



Advances and opportunities in materials science for scalable quantum computing

Vincenzo Lordi*¹ and John M. Nichol, Guest Editors

By harnessing unique quantum mechanical phenomena, such as superposition and entanglement, quantum computers offer the possibility to drastically outperform classical computers for certain classes of problems. The realization of this potential, however, presents a substantial challenge, because noise and imperfections associated with the materials used to fabricate devices can obscure the delicate quantum mechanical effects that enable quantum computing. Hence, progress in synthesis, characterization, and modeling of materials for quantum computing have driven many exciting advances in recent years and will become increasingly important in the years to come. As progressively more complex, multi-qubit systems come online, and as significant government and industrial investment drives research forward, new challenges and opportunities for materials science continue to emerge. The articles in this issue survey the current state of materials science progress and obstacles for some leading quantum computing platforms; opportunities for deeper involvement by materials scientists abound. Ultimate realization of the full potential of quantum computers will require a multidisciplinary effort spanning many traditional areas of expertise.

Introduction

Since initial proposals by Feynman¹ and others^{2,3} more than 40 years ago, the field of quantum information processing has experienced intense and sustained research, because of the potentially revolutionary technological applications. The ultimate goal of quantum computing research is to create a universal and fault-tolerant quantum computer. Such a device is predicted to enable an exponential speedup for certain types of calculations, such as integer factorization and quantum simulation, as compared to classical computers. In general, this goal has not yet been reached, but the global quantum information processing community has made great strides toward achieving this objective in the past decade. In recent years, larger scale but imperfect devices have come online, and they enable specific calculations, which are difficult, if not impossible, to perform on classical machines in practical time.⁴ This availability has opened up a wide variety of new opportunities and challenges.

Many physical embodiments can be used to implement a quantum bit, or qubit, the two-level quantum system that is the basic unit of a quantum computer (see [sidebar](#)). For example, trapped-ion qubits may make use of different hyperfine levels

in individual ions.⁵ Superconducting qubits make use of different ways that charge can flow in superconducting circuits.⁶ Other leading platforms include semiconductor quantum dot and dopant-based spin qubits,⁷ defects or color centers in semiconductors,⁸ neutral-atom qubits,⁹ qubits based on nuclear magnetic resonance,¹⁰ photonic qubits,¹¹ and possibly qubits based on topological states of matter.¹² Topological qubits, unlike the other qubit technologies, have not yet been conclusively demonstrated in the laboratory; however, they may offer significant long-term scaling advantages compared with conventional qubits. To this end, initial laboratory demonstrations and the development of topological qubits will greatly depend on materials advances, some of which are highlighted in the article by Scappucci et al. in this issue.¹³ Paradigms also have been proposed for distributed quantum computation using combinations of the approaches previously listed, with the quantum states transported between media, for example, by coupling superconducting qubits with color centers.^{14–17} Such a distributed quantum computing architecture may be an intermediate step to fully scaled systems, leveraging technology developments in quantum networking for storage and distribution of quantum information.

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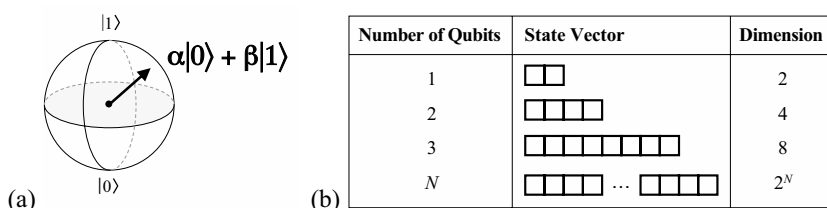
Sidebar: Quantum Information Processing and Quantum Advantage

The fundamental principles of quantum information processing and quantum computing are based on operations of few-level quantum systems, the most common of which is the quantum bit, or *qubit*. Qubits are the quantum analog of classical bits, which encode the 0s and 1s of binary digital information. The power of quantum information arises from the principles of *superposition* and *entanglement*. A qubit in a superposition state can exist in a coherent combination of both $|0\rangle$ and $|1\rangle$ simultaneously, where the $|\bullet\rangle$ notation signifies a quantum basis state corresponding to the 0 and 1 classical values. Further details of the basic principles of quantum computation can be found in Reference S1.

Figure (a) below depicts a representation of possible qubit states using a Bloch sphere. Multiple qubits, when entangled with each other, exhibit correlations that have no classical analog. The combination of superposition and entanglement leads to a collection of N qubits encoding information in a Hilbert space of dimension 2^N . The power of quantum computation derives from this exponential growth of encoded information with the number of qubits. Conversely, the challenges of harnessing this computational power are associated with initialization, manipulation, and readout of the quantum states^{S2}, which have finite lifetimes (quantum coherence) due to interactions with their environment that cause *decoherence*. The ability to perform useful quantum computations, particularly in large-scale systems, hinges on being able to protect the fragile quantum states during the sequence of operations that implement a quantum algorithm. Materials science advances largely aim to increase quantum coherence times by eliminating sources of decoherence associated with materials and fabrication.

S1. M.A. Nielsen, I. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, New York, 2000)

S2. D.P. DiVincenzo, *Fortschr. Phys.* **9**, 771 (2000).



(a) Qubits are often represented using a Bloch sphere representation, where points on the surface of the sphere, pointed by the arrow, represent the possible quantum states formed by complex superposition of the $|0\rangle$ and $|1\rangle$ basis states at the poles; α and β are complex numbers. (b) Entanglement of multiple qubits creates a quantum Hilbert space of 2^N dimensions, which encodes exponentially more information with each added qubit.

Progress, challenges, and scalability

Historically, the primary challenge confronting the architects and builders of quantum computers has been how to preserve the delicate and inherently quantum mechanical properties of qubits, such as superposition and entangled states, against the effects of environmental noise that inevitably perturb real-world quantum systems. This challenge has been previously discussed in detail,¹⁸ and it recurs in this issue. Often, these deleterious fluctuations originate from the materials themselves, which host the qubits. On the one hand, the clever quantum mechanic can sometimes mitigate these noise

sources either by clever qubit design or other engineering workarounds. On the other hand, a deeper understanding of these challenges and their potential solutions from a materials science perspective could propel quantum computing research definitively past these obstacles. (See also the October 2013 issue of *MRS Bulletin*.¹⁹) Although this issue focuses on quantum computing, quantum information processing also has other important real-world applications, including secure quantum networks with communication channels resistant to eavesdropping and quantum sensors that leverage the exquisite sensitivity of quantum systems. It is certain that a materials science perspective would benefit these areas too.

In the past few years, new opportunities and challenges in quantum computing have emerged. The demonstration of a 53-qubit quantum processor by Google⁴ heralded the start of the era of “noisy intermediate-scale quantum” (NISQ)²⁰ computing and a race toward scaling up systems to many qubits. Such devices can now begin to carry out calculations that are difficult or impossible to complete on even the most advanced classical supercomputers. Such NISQ devices, however, are not

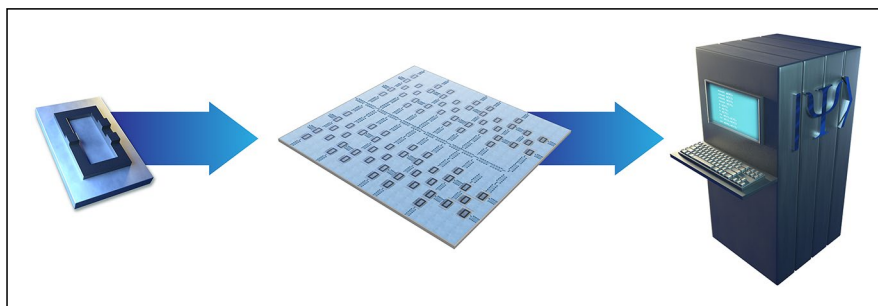
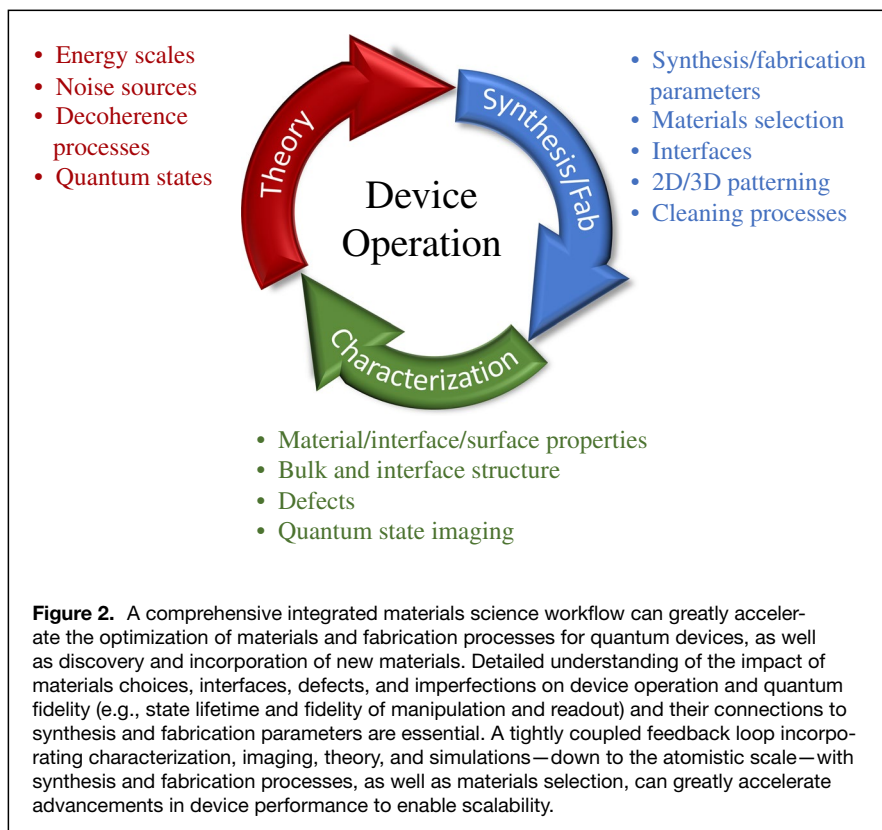


Figure 1. Materials science and engineering advances that drive ever-improved single qubit performance (left) are being leveraged to build modestly scaled noisy intermediate-scale quantum systems with 10 s to 100 s of qubits (middle), which begin to allow researchers to explore computational or simulation regimes with quantum advantage. Lessons learned from these small multi-qubit systems will help drive materials science research into the future to one day enable general purpose quantum computers (right), which likely will require a multitude of qubits to implement quantum error correction and perform useful computations.



error corrected and, while they may incorporate more qubits than can be simulated practically with classical computers, are a far cry from a universal quantum computer. For example, the device previously mentioned performs a specific computation that is difficult for a classical computer but that does not have a direct real-world application. It is thought that NISQ devices can enable advances in several specific areas, including applications related to optimization or even solving quantum chemistry problems. In addition, NISQ devices will allow hands-on exploration of materials issues in real quantum systems, which is expected to translate into enabling knowledge for development of larger scale quantum computing devices approaching general purpose. Besides quantum computers, quantum annealers (e.g., the D-Wave device) and simulators based on many-qubit systems also have emerged in recent years, providing complementary insights into new challenges of large-scale quantum systems, including challenges related to materials science.

Although the realization of a universal, fault-tolerant quantum computer seems a distant goal, NISQ technologies offer an essential opportunity for practical experimentation with powerful quantum devices in the near-term. While in principle, scientists today understand exactly how a quantum computer should function, just as scientists in the mid-twentieth century understood in principle how digital computers should operate, it seems likely that many more surprises lurk around the corner. Thus, NISQ technology is a critical milestone along the path to a universal quantum computer. In fact, this stepping

stone will provide much needed working experience toward building a full-scale quantum computer (**Figure 1**).

The fabrication and operation of these NISQ devices represent a substantial challenge, for many reasons. From a materials science perspective, the most important challenges center around how to fabricate many-qubit systems that simultaneously preserve the excellent properties demonstrated for single qubits (e.g., long quantum coherence times), but also enable high-fidelity interactions (quantum entanglement) between the qubits, required to execute complex quantum algorithms. Thus, although the materials science considerations relating to single- or few-qubit devices remain outstanding questions of importance, the creation of NISQ devices has uncovered a set of new problems to address. These problems are multidisciplinary and complex, rooted not only in the fundamental quantum interactions, but also intimately connected to the materials and fabrication

processes used to realize devices and systems. Thus, a dedicated, systematic, and comprehensive contribution from materials scientists—spanning synthesis, fabrication, characterization, theory, and modeling, as highlighted in **Figure 2**—will play an essential role in driving future advancements in both single-/few-qubit systems and the path to scale-up.

Expanded funding environment

Concomitant with today's technological crossroads of quantum technologies transitioning to NISQ and scaled-up functional systems is an influx of broad interest and funding for quantum research, across both public and private sectors. Major investments have been announced by governments around the world and private industry, including both large and start-up companies as well as significant venture capital. For example, the United States enacted the National Quantum Initiative Act (NQIA) in 2018 to accelerate quantum research and development across agencies, including the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and the US Department of Energy (DOE), with a goal to strengthen quantum information science (QIS) programs, centers, and consortia.²¹ Collaborations between industrial researchers and the academic community are becoming commonplace, particularly in areas of basic science research such as those related to fundamental materials issues. These emerging public-private partnerships are consistent with a recognized need to establish an educational

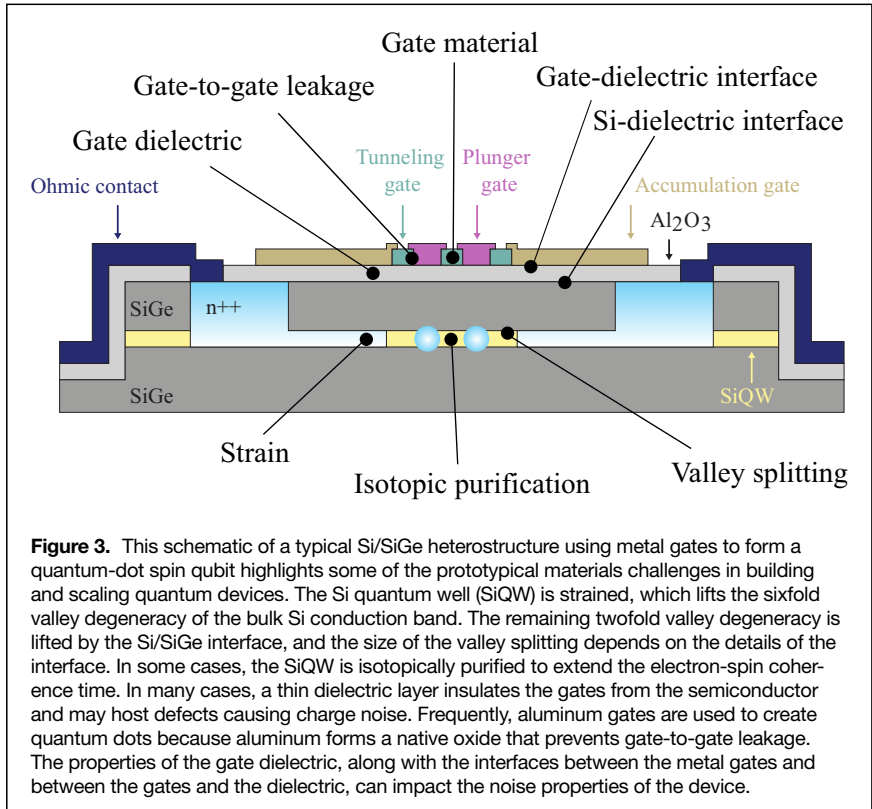


Figure 3. This schematic of a typical Si/SiGe heterostructure using metal gates to form a quantum-dot spin qubit highlights some of the prototypical materials challenges in building and scaling quantum devices. The Si quantum well (SiQW) is strained, which lifts the sixfold valley degeneracy of the bulk Si conduction band. The remaining twofold valley degeneracy is lifted by the Si/SiGe interface, and the size of the valley splitting depends on the details of the interface. In some cases, the SiQW is isotopically purified to extend the electron-spin coherence time. In many cases, a thin dielectric layer insulates the gates from the semiconductor and may host defects causing charge noise. Frequently, aluminum gates are used to create quantum dots because aluminum forms a native oxide that prevents gate-to-gate leakage. The properties of the gate dielectric, along with the interfaces between the metal gates and between the gates and the dielectric, can impact the noise properties of the device.

Materials science opportunities

To illustrate some of the materials science challenges associated with quantum computing,¹⁸ consider electron-spin qubits in silicon quantum dots, as an example (Figure 3). Silicon quantum-dot spin qubits possess extremely long coherence times,²⁵ enabling high-fidelity single- and two-qubit gates²⁶ and the implementation of quantum algorithms.²⁷ Because they are fabricated using common materials such as semiconductors, quantum-dot spin qubits are also potentially scalable, although specialized processing is required compared to traditional silicon fabrication. As with any quantum computing platform, multiple materials science challenges exist and limit the performance and scaling properties of silicon qubits. For example, the conduction band minima in Si quantum dots typically occur at multiple equivalent valleys, and the required splitting of this degeneracy,

or “valley splitting,” to enable the states to be used as qubits depends strongly on details of the interfaces in the device and can complicate the operation of Si spin qubits.²⁸ Silicon quantum wells are often grown under tensile strain, complicating large-scale fabrication,²⁸ and the best quantum wells are grown with isotopically purified sources to minimize magnetic noise resulting from residual nuclear spins.²⁹ Above the semiconductor itself, electrostatic potentials applied to multiple layers of overlapping gates confine the electrons. The choice and thickness of gate dielectric,³⁰ gate metal,^{31,32} and inter-gate insulation layer,³³ as well as the different interfaces in the device,^{34,35} are all critical aspects of the device design that can impact its performance. Analogous issues associated with materials choices, interfaces, defects, and fabrication processes affect all types of qubit technologies.

pipeline for a quantum workforce.²² Several recent government initiatives, such as by the NSF, include an explicit objective of education and workforce development, beginning as early as middle and high school. Academic researchers will continue to play an important role in scientific innovation to feed a quantum industrial sector, which will become more focused on building large systems geared toward revenue generation. Recent notable government investments in the US under the NQIA have included establishing three NSF Quantum Leap Challenge Institutes and five DOE QIS Research Centers, allocating \$75 million and \$625 million, respectively, over 5 years, with additional centers expected in the future.^{23,24} Corresponding initiatives have been announced in the United Kingdom, the European Union, Australia, and China. Major corporate investments in quantum computing include IBM, Google, Intel, Microsoft, Honeywell, Hitachi, Infineon, and Raytheon/BBN, although at least 100 start-up companies also are contributing, including major players such as Rigetti, IonQ, Xanadu, and PsiQuantum. Many of the corporate players are focused on superconducting quantum technologies, but major bets also include trapped-ion, silicon-based, topological, optical, and defect-center approaches; some companies are pursuing multiple technologies in parallel. The variety of companies and technologies being pursued highlights both the significant challenges and also the great perceived opportunities in this blossoming field.

The articles in this issue summarize the state of the art in materials advances for quantum computing devices, across a broad spectrum of qubit technologies and spanning issues of synthesis, fabrication, characterization, and theory, with an emphasis on current knowledge and opportunities for major materials science advances to push the field forward. The topics are not comprehensive and purposely omit important subjects that have been the focus of recent review articles, to which the reader is referred. In particular, materials issues for trapped-ion quantum information processors are reviewed in Brown et al.³⁶ In addition, so-called “two-level system”

sources of noise and decoherence associated with amorphous materials, particularly in superconducting circuit devices, are reviewed in Müller et al.,³⁷ these defects also are responsible for important effects in silicon-based devices, ion traps, and possibly other technologies. The fabrication, design, characterization, and operation of donor spins in silicon are reviewed in Morello et al.³⁸ Optical quantum computing technologies are not covered in this issue, since major materials science challenges and advances are still emerging in that field.

In this issue, the article by Scappucci et al.¹³ surveys the current state of semiconductor heterostructure growth for quantum-dot spin qubits, as well as the growth of topological insulator thin films and topological crystalline insulators. Advances in the fabrication of crystalline semiconductors have long spurred the development of quantum systems. Although semiconductor growth is generally a mature technology, the production of new single-crystal substrates, as well as the fabrication of novel low-dimensional and more exotic materials, for quantum technologies continues to push this technique in new directions, uncovering a host of new challenges and opportunities.

The article by Bussmann et al.³⁹ describes advanced fabrication techniques termed atomic-precision advanced manufacturing (APAM), which enable fabrication of single-spin quantum devices by placing individual dopant atoms in three-dimensions, using either scanning tunneling microscope-enabled “desorption” lithography or precise ion implantation approaches. Currently, the techniques are used mostly for small-scale prototyping, but opportunities toward scalable manufacturing are identified.

The article by Voisin et al.⁴⁰ describes how such atom-scale quantum devices can be characterized, through a combination of electrical transport measurements, scanning tunneling microscopy, and simulations. Although the phosphorous donor in silicon—the most common single-atom spin qubit—has been the focus of research through many years in the context of classical electronics, new insights into its quantum mechanical nature are being uncovered by these advanced characterization methods. As systems of single-atom spin qubits are poised to begin scaling up, characterization methods such as those described by Voisin et al. will be essential to understand the complexities of multi-qubit systems.

The article by Rodgers et al.⁴¹ focuses on nitrogen–vacancy (NV) centers in diamond. The NV center is a leading candidate for quantum sensing, owing to its small size and proximity to surfaces; quantum communication, because it couples to optical photons; and also quantum computation, because of its long coherence time and potential to interact with other spins in the diamond substrate. Rodgers et al. describe the key metrics, progress, and challenges for each of these applications of NV centers. Underlying grand challenges include understanding and controlling the effects of surfaces on NV center metrics and the creation of NV centers in diamond with subnanometer precision. The sensing aspect of NV centers may also play a role as a future materials science probe.

The article by Gyure et al.⁴² summarizes how theoretical understanding has helped inform the design of highly successful silicon-based electrostatic quantum-dot qubits. In particular, the authors not only focus on fundamental materials issues associated with silicon and silicon–germanium alloys that make them superior host materials compared to earlier III–V materials, but also describe the challenges that created delays in adoption of these materials compared to the previous technology. Theoretical exploration of relevant properties, including carrier transport, band structure, quantum state engineering, and coupling processes that cause decoherence, in silicon and silicon–germanium quantum-dot qubits is specifically highlighted in the context of designing and fabricating highly controlled and performant devices.

Perspectives and outlook

Materials science opportunities exist both for optimizing current materials and fabrication processes, as well as leapfrogging present technology by discovering and designing new materials systems for the fabrication of quantum information devices, along with developing novel fabrication processes that are uniquely precise and scalable. These parallel opportunities mirror the concept that the NISQ era has uncovered new and unique challenges associated with multi-qubit systems and scale-up, while existing challenges and approaches remain for improving single- and few-qubit systems in the short term. Clearly, detailed understanding down to the atomic scale—as afforded by coordinated efforts in synthesis, characterization, and theory/simulation—will enable this path. The articles in this issue elucidate various examples of this paradigm across qubit technologies.

For example, as previously mentioned, the most common single-atom qubit consists of a phosphorous donor in silicon, which has been studied in great detail over the past decades. This research has led to significant advances for electronic devices, but significant additional work is required across synthesis, characterization, and modeling to achieve the precision needed to create reliable multi-qubit devices at-scale. In addition, novel dopants, including acceptors, optically active dopants, and dopants with high-spin nuclei, may be explored to enable new types of functionality, such as all-electrical control and optical readout of spin qubit arrays, which may prove especially beneficial for many-qubit systems.

This theme also occurs in the article of Rodgers et al.⁴¹ The capabilities of NV centers have improved dramatically in the past years, but key obstacles remain. Understanding the surfaces and interfaces involved in NV center systems will be essential for their continued improvement. In addition, reliable fabrication to create multi-qubit devices is another significant challenge. At the same time, exploring new types of defects, such as the silicon–vacancy center, may enable new capabilities, such as high optical cooperativity, which is a potential game changer for modular or networked quantum systems.

Similar examples exist for all qubit technology platforms. Indeed, we expect that creative ideas will uncover new ways

to encode quantum information in materials and devices for emerging and as-yet undiscovered qubit modalities. Topological qubits comprise one example of such novel modalities that not only expose a new set of materials challenges, but also impart novel use of materials for quantum information storage and manipulation. Intensified application of the tools and techniques of materials science will be essential for major advancements in these areas. In fact, quantum information devices themselves may play an essential role in enabling the exquisite materials characterization needed, since their extreme sensitivity to their environment makes them excellent probes of test materials as well. We already see examples of this with NV centers used to probe test surfaces and electromagnetic environments, as mentioned in the article by Rodgers et al.,⁴¹ and also recent work using trapped ions as surface science probes.^{43,44}

Going forward, we expect increased collaboration among diverse specialists, including within various sub-fields of material science and other fields, to play an essential role in advancing QIS devices in the race to scale-up. Advancements in high-throughput fabrication, testing, characterization, and simulation will improve understanding of tolerances and intrinsic materials limitations for scale-up.¹⁸ Equally important may be sharing of data and samples among laboratories, not only to access complementary capabilities, but also to cross-validate, corroborate, and collate a broad range of data.

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Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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