Quantum Computers: Importance, Materials Science Challenges, and the Promise of Two-Dimensional Materials

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Abstract: Quantum computing offers a fundamentally different approach to information processing by exploiting quantum phenomena such as superposition and entanglement. These effects enable efficient treatment of computational problems that become prohibitive for classical architectures, including molecular simulation, cryptography, optimization, and materials discovery. Despite rapid theoretical and algorithmic advances, the realization of practical quantum computers is constrained primarily by hardware limitations rooted in materials science. Qubit performance is highly sensitive to defects, impurities, and interfacial disorder, which induce decoherence and limit scalability across leading platforms such as superconducting, spin-based, and topological qubits. Consequently, advances in materials synthesis, defect control, and interface engineering are critical to achieving long coherence times and low error rates.

Two-dimensional (2D) materials provide an attractive experimental platform for quantum devices due to their atomic thickness, reduced bulk disorder, and high tunability via electrostatic gating, strain, and layer stacking. The ability to assemble van der Waals heterostructures without lattice-matching constraints enables flexible device architectures, positioning 2D materials as promising building blocks for scalable quantum computing hardware.

Keywords: Quantum computer, Materials science, Decoherence; Van der Waals heterostructures

1. Introduction

Quantum computing represents a paradigm shift in information processing, leveraging quantum mechanical phenomena as physical resources for computation (Simon, n.d.). Unlike classical bits, which are realized using macroscopic voltage levels, quantum bits (qubits) are based on fragile microscopic systems such as superconducting currents, electron spins,

trapped ions, or atomic states. Superposition enables a single qubit to represent a continuous spectrum of quantum amplitudes, while entanglement enables correlations that cannot be captured by classical probability theory (Sergei Kurgalin & Sergei Borzunov, 2021). These phenomena are harnessed using carefully designed control pulses and measurement protocols, allowing quantum computers to explore computational spaces that scale exponentially with system size (Bluvstein et al., 2024).

The primary motivation for quantum computing arises from problems where classical approaches fail due to exponential scaling, most notably in the simulation of quantum matter. Accurate modeling of molecular electronic structure, strongly correlated materials, and reaction pathways becomes prohibitively expensive on classical supercomputers as the number of interacting particles increases. Quantum processors, by directly implementing quantum Hamiltonians, offer a physically natural platform for such simulations. Beyond simulation, algorithmic developments such as Shor's factoring algorithm (Shor, n.d.) and Grover's search (Lov K. Grover, 1996) have established formal performance advantages, motivating experimental efforts to demonstrate quantum advantage in controlled settings.

However, the achievement of scalable quantum hardware is still hampered by decoherence and operational errors(Camino et al., 2023). In other words, the coherence times of qubits, the fidelity of quantum gates, and the device reproducibility are currently limited by material defects, interfaces, and electromagnetic interference. As a result, material synthesis, nanofabrication, and interface engineering have become critical to the performance of quantum processors. In this materials-science paradigm, two-dimensional materials have been identified as promising for next-generation quantum technology due to their high-quality interfaces, property tunability, and suitability for heterogeneous quantum architectures.

2. Why Quantum Computers Are Important

The power of quantum computing is essentially based on its capability to solve computational problems that are exponentially dependent on the size of the system for classical computers. For example, quantum simulation, which involves the simulation of quantum systems such as molecules and materials, is fundamentally difficult for classical computers because of the exponentially increasing memory and computation requirements with the size of the system. Quantum computers (Davide Castelvecchi, 2026), on the other hand, are expected to simulate

these systems in a more natural way, which could potentially shorten tasks that would take centuries on classical computers to minutes or seconds on a quantum computer. This has profound implications for drug discovery, materials design, and chemical catalysis, where accurate simulations could uncover novel compounds or reactions that classical methods struggle to predict.

Furthermore, quantum algorithms (Lov K. Grover, 1996; Shor, n.d.) like Shor's algorithm and Grover's search algorithm have shown theoretically important speedup advantages over their classical counterparts: Shor's algorithm can factor large numbers exponentially faster than the best known classical algorithms, which directly threatens modern cryptography; Grover's algorithm offers a quadratic speedup for search problems. The ability to offer such advantages in practice would be a paradigm-shifting event for many areas of study, including cybersecurity and artificial intelligence research.

However, the development of a practical quantum advantage in solving real-world problems has been an active area of research, and recent examples such as Google's "Quantum Echoes" algorithm (Hartmut Neven & Vadim Smelyanskiy, 2025) have shown improvements in velocity for solving specific problems, but scalable fault-tolerant quantum computers are still being developed.

3. Materials Science: The Keystone of Quantum Computing Hardware

At the core of quantum computers are qubits, physical systems that can maintain a coherent quantum state for a sufficient amount of time to solve computations. These qubits take many forms: superconducting circuits, ion traps, neutral atoms, spin qubits, and topological qubits, each of which has its own set of materials challenges.

A central theme in quantum hardware is quantum coherence: the ability of a qubit to maintain its quantum state without decohering due to interactions with its environment. Coherence times depend critically on materials purity, defect densities, and interfaces within the quantum device. Even tiny imperfections can introduce noise that collapses the fragile superposition state, leading to errors in computation. Therefore, state-of-the-art quantum systems demand materials with extremely low defect densities, precise control at the atomic scale, and interfaces engineered to minimize decoherence(Banerjee et al., 2025; Meziani et al., 2026).

A comprehensive materials perspective, spanning synthesis, characterization, and modeling, is therefore pivotal to advancing quantum computing performance. For instance:

- **Superconducting qubits(Kjaergaard et al., 2020; Siddiqi, 2021)**, widely used in current prototype machines, rely on materials like aluminum or niobium patterned with Josephson junctions. Two-level systems arising from oxides or surface defects can significantly shorten coherence times, demanding meticulous materials selection and interface engineering.

- **Spin qubits(Burkard et al., 2023)** in semiconductors require ultra-pure crystals with controlled dopants, often at the single-atom level. Fabricating such systems necessitates advances in crystal growth, defect control, and atomic-scale lithography.

- **Topological qubits(Lee et al., 2019)**, an emerging approach to reduce environmental sensitivity, depend on exotic materials such as topological insulators or superconductors hosting Majorana modes, again underscoring the interplay of materials innovation with quantum performance.

In summary, materials science is not a peripheral concern but a core discipline driving quantum computing's evolution from laboratory prototypes to scalable systems.

4. Two-Dimensional (2D) Materials and Quantum Computing

Among the vast landscape of materials being explored for quantum technologies, two-dimensional (2D) materials have emerged as especially promising due to their atomic thickness, tunable properties, and ability to form heterostructures with engineered quantum behavior. 2D materials, e.g., graphene, transition metal dichalcogenides, hexagonal boron nitride (hBN), etc consist of layers just one or a few atoms thick with strong in-plane bonds and weak van-der-Waals interactions between layers. The potential relevance of 2D materials to quantum computing arises from several intrinsic characteristics:

1. **Long coherence and low-defect interfaces**

   Atomically thin 2D materials naturally eliminate bulk defects and dangling bonds, leading to exceptionally clean interfaces. A prominent example is hexagonal boron nitride (hBN) used as an encapsulating dielectric for graphene and semiconductor qubits. hBN has been shown to suppress charge noise and substrate-induced disorder, resulting in improved carrier mobility and longer coherence times in spin and superconducting qubit

architectures. In superconducting resonators, hBN-based interfaces exhibit reduced two-level-system (TLS) losses compared to amorphous oxides(Dean et al., 2010; Tran et al., 2016).

2. Tunable electronic and spin properties

2D materials offer unparalleled tunability through electrostatic gating, strain engineering, and compositional control. Transition metal dichalcogenides (TMDCs) such as MoS_2 and WSe_2 exhibit strong spin-orbit coupling and valley polarization, enabling electrical control of spin and valley degrees of freedom, key resources for qubit encoding and manipulation. Strain has been experimentally used to modify band gaps and spin splitting, directly affecting qubit addressability(Xu et al., 2014).

3. Van der Waals heterostructures and integration

Stacking dissimilar 2D layers enables atomically precise heterostructures without lattice-matching constraints. Graphene/hBN/TMDC stacks have been used to integrate conducting channels, tunnel barriers, and spin–orbit layers in a single device, forming custom quantum architectures with reduced interfacial disorder (Islam et al., 2025; Wang et al., 2015).

4. Quantum dots and spin qubits

Gate-defined quantum dots have been experimentally realized in graphene and MoS_2, enabling confinement of single electrons with electrically tunable energy levels. These systems are attractive for scalable spin qubits due to compatibility with planar device fabrication and reduced hyperfine interactions (Burkard et al., 2023; Eich et al., 2018; Xu et al., 2014).

5. Photonic quantum elements

Defect centers in hBN and WSe_2 act as stable single-photon emitters at room and cryogenic temperatures, making them promising for quantum communication and on-chip photonic interconnects(Tran et al., 2016).

One recent review reports that 2D heterostructures such as graphene combined with TMDC layers can achieve increased qubit fidelity, longer coherence, and scalable integration, addressing some core obstacles in quantum hardware(Islam et al., 2025).

4.3 Challenges and Outlook

However, the integration of 2D materials into a complete quantum system is still an issue. This is due to the reproducible synthesis of high-quality monolayers, the uncontrolled defects

that can cause noise, and the integration of 2D materials with other materials and control electronics. Further advancements in chemical vapor deposition and other growth methods, as well as sophisticated interface engineering, will be essential in unlocking the full potential of 2D materials in commercial quantum computing systems.

5. Conclusion

Quantum computing is a paradigm shift in computing power, which has the potential to transform various areas of research, including chemistry, optimization problems, and cryptography. However, the unlocking of this potential is contingent on advances in materials science. The development of qubits with long coherence times, low error rates, and scalable architectures requires advances in advanced materials research. Two-dimensional materials are atomically thin, tunable, and uniquely quantum. They provide a promising route to overcoming the most significant challenges in quantum hardware and unlocking the transition from quantum concepts to practical quantum use.

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