, structural modification, and quantum-mechanical behaviour** remains comparatively limited. A major challenge is that theoretical predictions can vary considerably depending on the computational methodology, exchange–correlation treatment, model dimensions, boundary conditions, and structural assumptions employed. Consequently, results obtained for nominally similar systems may not always be directly comparable. A systematic theoretical framework is required to understand how methodological and structural factors influence predicted properties.

Another important gap concerns the simultaneous consideration of several interacting factors. For example, dimensionality may alter electronic states, while defects, strain, edge effects, or chemical functionalization can further modify those states. Many investigations examine these parameters independently, whereas their combined influence can be important for realistic low-dimensional systems. There is also a need for more detailed **structure–property correlations**. Reporting calculated band gaps or density-of-states profiles alone does not necessarily explain the microscopic origin of the observed changes. Analysis of charge redistribution, bonding characteristics, atomic configuration, and electronic states can provide deeper insight into why particular modifications produce specific quantum responses. Furthermore, the rapid development of new low-dimensional material architectures creates a continuing need for computational screening of candidate systems. Theoretical investigations can narrow the range of materials requiring experimental validation and can help identify configurations with potentially useful electronic, magnetic, or optical properties. Therefore, the present study is needed to provide a **systematic and comparative theoretical investigation** of selected low-dimensional materials, focusing on the influence of dimensionality and controlled structural modifications on their quantum-mechanical properties. The study seeks to address the existing gap by integrating structural optimization, electronic-structure analysis, and selected quantum-mechanical property calculations within a consistent computational framework.

Delimitations of the Study

The study will be subject to the following delimitations:

1. **Material Selection:** The investigation will be restricted to a defined set of representative low-dimensional materials selected according to their structural relevance, theoretical significance, and suitability for computational analysis.
2. **Dimensionality:** The study will primarily focus on selected **two-dimensional and/or one-dimensional systems**, depending on the specific material models adopted. Bulk three-dimensional materials will be considered mainly for comparison where required.
3. **Theoretical Approach:** The investigation will be limited to selected quantum-mechanical computational methods, such as density functional theory, tight-binding calculations, or other appropriate first-principles approaches, rather than attempting to employ every available theoretical methodology.
4. **Structural Models:** The calculations will generally employ idealized or systematically modified atomic structures. Highly complex experimental morphologies, uncontrolled disorder, and large-scale structural imperfections may not be explicitly represented.
5. **Defects and Modifications:** Only selected defects, substitutions, functional groups, edge configurations, or structural modifications will be examined. The study will not attempt to evaluate every possible defect or chemical modification.
6. **External Conditions:** Where investigated, strain and external electric or magnetic fields will be considered within predefined theoretical ranges. Extreme conditions beyond the selected computational range will fall outside the scope of the study.
7. **Properties Examined:** The investigation will primarily emphasize structural stability, electronic structure, density of states, band-gap behaviour, charge distribution, and selected optical or magnetic properties. Other properties, such as detailed thermal transport, large-scale mechanical behaviour, or full device-level performance, will not be comprehensively addressed.
8. **Computational Scale:** The calculations will be performed on finite and computationally manageable models. Therefore, extremely large systems and long-time dynamical processes may not be included.
9. **Experimental Validation:** The research is primarily theoretical. Experimental synthesis and direct laboratory characterization of the investigated materials will remain outside the principal scope, although published experimental data may be used for comparison and validation.
10. **Application Analysis:** Potential technological applications will be discussed on the basis of theoretically calculated properties rather than through complete device fabrication and performance testing.

II. Review of Literature

The development of low-dimensional materials has significantly expanded the scope of modern condensed-matter physics and computational materials science. The discovery of graphene by Novoselov et al. (2004) demonstrated that atomically thin materials can possess electronic characteristics substantially different from those of their bulk counterparts. Castro Neto et al. (2009) subsequently provided a comprehensive theoretical description of graphene, demonstrating the importance of its linear electronic dispersion and unusual carrier dynamics. These studies established reduced dimensionality as an important route for exploring quantum-mechanical phenomena. Hohenberg and Kohn (1964) and Kohn and Sham (1965) provided the theoretical foundation for modern density functional theory (DFT), which has subsequently become one of the most widely used approaches for calculating the electronic and structural properties of condensed-matter systems. Perdew et al. (1996) further developed the generalized-gradient approximation, providing a computationally efficient approach for practical materials investigations. Research subsequently expanded from graphene to transition-metal dichalcogenides and other layered compounds. Splendiani et al. (2010) demonstrated strong photoluminescence in monolayer MoS_2, highlighting the profound influence of dimensionality on optical and electronic behaviour. Radisavljevic et al. (2011) demonstrated the potential of monolayer MoS_2 for field-effect transistor applications, while Wang et al. (2012) reviewed the emerging electronic and optoelectronic properties of two-dimensional transition-metal dichalcogenides. Chhowalla et al. (2013) emphasized the chemical diversity of layered transition-metal dichalcogenides and their potential for engineering functional properties. Butler et al. (2013) further demonstrated that the field extends considerably beyond graphene, with numerous two-dimensional materials exhibiting distinctive electronic, optical, mechanical, and chemical characteristics.

Theoretical investigations have increasingly focused on the ability to manipulate these properties through structural modification. Liu et al. (2014) investigated phosphorene and highlighted its unusual electronic structure and potentially high carrier mobility. Li et al. (2014) experimentally demonstrated field-effect behaviour in black phosphorus, further establishing the importance of low-dimensional semiconductors. Fiori et al. (2014) discussed the prospects of two-dimensional materials for future electronic technologies. Kormányos et al. (2015) developed a theoretical framework for understanding the electronic structure of transition-metal dichalcogenides, including the role of spin and valley degrees of freedom. Manzeli et al. (2017) reviewed the rapidly developing field of two-

dimensional transition-metal dichalcogenides and identified opportunities for controlling their properties through thickness, strain, defects, and external perturbations. Computational studies have also demonstrated the importance of methodological accuracy. Kresse and Furthmüller (1996) established efficient plane-wave approaches for first-principles calculations, while Giannozzi et al. (2009, 2020) developed the Quantum ESPRESSO framework for large-scale quantum simulations. Grimme (2006) introduced a dispersion correction that can improve the treatment of long-range interactions, which is particularly relevant for layered and van der Waals materials. Marzari et al. (2012) demonstrated the usefulness of Wannier functions for analysing electronic structures and constructing effective models. Recent research has increasingly emphasized defect engineering, strain tuning, charge redistribution, and computational screening as routes for tailoring low-dimensional materials. Nevertheless, much of the existing literature remains focused on individual material classes or isolated physical properties. A comprehensive framework simultaneously relating dimensionality, structural configuration, defects, chemical modification, strain, electronic states, charge distribution, and magnetic behaviour remains necessary. The proposed study addresses this need through an integrated first-principles investigation designed to establish quantitative structure–property relationships in selected low-dimensional systems.

III. Research Methodology

The proposed investigation will employ a **theoretical and computational research methodology** based primarily on first-principles quantum-mechanical calculations. Selected low-dimensional materials, particularly representative two-dimensional and one-dimensional systems, will first be identified through a systematic literature review based on their structural stability, electronic characteristics, and technological relevance. Atomic models of pristine materials will be constructed using reported crystal structures or established theoretical configurations. Appropriate vacuum spacing will be introduced to minimize interactions between periodically repeated images. The structures will then be subjected to geometry optimization using Density Functional Theory (DFT), with an appropriate exchange-correlation functional such as GGA-PBE. Convergence tests will be performed for plane-wave cutoff energy, k-point sampling, vacuum spacing, total energy, and atomic forces before production calculations are undertaken. Following optimization, structural stability will be evaluated using total energy, formation energy, cohesive energy, lattice parameters, bond lengths, and bond angles. Electronic properties will subsequently be investigated through band-structure calculations, band-gap determination, total and projected density of states, Fermi-level analysis, and charge-density calculations. Selected vacancies, substitutional atoms, and chemical modifications will be introduced systematically to investigate defect-induced changes in electronic and structural properties. Mechanical strain will also be applied within predefined tensile and compressive ranges to examine strain-dependent band-gap and electronic-state modulation. Spin-polarized calculations will be conducted for systems showing possible magnetic behaviour, while selected optical properties will be evaluated where computationally appropriate. Charge-density-difference analysis will be used to identify electron accumulation, depletion, and charge transfer. The calculated results will be organized into comparative datasets and analysed using percentage changes, correlations, and regression approaches where statistically appropriate. Band structures, DOS/PDOS profiles, charge-density maps, and comparative graphs will be used for interpretation. Finally, selected results will be compared with reliable published theoretical or experimental data to assess computational consistency and establish the scientific validity of the predicted structure–property relationships.

IV. Results and Data Analysis

The results of the proposed theoretical investigation will be analysed systematically to establish relationships between the structural characteristics and quantum-mechanical properties of selected low-dimensional materials. The analysis will begin with structural optimization and energetic stability, followed by investigation of electronic structure, density of states, charge redistribution, defect effects, strain dependence, and magnetic properties. For each material, the optimized configuration will be used as the reference structure. Modified configurations will then be compared with the pristine system under identical computational conditions. Quantitative parameters such as lattice constant, bond length, formation energy, band gap, Fermi energy, magnetic moment, and charge transfer will be examined together with graphical outputs including band structures, DOS/PDOS plots, charge-density maps, and strain-dependent curves.

Table 1. Illustrative Structural Parameters of Selected Low-Dimensional Material Systems

Material System	Lattice Parameter (Å)	Average Bond Length (Å)	Bond Angle (°)	Total Energy (eV)	Structural Status
Material A	2.46	1.42	120.0	-154.82	Stable
Material B	3.18	2.41	121.6	-286.47	Stable
Material C	3.52	2.36	109.8	-319.74	Stable
Material D	3.91	2.52	118.4	-402.61	Stable
Material E	4.12	2.61	116.7	-438.35	Stable

The illustrative data in Table 1 demonstrate the type of structural information that will be obtained after geometry optimization. The lattice parameter and average bond length provide fundamental information concerning the equilibrium geometry of the investigated systems. Differences among the materials indicate that chemical composition and atomic arrangement strongly influence the optimized structural configuration. The bond-angle values provide additional information about the local bonding environment. Values close to characteristic geometrical configurations indicate that the optimized structures retain their expected structural symmetry, whereas substantial deviations may indicate local distortion. Such distortions are particularly important in low-dimensional systems because even small changes in atomic geometry can modify orbital overlap and consequently alter the electronic structure. The total-energy values will primarily be useful for comparing different configurations of the **same chemical system** under identical computational conditions. A lower relative energy generally indicates a more energetically favourable configuration. However, absolute total energies between chemically different systems should not be interpreted directly as a measure of which material is more stable. The optimized geometries obtained from this stage will serve as the basis for subsequent electronic-structure calculations. Correlation between bond-length changes and electronic parameters such as band gap and density of states will subsequently be examined. Thus, structural optimization represents the essential first stage for establishing reliable structure–property relationships.

Table 2. Illustrative Energetic Stability and Defect Formation Analysis

Configuration	Total Energy (eV)	Formation Energy (eV)	Defect Formation Energy (eV)	Relative Stability
Pristine	-286.47	-3.82	—	Highest
Single Vacancy	-281.63	-2.91	2.14	Moderate
Double Vacancy	-276.12	-1.84	3.76	Lower
Substitution-1	-284.92	-3.21	1.55	High
Substitution-2	-283.74	-3.05	1.82	High–Moderate

Table 2 illustrates how energetic calculations can be used to compare pristine, vacancy-containing, and substitutionally modified structures. The pristine configuration represents the reference system, whereas the defective structures contain controlled atomic modifications. Defect formation energy is particularly important because the removal or replacement of an atom does not necessarily result in an energetically favourable structure. Lower defect formation energy indicates that the corresponding defect is comparatively easier to form under the assumed chemical-potential conditions. Conversely, a higher value suggests that the configuration is energetically less favourable. The illustrative results suggest that the single-vacancy configuration has a lower energetic cost than the double-vacancy configuration. This type of result would indicate that increasing defect concentration may reduce structural stability. However, the relationship should not be generalized without considering the specific chemical potentials and defect environment. Substitutional configurations can sometimes exhibit lower formation energies than vacancies because the introduced atom may establish favourable chemical interactions with neighbouring atoms. Therefore, defect engineering may provide a mechanism for modifying material properties while retaining reasonable structural stability. The formation-energy analysis will subsequently be combined with electronic-structure calculations. A particularly important question will be whether energetically accessible defects introduce desirable electronic states without causing excessive structural destabilization.

Table 3. Illustrative Electronic Properties of Pristine and Modified Systems

Configuration	Band Gap (eV)	Fermi Energy (eV)	Electronic Character	VBM (eV)	CBM (eV)
Pristine	1.82	-4.61	Semiconductor	-5.52	-3.70
Vacancy	1.24	-4.43	Semiconductor	-5.05	-3.81
Double Vacancy	0.76	-4.21	Narrow-gap semiconductor	-4.82	-4.06
Substitution-1	1.46	-4.52	Semiconductor	-5.19	-3.73
Substitution-2	1.08	-4.36	Semiconductor	-4.94	-3.86

The electronic properties presented in Table 3 illustrate how structural modifications may influence the electronic band structure. The pristine system possesses an illustrative band gap of 1.82 eV, whereas the introduction of defects progressively reduces the calculated gap. Such reduction may originate from defect-induced electronic states appearing within the forbidden energy region. A vacancy can modify the local coordination environment and alter orbital overlap, resulting in localized states near the valence- or conduction-band edges. The hypothetical double-vacancy configuration exhibits the smallest band gap among the configurations considered. If confirmed through actual calculations, this behaviour would suggest that defect concentration provides an effective mechanism for tuning the electronic response. The positions of the valence-band maximum (VBM) and conduction-band minimum (CBM) will also be examined to determine whether the modification changes the direct or indirect nature of the band gap. This distinction is important when considering potential optoelectronic applications. However, calculated band gaps obtained using conventional semilocal DFT should be interpreted cautiously because such methods can underestimate experimental band gaps. Where accurate

band-gap prediction is central to the study, higher-level computational methods may be used for selected structures.

Table 4. Illustrative Density of States and Orbital Contributions

System	Dominant VBM Contribution	Dominant CBM Contribution	Defect States	Fermi-Level DOS
Pristine	p-orbital	p-orbital	Absent	0.00
Vacancy	p-orbital	p/d mixed	Present	0.12
Double Vacancy	p/d mixed	d-orbital	Strong	0.28
Substitution-1	p-orbital	p/d mixed	Moderate	0.09
Substitution-2	p/d mixed	d-orbital	Moderate–Strong	0.17

The density-of-states analysis will provide information about the atomic and orbital origin of the electronic states identified from the band-structure calculations. In the pristine configuration, the states near the valence- and conduction-band edges are expected to arise primarily from the orbitals associated with the constituent atoms. Defects can introduce additional electronic states within the band gap or near the Fermi level. Such states can substantially modify the electronic response even when the overall crystal structure remains relatively unchanged. The projected density of states will therefore be particularly useful for determining whether these states originate from neighbouring atoms, the defect site, or the substituted species. The illustrative increase in Fermi-level DOS from the pristine system toward defective configurations suggests progressively stronger electronic-state contributions around the Fermi energy. If sufficiently strong, such modifications could influence conductivity and carrier behaviour. The PDOS analysis will be combined with charge-density plots to distinguish between localized defect states and extended electronic states. This combined approach will provide a more complete interpretation than band-gap analysis alone.

Table 5. Illustrative Effect of Mechanical Strain on Band Gap

Applied Strain (%)	Lattice Parameter (Å)	Band Gap (eV)	Relative Change (%)	Electronic Character
-5	3.02	1.51	-17.0	Semiconductor
-3	3.08	1.63	-10.4	Semiconductor
-1	3.14	1.75	-3.8	Semiconductor
0	3.18	1.82	0.0	Semiconductor
+1	3.21	1.91	+4.9	Semiconductor
+3	3.28	2.04	+12.1	Semiconductor
+5	3.34	2.17	+19.2	Semiconductor

Table 5 demonstrates the proposed approach for investigating strain-dependent electronic properties. The equilibrium structure at 0% strain serves as the reference configuration. Both compressive and tensile strain are then introduced systematically. The illustrative results show a gradual reduction in band gap under compressive strain and an increase under tensile strain. Such behaviour could arise from strain-induced changes in interatomic distances and orbital overlap. The modification of orbital interactions can shift the positions of the valence and conduction bands. The percentage-change analysis provides an additional quantitative measure of the sensitivity of the electronic structure to strain. In the illustrative dataset, the +5% tensile condition produces a considerably larger band gap than the unstrained system. The actual relationship may not necessarily be linear. At larger strain values, structural reconstruction, phase transformation, band crossing, or metallization may occur. Therefore, every strained configuration should be structurally optimized before its electronic properties are interpreted. A strain-dependent study can consequently determine whether mechanical deformation provides a practical theoretical mechanism for controlling electronic properties in low-dimensional materials.

Table 6. Illustrative Charge-Transfer Analysis

Configuration	Charge Transfer (e)	Maximum Charge Accumulation	Maximum Charge Depletion	Principal Charge-Transfer Region
Pristine	0.00	Low	Low	Uniform
Vacancy	0.18	Moderate	High	Neighbouring atoms
Substitution-1	0.31	High	Moderate	Substituent–host region
Substitution-2	0.44	High	High	Interface region
Functionalized	0.52	Very High	High	Functional group region

Charge-density analysis will be used to understand the microscopic mechanism responsible for changes in electronic behaviour. The amount and spatial distribution of charge transfer can reveal whether a chemical modification produces electron donation, electron withdrawal, or localized polarization. The illustrative data show progressively greater charge redistribution for the modified systems. Such redistribution can alter the local electrostatic potential and modify orbital energies, which may subsequently influence the band gap and density of states. Charge-density-difference maps will be particularly valuable because numerical charge-transfer values alone cannot identify where the electrons are accumulated or depleted. Visualization of the three-dimensional or

planar charge-density difference will therefore complement the quantitative analysis. For substituted and functionalized systems, the charge-transfer analysis can also help establish relationships between chemical composition and electronic properties. A strong correlation between charge transfer and band-gap modification would provide evidence that electronic tuning originates partly from redistribution of electron density.

Table 7. Illustrative Magnetic Properties of Defective Systems

Configuration	Magnetic Moment (μB\mu_B)	Spin Polarization	Magnetic State
Pristine	0.00	No	Non-magnetic
Single Vacancy	0.74	Moderate	Magnetic
Double Vacancy	1.36	Strong	Magnetic
Substitution-1	0.48	Moderate	Magnetic
Substitution-2	1.02	Strong	Magnetic

The magnetic-property analysis will focus on systems in which defects, substitutions, or edge configurations may generate unpaired electrons. The pristine structure may exhibit a non-magnetic ground state, while structural modifications can break local symmetry and generate spin-polarized states. The illustrative magnetic moments indicate that vacancy formation can induce a magnetic response. Such behaviour may originate from unsaturated bonds or localized electronic states associated with the defect. Spin-resolved density-of-states calculations will be used to determine whether the spin-up and spin-down electronic states are energetically equivalent. Differences between the two spin channels will provide evidence for spin polarization. Spin-density visualization will further identify the spatial location of the magnetic states. If the magnetic density is strongly localized around a defect, the result would suggest a defect-induced magnetic mechanism rather than a bulk-like magnetic state. These findings could be relevant to theoretical investigations of spin-dependent electronic behaviour and potential spintronic applications, although application claims would require further device-level investigation.

Table 8. Illustrative Comparative Assessment of Material Configurations

Configuration	Stability	Band Gap	Defect States	Charge Redistribution	Magnetic Response	Overall Potential
Pristine	High	1.82	No	Low	Low	High
Vacancy	Moderate	1.24	Yes	Moderate	Moderate	High
Double Vacancy	Lower	0.76	Strong	High	Strong	Moderate
Substitution-1	High	1.46	Moderate	High	Moderate	Very High
Substitution-2	Moderate	1.08	Strong	Very High	Strong	High

Table 8 provides an integrated framework for identifying promising material configurations. No single quantum-mechanical parameter is sufficient to determine the overall suitability of a low-dimensional material. A configuration may possess a desirable band gap but poor structural stability, or it may demonstrate strong magnetic behaviour while having energetically unfavourable defect formation. The comparative framework therefore combines structural stability, electronic properties, defect states, charge redistribution, and magnetic response. Configurations demonstrating a favourable balance between these parameters can be identified for more detailed investigation. The illustrative data suggest that Substitution-1 provides a favourable combination of stability, moderate band-gap modification, charge redistribution, and magnetic response. Such a configuration could subsequently be subjected to higher-accuracy electronic calculations or additional external-perturbation studies. Importantly, the term **"promising"** should be based on predefined criteria rather than subjective interpretation. The final research should therefore establish quantitative screening criteria before ranking candidate systems.

V. Conclusion

The proposed research presents a systematic theoretical framework for investigating the quantum-mechanical properties of low-dimensional materials through first-principles computational modelling. The study is designed to address the increasing need for an atomistic understanding of how reduced dimensionality and controlled structural modifications influence the fundamental properties of nanoscale materials. By integrating structural optimization, energetic analysis, electronic-structure calculations, charge-density investigations, defect engineering, strain analysis, and selected magnetic and optical calculations, the research will provide a comprehensive assessment of the relationship between atomic structure and quantum response. A major strength of the proposed investigation is its emphasis on **structure–property relationships rather than isolated property calculations**. Dimensionality, vacancies, substitutional atoms, chemical functionalization, and mechanical strain will be treated as controllable factors, while band gap, density of states, charge redistribution, formation energy, magnetic moment, and related properties will be considered as measurable responses. This approach will enable the identification of the microscopic mechanisms responsible for changes in the quantum-mechanical behaviour of the investigated systems.

The study is also expected to demonstrate the usefulness of computational materials science for predicting potentially desirable material characteristics before experimental synthesis. Systematic convergence testing and comparison with reliable published results will be incorporated to improve the reliability and reproducibility of the theoretical predictions. The findings may reveal configurations in which electronic or magnetic properties can be effectively tuned through defect engineering, chemical modification, or mechanical strain. Overall, the research is expected to contribute to the theoretical understanding of low-dimensional quantum systems and provide a computational basis for designing materials with tailored properties. The outcomes may have relevance to emerging areas including nanoelectronics, optoelectronics, sensing, spintronics, energy conversion, and quantum technologies. The predicted structures and properties can further serve as a foundation for future experimental validation and more advanced theoretical investigations.

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