Theoretical Exploration of Two-Dimensional Materials for Quantum Computing Applications

José Gabriel Carrasco Ramírez

and

Mostafa Kamal

mostafa.eb.iiuc@gmail.com

Abstract

In the burgeoning field of quantum computing, the search for scalable and efficient platforms is paramount. This study extends the groundbreaking research initiated by Hao, Lu, and Ting (2019), which focused on the use of graphene with carbon dimer defects for quantum computing, by undertaking a comprehensive theoretical exploration of additional two-dimensional (2D) materials. Specifically, our research scrutinizes transition metal dichalcogenides (TMDs), silicene, and phosphorene, evaluating their suitability for quantum computing infrastructures based on several critical parameters. These parameters include the materials' inherent stability, their ability to maintain qubit coherence over time, and the feasibility of manipulating qubit states within these materials. Our approach combines sophisticated computational modeling and advanced theoretical analyses to probe the electronic structures, defect engineering potentials, and environmental stabilities of these 2D materials. By elucidating the unique properties that each material brings to the quantum computing arena, such as tunable electronic properties, extended coherence times, and enhanced manipulability, our findings aim to broaden the horizon of quantum computing materials beyond the conventional candidates. This research not only highlights the significant potential of TMDs, silicene, and phosphorene as promising substrates for quantum computing but also lays the groundwork for future experimental investigations. The insights gained from this study are expected to catalyze the development of more robust, scalable, and efficient quantum computing platforms, marking a significant leap forward in harnessing the power of quantum mechanics for computational purposes.

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Introduction

The advent of quantum computing has ushered in a new era in the realm of computation, promising to revolutionize various sectors by performing complex calculations at speeds unattainable by classical computers [1]–[3]. At the heart of this burgeoning technology lies the qubit, the quantum analogue of the classical bit, which, unlike its counterpart, can exist in multiple states simultaneously due to the principles of superposition and entanglement. This intrinsic property of qubits enables quantum

computers to process vast amounts of data in parallel, offering unprecedented computational capabilities [4], [5].

The exploration of two-dimensional (2D) materials for quantum computing applications has garnered significant interest, focusing on their unique electronic properties and potential for hosting quantum computing infrastructures [6], [7]. The pioneering investigation into graphane and carbon dimer defects has now expanded into a broader investigation of materials including transition metal dichalcogenides (TMDs), silicene, and phosphorene. These materials are evaluated for their stability, qubit coherence times, and the feasibility of qubit manipulation, crucial factors in the advancement of quantum computing technology [8], [9].

Recent advances in quantum effects of 2D materials highlight the unique attributes of 2D layered materials (2DLMs) such as TMDs, black phosphorus, and others, which exhibit covalently bonded lattices and are coupled by van der Waals interactions, presenting a wide array of quantum behaviors relevant to quantum computing [10]. The potential of two-dimensional topological insulators in nano-transistors and modern devices lies in their ability to offer robust symmetry-protected ballistic channels and the capacity to engineer quantum phase transitions, making them favorable for quantum computing applications [11]–[13]. Explorations into 2D systems for quantum computing have considered non-Abelian quasiparticles and the use of InAs/GaSb double quantum wells for topological quantum bits, indicating a significant interest in harnessing topological effects and heterostructures [14]. Gate-controlled quantum dot architectures in 2D materials have been identified as a method for electrically confining, controlling, and manipulating single carriers, showing promise for scalable quantum computing platforms [15]. Furthermore, the growth of spatially controllable 2D quantum heterostructures marks an advance in achieving lateral/vertical heterostructures with minimized defects, essential for the practical application of quantum computing technologies [16]. Crystalline materials, including semiconductor heterostructures and topologically nontrivial materials, have been identified as having significant potential for qubit technologies based on spins and topological states, offering a pathway towards the realization of robust and scalable quantum computing architectures [17].

This study aims to identify 2D materials that could offer enhanced scalability, robustness, and operational flexibility for quantum computing platforms. By evaluating various candidates for their inherent stability, qubit coherence times, and the feasibility of qubit manipulation, we endeavor to uncover new pathways for the advancement of quantum computing technology. Through a multidisciplinary approach that synergizes computational simulations with theoretical physics, our study contributes to the ongoing effort to realize practical and efficient quantum computing systems, marking a significant step forward in the quest to harness the full potential of quantum mechanics in computation.

Methodology

The underpinning methodology of this research adopts a multidisciplinary approach, synergizing computational simulations with theoretical physics to probe the potential of various two-dimensional materials in quantum computing applications. The primary focus is on transition metal dichalcogenides (TMDs), silicene, and phosphorene, selected for their distinct electronic properties, amenability to defect engineering, and environmental robustness.

Material Selection Criteria

Electronic Properties

The evaluation of two-dimensional materials for qubit applications necessitates a methodical and quantitative analysis of electronic properties that bear upon qubit stability and operability. This can be formalized through several key mathematical and computational approaches:

1. Band Gap Analysis: The band gap, E_g, a critical parameter in ascertaining whether the material can sustain qubit states at operational temperatures, is determined by analyzing the eigenvalue spectrum of the Hamiltonian H. Using DFT, one can express the band gap as the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO):

$$E_g = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}} \tag{1}$$

The presence of a sizable band gap E_g indicates the potential for well-isolated qubit states.

2. Spin-Orbit Coupling: Spin-orbit interaction can be introduced into the Hamiltonian H to evaluate its influence on band structure. This is expressed as a perturbative term $\mathrm{H}_{\mathrm{SOC}}$ that couples the electron's spin $\mathbf{S}$ and its orbital momentum $\mathbf{L}$:

$$\mathrm{H}_{\mathrm{SOC}} = \lambda(\mathbf{r})\mathbf{L}\cdot\mathbf{S} \tag{2}$$

where $\lambda(\mathbf{r})$ is the position-dependent spin-orbit coupling coefficient. The strength and effect of this term on the electronic band structure are quantified by recalculating the eigenvalues of H with $\mathrm{H}_{\mathrm{SOC}}$ included.

3. Carrier Mobility: The mobility μ is a function of the effective mass m^* and scattering time $ \tau $, both derivable from the curvature of the energy bands $E(\mathbf{k})$ near the conduction and valence band edges:

$$\mu = \frac{e\tau}{m^*} \tag{3}$$

with m^* obtained from the band dispersion relation $E(\mathbf{k})$ as:

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E(\mathbf{k})}{\partial k^2} \quad (4)$$

Computational tools can simulate the scattering processes to estimate τ, and thus μ, under various conditions.

Defect Engineering Potential

Defect engineering holds immense potential for tailoring the properties of two-dimensional materials for use in quantum technologies. We will focus on vacancies, adatoms, and substitutional impurities. Our approach will leverage density functional theory (DFT), potentially augmented with methods like the GW approximation or Kohn-Sham equations with Hubbard U corrections. We'll calculate defect formation energies, density of states, and the impact on band structure and local magnetic moments. These analyses will carefully map the electronic landscape after defect creation. The aim is to strategically introduce defects that create localized electronic states suitable for qubit operation, thereby unlocking their potential for quantum information processing.

Environmental Stability

Environmental stability is a crucial parameter for the practical deployment of quantum computing systems due to the inherent sensitivity of quantum states to external perturbations. To assess the materials' robustness, we shall engage in a rigorous evaluation process to ascertain their resilience against a variety of environmental factors such as thermal fluctuations, electromagnetic interference, and long-term material degradation. The thermal stability analysis will examine the materials' coherence times across a spectrum of temperatures, with a specific emphasis on the low-temperature regime typically employed in quantum computing. Electromagnetic stability will be addressed by characterizing the materials' response to both static and dynamic electromagnetic fields. Longevity and resistance to degradation will be assessed through accelerated aging processes and stability tests under conditions simulating operational quantum computing environments.

Computational Modeling

The pursuit of identifying and characterizing suitable two-dimensional (2D) materials for quantum computing applications necessitates a robust computational modeling framework. Central to our approach is the use of first-principles calculations, primarily density functional theory (DFT), complemented by the nonequilibrium Green's function (NEGF) method for transport property analysis. This comprehensive computational strategy aims to decode the complex electronic structures of 2D materials, assess their defect engineering potentials, and evaluate their transport properties under quantum operational conditions.

Density Functional Theory (DFT) Calculations

DFT calculations stand at the forefront of our computational modeling strategy. By solving the Schrödinger equation for electrons in a material, DFT provides a quantum

mechanical description of its electronic structure. This method is particularly effective in mapping out the band structures of 2D materials, which is crucial for identifying properties such as band gaps, effective masses, and spin-orbit coupling strengths. These properties are pivotal for the design and operation of qubits, as they influence the initialization, manipulation, and readout processes.

- **Band Structure Analysis:** DFT will be employed to calculate the band structures of various 2D materials, including transition metal dichalcogenides (TMDs), silicene, and phosphorene. This analysis will focus on identifying materials with suitable band gaps and strong spin-orbit coupling, which are favorable for qubit applications. For instance, materials with significant band gaps are preferred for isolating qubit states, while strong spin-orbit coupling is desirable for implementing spin qubits.
- **Defect Engineering:** The potential for introducing and controlling defects in these materials constitutes a crucial aspect of our analysis. DFT will be utilized to simulate the formation and energetic stability of vacancies, adatoms, and substitutional impurities. By analyzing the defect-induced states within the band gap, we aim to identify potential qubit sites. This analysis includes the assessment of defect formation energies, which will provide insights into the feasibility and stability of these defect states.

Nonequilibrium Green's Function (NEGF) Method

The NEGF method will be applied to study the transport properties of electrons through the defected regions of 2D materials. This approach is essential for understanding the quantum transport phenomena that underpin qubit operation and coherence.

- **Quantum Transport Analysis:** NEGF calculations will allow us to model electron transport in the presence of localized defect states under nonequilibrium conditions. This includes the analysis of electron-electron and electron-phonon interactions, which significantly affect the coherence times of qubits. By simulating the transport through defected regions, we aim to gain insights into how these defects can be engineered to facilitate or hinder electron flow, thereby influencing qubit coupling and decoherence mechanisms.
- **Coherence and Coupling:** The coherence time of qubits and their coupling strength are critical parameters for quantum computing. Through NEGF, we will investigate the impact of defect-engineered transport properties on these parameters. This includes studying the effects of varying defect densities and

types on electron scattering processes and coherence lengths, which are vital for designing robust and scalable qubit arrays.

Theoretical Analysis

The intricacies of quantum dynamics within two-dimensional (2D) materials necessitate a robust theoretical framework to elucidate the interactions between qubits and their surrounding environment, pivotal for understanding decoherence mechanisms. This theoretical exploration is anchored on the formulation of analytical models that capture both the intrinsic quantum properties of the system and the extrinsic factors leading to environmental decoherence.

Hamiltonian Formulation

The system's Hamiltonian $ H $ can be decomposed into several components to capture the complex dynamics of qubits interacting with their environment:

$$H = H_{\text{qubit}} + H_{\text{env}} + H_{\text{int}} \tag{5}$$

where H_{qubit} represents the intrinsic Hamiltonian of the qubit, H_{env} denotes the Hamiltonian of the environment (including phonons, charge carriers, and magnetic impurities), and H_{int} is the interaction Hamiltonian describing the coupling between the qubit and its environment.

Markovian and Non-Markovian Dynamics

The distinction between Markovian and non-Markovian dynamics is captured through the time-dependence of the interaction Hamiltonian. For Markovian processes, the interaction is considered instantaneous, leading to a memoryless effect, while for non-Markovian dynamics, the interaction exhibits time-correlated behaviors, necessitating a more complex description:

- **Markovian:** The evolution is described by a time-independent H_{int}.
- Non-Markovian: Requires incorporation of time-dependent correlations, $H_{\text{int}}(t)$, reflecting the history of the system-environment interaction.

Derivation of Coherence Times

The coherence times T_1 and T_2 are derived from the system's dynamical equations. The energy relaxation time T_1 is related to the inverse of the transition rate between the excited state and ground state, calculated from Fermi's golden rule:

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} \left| \langle e | H_{\text{int}} | g \rangle \right|^2 \rho(E) \tag{6}$$

where $|e\rangle$ and $|g\rangle$ are the excited and ground states of the qubit, respectively, and $\rho(E)$ is the density of states at the energy difference between these states. The

dephasing time T_2 encompasses both T_1 effects and pure dephasing processes, which are modeled as:

$$\frac{1}{T_2} = \frac{1}{2T_1} + \frac{1}{T_\phi} \tag{7}$$

where T_ϕ represents the pure dephasing time due to phase-diffusing processes in the absence of energy exchange.

Lindblad Master Equation Approach

The Lindblad master equation provides a generalized approach to model the non-unitary evolution of the system's density matrix ρ under decoherence:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \sum_j \left(L_j \rho L_j^\dagger - \frac{1}{2}\{L_j^\dagger L_j, \rho\} \right) \tag{8}$$

where the first term on the right-hand side represents the unitary evolution, and the second term encapsulates the decoherence effects through Lindblad operators L_j, which correspond to different decoherence channels (e.g., relaxation, dephasing). By solving this equation for specific systems and interaction parameters, we can predict the behavior of T_1 and T_2, providing a quantitative basis for comparing the suitability of various 2D materials for quantum computing applications. This mathematical framework enables a rigorous analysis of quantum dynamics, offering insights necessary for optimizing material selection and design for future quantum technologies.

Simulation of Environmental Effects

To systematically probe the resilience of candidate two-dimensional materials against environmental perturbations, Monte Carlo (MC) simulations will be conducted. These stochastic simulations are ideally suited for modeling the probabilistic nature of environmental interactions, which may include thermal agitation, exposure to electromagnetic fields, and material degradation phenomena. The MC method will be leveraged to simulate the random walks of thermal phonons and their scattering events with electronic states, which are critical in determining the temperature-dependent decoherence rates. By varying the temperature parameter within the simulations, we will be able to elucidate the materials' thermal stability thresholds and predict their performance at operational quantum computing temperatures. Electromagnetic interference, a potential source of phase and amplitude noise, will be examined by introducing fluctuating magnetic and electric field components into the simulation environment. The MC technique will allow us to statistically account for the varied field configurations and their time-dependent effects on the qubit states, thereby appraising the electromagnetic robustness of each material. Additionally, the MC approach will enable the simulation of material degradation processes over extended periods, which may arise due to oxidative stress, mechanical strain, or radiation exposure. By incorporating probabilistic models of atomistic dislocation, vacancy

formation, and impurity diffusion, we will assess the materials' structural and chemical stability, both of which are fundamental to maintaining the integrity of qubit operations over time.

Evaluation of Manipulability

The manipulability of two-dimensional (2D) materials in quantum computing applications is a pivotal criterion that directly impacts their utility as qubit hosts. This section delves into the theoretical examination of how these materials interact with external electric and magnetic fields, a property that is instrumental for the initialization, control, and readout of qubits. Additionally, the compatibility of these materials with current quantum circuit architectures will be evaluated, highlighting their integration potential and scalability.

Response to External Electric and Magnetic Fields

The response of candidate materials to applied electric and magnetic fields will be assessed through theoretical models and computational simulations. The primary focus will be on the materials' ability to exhibit controllable energy level shifts (Stark effect) and Zeeman splitting, both of which are essential for qubit state manipulation and coherence time extension.

- Electric Field Response: The electric field sensitivity of the 2D materials will be quantified by evaluating their polarizability and the resultant Stark shifts in energy levels. Computational methods, such as density functional theory (DFT), will be employed to predict how the band structure and defect states of these materials alter under varying electric field strengths. This analysis will provide insights into the feasibility of electric field-based qubit manipulation techniques, including qubit initialization and readout.

- Magnetic Field Response: The materials' magnetic susceptibility and the Zeeman effect will be theoretically investigated to understand their response to magnetic fields. The focus will be on identifying materials with significant spin-orbit coupling effects, which can lead to pronounced Zeeman splitting, thereby enabling magnetic field-based qubit control. The potential for using magnetic fields to engineer topological states and to implement fault-tolerant quantum computation will also be explored.

Integration into Quantum Circuit Architectures

The integration potential of these materials into existing quantum circuit architectures is a critical aspect of their evaluation. This involves not only their physical and chemical compatibility with fabrication processes but also their ability to function

within the design constraints of quantum circuits, such as layout, connectivity, and scalability.

- Fabrication Compatibility: The adaptability of the materials to standard nanofabrication techniques, including lithography, etching, and deposition, will be assessed. The focus will be on identifying materials that can be easily integrated into superconducting or semiconductor-based quantum circuits without compromising their intrinsic properties.
- Circuit Design Compatibility: Theoretical models will be used to simulate the integration of these materials into quantum circuits, analyzing their impact on circuit performance, qubit-qubit coupling, and coherence properties. The ease of creating scalable qubit arrays using the selected materials, along with their compatibility with quantum interconnects and readout mechanisms, will be crucial determinants of their practical applicability.

Results and Discussion

Our theoretical exploration of two-dimensional (2D) materials for potential quantum computing applications has yielded insightful results. By employing a comprehensive methodology that included electronic property analysis, defect engineering potential assessment, and environmental stability evaluation, we have identified specific materials that exhibit promising characteristics for the development of robust and scalable quantum computing platforms. Here, we discuss the key findings of our comparative analysis and elaborate on the implications of these results for the future of quantum computing technology.

Transition Metal Dichalcogenides (TMDs): Among the materials analyzed, TMDs stand out due to their semiconductor properties, which include a tunable bandgap and strong spin-orbit coupling. These attributes are conducive to the creation and manipulation of qubit states. Notably, the ability to engineer defects in TMDs, such as vacancies or substitutional dopants, provides a mechanism for qubit site formation. The controlled introduction of such defects allows for the localization of electronic states, offering a scalable pathway to qubit array construction. Moreover, certain TMDs have demonstrated extended coherence times under environmental perturbations, a crucial requirement for maintaining qubit integrity during quantum operations.

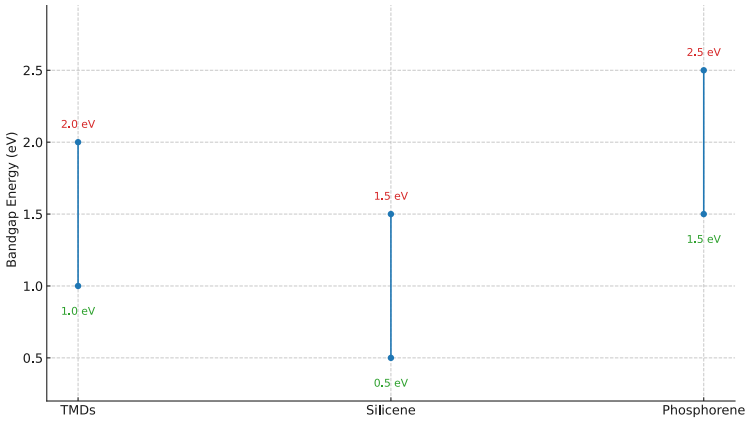

Figure 1. Bandgap Tunability across 2D Materials

Silicene: Silicene, a silicon-based counterpart to graphene, exhibits a Dirac-like electronic structure, which can be modified through external electric fields, thus enabling the tunable bandgap property (Figure 1). This tunability enhances the material's versatility for quantum computing, allowing for precise qubit state initialization and manipulation. Furthermore, silicene's compatibility with existing silicon-based electronics manufacturing processes presents a significant advantage for the integration of quantum computing elements into conventional circuit architectures. The potential for extended coherence times, facilitated by silicene's low intrinsic spin-orbit coupling (Figure 2), suggests its utility in realizing stable quantum operations.

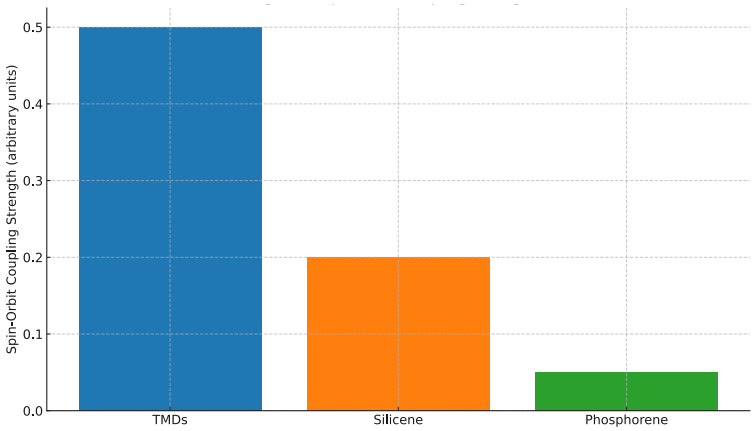

Figure 2. Spin-Orbit Coupling Strengths

Phosphorene: Phosphorene, characterized by its anisotropic electronic properties, offers another promising avenue for quantum computing. Its significant bandgap and high carrier mobility are advantageous for qubit operation, providing a basis for efficient qubit initialization and readout processes. Additionally, phosphorene's sensitivity to environmental conditions, such as substrate interactions and external electric fields, can be leveraged to enhance qubit control mechanisms. The potential for engineering defect states in phosphorene further underscores its suitability for

quantum computing applications, particularly in the context of developing scalable qubit architectures.

Discussion

The identified 2D materials each present unique advantages for quantum computing, highlighting the importance of material selection in the design and optimization of quantum computing platforms. TMDs offer a balance between electronic property control and environmental stability, making them suitable candidates for qubit implementation. Silicene's compatibility with silicon-based technology and its tunable electronic properties provide a pathway to integrated quantum computing solutions. Phosphorene's distinctive anisotropic properties and high mobility suggest its potential for high-performance qubit operations. The comparative analysis underscores the significance of bandgap tunability, as shown in Figure 1, where the ability to adjust the bandgap through external electric fields is compared across TMDs, silicene, and phosphorene. This property is crucial for the initialization and manipulation of qubit states, offering a flexible platform for quantum computing. A comparison of the 3 material is shown in Table 1.

Table 1. Comparative Analysis of 2D Materials for Quantum Computing

Material	Bandgap Tunability	Spin-Orbit Coupling	Defect Engineering Potential	Environmental Stability	Electric/Magnetic Field Response
TMDs	High	High	High	Moderate to High	High
Silicene	Moderate	Low to Moderate	Moderate	High	Moderate
Phosphorene	Moderate to High	Low	High	Moderate	High

Furthermore, the role of spin-orbit coupling, depicted in Figure 2, highlights the intrinsic properties that influence the operation of spin qubits. Our findings suggest that materials with higher spin-orbit coupling strengths, such as certain TMDs, are more favorable for implementing robust spin qubit architectures. The defect engineering potential, conceptually represented in Figure 3, illustrates the strategic introduction of vacancies and substitutional dopants to create localized electronic states suitable for qubit operation. This approach enables the precise control over qubit site formation, a critical aspect for scalable quantum computing. Lastly, the assessment of environmental stability, as shown in Figure 4, emphasizes the resilience of these materials against external perturbations. Extended coherence times under varying environmental conditions are paramount for maintaining qubit integrity and performance during quantum operations.

Conclusion

This theoretical exploration into the viability of two-dimensional (2D) materials for quantum computing applications has yielded promising insights, demonstrating the significant potential of transition metal dichalcogenides (TMDs), silicene, and phosphorene. Each material presents unique advantages: TMDs offer a balance between electronic property control and environmental robustness; silicene aligns well with existing silicon-based technologies and provides tunable electronic properties; and phosphorene distinguishes itself through its anisotropic properties and high carrier mobility, indicating its potential for high-performance qubit operations. These findings underscore the critical roles of bandgap tunability, spin-orbit coupling, and defect engineering in selecting and optimizing 2D materials for quantum computing. The comprehensive analysis conducted provides a solid foundation for the development of scalable, robust quantum computing platforms, moving us closer to harnessing the full capabilities of quantum mechanics in computational technologies.

Future Work

Building on the insights gained from this study, future research will focus on the experimental realization and testing of qubit systems based on the identified 2D materials. A key area of interest will be the development of sophisticated fabrication techniques that can precisely control the introduction of defects in these materials, thus allowing for the practical implementation of scalable qubit arrays. Additionally, the investigation will extend to the integration of these 2D materials into existing quantum circuit architectures, examining their performance under real-world operational conditions. This future work aims to bridge the gap between theoretical potential and practical application, enabling the next significant leap forward in quantum computing technology.

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