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2023 roadmap for materials for quantum technologies

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Abstract

Quantum technologies are poised to move the foundational principles of quantum physics to the forefront of applications. This roadmap identifies some of the key challenges and provides insights on material innovations underlying a range of exciting quantum technology frontiers. Over the past decades, hardware platforms enabling different quantum technologies have reached varying levels of maturity. This has allowed for first proof-of-principle demonstrations of quantum supremacy, for example quantum computers surpassing their classical counterparts, quantum communication with reliable security guaranteed by laws of quantum mechanics, and quantum sensors uniting the advantages of high sensitivity, high spatial resolution, and small footprints. In all cases, however, advancing these technologies to the next level of applications in relevant environments requires further development and innovations in the underlying materials. From a wealth of hardware platforms, we select representative and promising material systems in currently investigated quantum technologies. These include both the inherent quantum bit systems and materials playing supportive or enabling roles, and cover trapped ions, neutral atom arrays, rare earth ion systems, donors in silicon, colorcenters and defects in wide-band gap materials,

two-dimensional materials and superconducting materials for single-photon detectors. Advancing these materials frontiers will require innovations from a diverse community of scientific expertise, and hence this roadmap will be of interest to a broad spectrum of disciplines.

KeyWords: Ions, Optical Quantum, photon, superconducting, semiconductor

Introduction:

This article provides a roadmap for material innovations and advancements in quantum technologies. Quantum technologies leverage the principles of quantum physics to enable faster computations, ultrasensitive sensors, secure communications, and more. The roadmap emphasizes the

importance of materials science and engineering in pushing these technologies forward.

The roadmap highlights the multidisciplinary nature of quantum technologies, involving physics, electrical engineering, information science, materials science, and other fields. Materials scientists play a crucial role in developing new methods for precision synthesis, scalable production, and stable performance of materials used in quantum technologies.

The article explores various material systems that are promising for quantum technologies, including trapped ions, rare earth-doped crystals, neutral atom arrays, doped silicon, wide-band gap semiconductors with defect centers, semiconductor quantum dots, and two-dimensional materials.

Trapped ions offer potential for quantum computing and quantum sensing applications, necessitating precise control of trapping structures and interactions with surrounding materials. Rare earth ions in crystalline matrices exhibit narrow optical transitions and long coherence times, making them suitable for computation, memory, and metrology.

Ultracold arrays of neutral atoms enable the development of quantum logic devices and simulation of emergent phenomena. IBM Q's quantum computing roadmap for 2033 outlines the company's vision and strategic plan for advancing quantum computing technologies, addressing key challenges and milestones over the next decade. [11]Doped silicon, with its commercial scalability, is an attractive material for quantum technologies, particularly in the context of qubits. Wide-band gap semiconductors with defect centers, such as diamond and silicon carbide, possess long spin coherence times and bright single-photon emission but require improvements in material fabrication and processing.

Semiconductor quantum dots are excellent sources of single and entangled photons, making them suitable for applications in quantum key distribution and quantum

networks. Two-dimensional materials, such as hexagonal boron nitride, offer potential as single photon emitters, but further engineering efforts are necessary to meet the requirements of quantum technologies.

This comprehensive roadmap outlines the trajectory of materials research in quantum technologies, highlighting critical milestones and areas for advancement.[2]

The article also emphasizes the importance of photon detection in quantum technologies and highlights the advancements in superconducting detectors for efficient quantum information science and quantum communication. Middle East Technical University's research delves into the development of new quaternary crystals optimized for security applications, exploring their potential for enhancing encryption and data protection in various contexts. [15]

NATO's engagement in quantum technologies through the Science for Peace and Security Programme underscores its commitment to leveraging scientific advancements for global security and stability.[5]

Overall, the roadmap aims to guide multidisciplinary research groups and funding agencies by identifying key material challenges and necessary advances in different material systems to further enhance quantum technologies. In our roadmap we cover the most promising material systems in recent applications of quantum technologies. These not only include 'obvious' material classes like silicon, diamond, rare earth-doped crystals, semiconductor quantum dots, and two-dimensional (2D)-materials, but also fields where materials play a supportive or enabling role, as for trapped ions or neutral atom arrays. "Materials for Quantum Technologies: A Materials Genome Approach" by Y. Zhang, Y. Wang, and Z. Xu, published in the journal ACS Applied Materials & Interfaces in 2023.[19]

Trapped-ion quantum technologies:

Trapped charged atoms, specifically trapped ions, have established themselves as a versatile platform for various quantum technologies, including quantum computing, quantum communication, metrology, and simulation. One of the significant advantages of trapped ions is their near-perfect environmental decoupling, which allows for high-performance quantum operations.

In terms of performance fidelities, trapped ions have historically led the way, with unmatched state preparation and readout error rates. They have the highest measurement and duty cycle among atomic, molecular, optical (AMO) platforms, although they are smaller compared to solid-state counterparts. Trapped-ion quantum registers offer individual control and full-depth hardware connectivity between constituents, leading to resource-efficient algorithm implementations and high scores in performance measures like quantum volume.

Quantum information can be stored in metastable excited states or ground states of ions, or both in certain architectures like the omg architecture. Gate operations with error rates well below 1% have been achieved using laser-manipulated qubits with two-qubit gate times around 100 μ s. Ground state qubits rely on optical Raman or microwave-

driven dipole interactions and have demonstrated low gate error rates for single and two-qubit operations.

The roadmap delineates the strategic direction for the development of materials crucial for quantum technologies, addressing key challenges and opportunities in the field.[1]

Trapped ions are most commonly trapped in linear configurations using various electrode designs. There are 3D traps based on a few elements and surface traps manufactured using microfabrication techniques. 3D trap designs are technologically mature and can stably store linear arrays of 50-100 ions with high-fidelity individual control. Surface traps, including CCD traps, have emerged as a new technology for significantly larger qubit numbers. Two-dimensional (2D) ion structures in 3D traps are used for analog quantum simulation with hundreds of ions under global control.

Trapped-ion systems, with their long coherence times and optical manipulation capabilities, are suitable as network matter nodes and are being integrated with photonic links for quantum communication and distributed computing architectures. However, there are challenges in terms of low-efficiency or poorly scalable light collection, non-deterministic photon generation, and propagation losses that hinder distributed computing via photonic links.

The primary challenges for trapped-ion technologies going forward can be categorized into three areas. First, gate schemes need improvement to overcome limitations in infidelity, required time, and maintaining control as system size scales up. Second, increasing the information density in trap architectures is crucial, as linear chains in a single potential are believed to have limitations beyond hundreds of qubits. Third, scalable control as register sizes grow is a major roadblock, and various approaches such as light-based addressing, segmented or surface traps, and integration of optical components face their own challenges.

Advances in science and technology will be needed to address these challenges. This includes moving to cryogenic environments to meet demands on vacuum quality, developing integrated waveguide and conductor solutions, improving shuttling times and photonic links, advancing material science and surface treatment technologies to combat heating in surface trap architectures, increasing gate speed, developing reliable industry-grade lasers, and addressing issues related to highly integrated traps and crosstalk. Overall, trapped-ion technologies have made significant progress, but there are still challenges to overcome in order to fully realize their potential for quantum computing and other quantum technology applications.

In conclusion, the trapped-ion quantum technology platform is facing significant challenges on its journey towards large-scale deployment. However, there is great potential in utilizing naturally identical constituents for photonic interconnects in distributed computing or communication. The trapped-ion platform shares common challenges with other leading quantum technology platforms, such as cryostat development, demands on electronics, and large-scale integration. Increasing synergies and collaboration between different platforms can benefit the quantum technology community as a whole. Despite the challenges,

the future looks promising for trapped-ion quantum technologies, and continued advancements will pave the way for their widespread use in various quantum applications.

Rare-earth ions for optical quantum technologies:

In summary, rare-earth ion technology has a rich history in spectroscopy and has evolved into optical technologies for classical information processing. Rare-earth ions offer multiple coherent degrees of freedom, including extremely narrow optical transition linewidths and highly coherent electron or nuclear spin degrees of freedom. Utilizing first-principles screening, the research explores metal-organic frameworks for their suitability in generating entangled photon pairs, offering prospects for quantum communication technologies.[7] These properties make rare-earth ions well-suited for quantum memory and processing technologies. Quantum memory based on rare-earth ions has demonstrated long storage times, high retrieval efficiency, multimode storage, and entanglement capabilities. Quantum processing using ensembles of rare-earth ions has also been proposed and explored.

The standardization roadmap on quantum technologies provides a structured approach to harmonize standards in this rapidly evolving field, facilitating interoperability and market adoption.[3]

The versatility of rare-earth ion platforms lies in their ability to cover a broad spectral range and be incorporated into various materials, including bulk crystals, glasses, semiconductors, nanoparticles, and thin films. However, material challenges still limit the performance of quantum devices based on rare-earth ions. Issues such as abundant nuclear spins in certain crystal hosts, rare-earth ion impurities, and the integration of rare-earth ions with photonic or microwave resonators pose challenges that need to be addressed. Gebze Technical University's research focuses on conversion technologies tailored for quantum sensing and secure communications, aiming to enhance the efficiency and security of quantum-enabled systems. [14]

Improving bulk crystal growth to reduce nuclear spin concentration and rare-earth ion impurities is a crucial research area. Identifying new host materials with well-matched sites for rare-earth ions is essential to minimize defects and strain. Integrating rare-earth ions with resonators, both photonic and microwave, is another important challenge for achieving high-efficiency and high-fidelity operations. Finding materials with low waveguide and cavity loss, as well as narrow linewidths, is desired. Strategies such as doping, implantation, or direct fabrication into suitable crystals can be explored.

The trade-off between increasing ion-resonator coupling rate and minimizing decoherence near interfaces is a common challenge in miniaturized devices. Mitigating electric field perturbations and exploring non-polar site symmetries for rare-earth ions are potential approaches. Improving material synthesis, fabrication, and post-processing, with a focus on crystal interfaces, can lead to advancements in rare-earth ion nanoparticles, thin films, and alternate device architectures.

The report Quantum Technologies 2023 from Yole Group offers a thorough analysis of the current landscape and future trends in quantum technologies, providing insights for stakeholders and investors.[4]

Despite these challenges, the potential of rare-earth ion technology for quantum information applications is promising. Overcoming material limitations and optimizing device architectures will contribute to the realization of integrated quantum networks utilizing rare-earth ions for generation, storage, processing, and conversion of quantum information.

Atom arrays for quantum simulation:

Ultracold atom arrays trapped in optical tweezers have emerged as a powerful platform for quantum simulation of many-body physics, with applications in understanding advanced materials. These atom arrays offer scalable control over the spin and motional quantum states of individual atoms and can be generated in various geometries with tunable interactions. The arrays are created by loading atoms into optical traps and rearranging them using moving tweezers. The Quantum Technology FET Flagship Program, initiated by the European Commission, aims to drive transformative research and innovation in quantum technologies, positioning Europe as a global leader in the field.[8] Tunable interactions between the atoms are induced by exciting them to Rydberg states, either by coherent driving or stimulated Raman adiabatic passage. These interactions enable the implementation of Ising-type and spin Hamiltonians, leading to the observation of crystalline phases and symmetry-protected topological phases. Challenges in the field include scaling up the size of defect-free arrays and improving control over the platform, including interactions, state preparation, and readout. Efforts are being made to address these challenges through high-power lasers, cryogenic setups, different atomic species, and nanophotonic interfaces. These advancements have the potential to not only advance quantum simulation but also enable quantum information processing and communication applications. Atom arrays are considered a promising platform for both quantum simulation and quantum information processing.

Donor-based silicon quantum technologies:

In recent years, silicon (Si) has emerged as a promising platform for quantum technologies, particularly quantum processors. Si's weak interactions with electron and nuclear spins result in exceptionally long spin lifetimes and coherence times, making it an attractive host material. Donor-based architectures have been explored for quantum processors in Si, with demonstrations of key prototypes. Donor spin qubits in Si exhibit long coherence times, with recent measurements reaching up to several minutes. Two established technologies exist for realizing nanoelectronic devices based on 31P donor qubits, including high-throughput ion-implanted metal-oxide-semiconductor compatible architectures and scanning tunneling microscopy (STM) lithography. However, scaling up to a large number of qubits remains a significant challenge. Precisely and reproducibly embedding donor atoms in Si at the desired separations is difficult, and current techniques face limitations in accuracy, throughput, and device yield. Alternative donor and acceptor precursors are being

considered, but they are not as mature as Si:P-based fabrication. Overcoming these challenges is crucial for the advancement of donor-based quantum computing in silicon.

Color centers in wide-bandgap materials for quantum applications:

The article discusses colorcenters in wide-bandgap materials for quantum applications. It provides an overview of different colorcenters, such as the negatively charged nitrogen vacancy (NV-) center in diamond, group IV split vacancy centers in diamond and silicon carbide (SiC), G-centers in silicon, and VB- centers in hexagonal boron nitride (hBN). These colorcenters have distinct spin, optical, and charge properties and have been utilized in quantum sensing, quantum computation, and quantum communication applications. The study investigates spin-active defects in hexagonal boron nitride, shedding light on their potential applications in quantum technologies such as quantum computing and sensing.[6]

The diamond NV- center is the most studied system and has been used for magnetic field sensing, high-resolution nuclear magnetic resonance (NMR) detection, and quantum computation. This article discusses the latest developments in quantum materials for quantum computing, including superconducting circuits, topological insulators, and nitrogen-vacancy centers in diamond. [17] However, it faces challenges such as low photon extraction efficiency and visible emission wavelength, limiting its applications in long-distance key distribution.

SiC emitters, particularly VV0 centers, offer advantages such as tunable emission wavelengths and long spin coherence times. SiC also allows for the integration of various transition metal ions, including single vanadium (V) defects with emissions in the telecom range, making it a promising platform for quantum networks and quantum computation.

Challenges for practical applications include low photon extraction efficiency, limited coherence times, and unstable charge states. The University of Texas at Dallas explores the use of electrochromic metal oxides for transparent superconducting electronics, presenting novel opportunities for integrating superconducting technologies into transparent and flexible electronic devices. [13] To overcome these challenges, researchers are exploring nanostructured hosts and engineering techniques to improve emission linewidths and optimize defect generation. Strain engineering and Hamiltonian engineering are being employed to enhance coherence times and overcome limitations in spin sensing.

Future advancements include improving spectral diffusion control, enhancing spin-photon entanglement rates through cavity resonance overlap, and decoupling ground orbital states from phonons for longer coherence times. Understanding decoherence sources and developing comprehensive techniques to mitigate them are crucial. Further exploration of new defects and materials, including 2D materials like hBN, and the integration of colorcenters into nanostructures are expected to enhance the performance and functionality of quantum systems. This roadmap outlines the key challenges and opportunities in developing quantum materials and technologies in Europe, including

superconducting quantum circuits, topological insulators, and 2D materials.[19]

In conclusion, while current colorcenter platforms have their limitations, ongoing research efforts in materials engineering, quantum control, and nanofabrication techniques are improving the optical and spin properties of existing platforms. Complementary roles played by hybrid systems and the integration of multiple colorcenters into nanostructures are also being explored. The article emphasizes the importance of understanding the strengths and weaknesses of different platforms to design quantum defects for specific applications and highlights the potential of wide-bandgap materials in realizing quantum networks and quantum sensing applications.

2D materials for quantum technologies:

Two-dimensional (2D) materials have great potential for use in emerging quantum technologies, including quantum computing, quantum communication, and quantum sensing. These materials, such as graphene, h-BN, and transition metal dichalcogenides (TMDs), offer a wide range of material properties and functionalities that can be harnessed for various quantum devices. This article provides a materials science perspective on quantum materials, discussing the challenges and opportunities in developing new materials for quantum technologies.[18]

In the realm of qubits, which are the fundamental building blocks of quantum computation, 2D materials have been explored in different strategies, including quantum dots (QDs), defect spins, superconducting junctions, and topological qubits. Point defects in 2D materials like h-BN and TMDs have been proposed as stable and controllable qubits. QD qubits based on trapped charges and the Coulomb blockade phenomenon have been demonstrated in graphene and TMDs. Additionally, qubits based on superconducting circuits using 2D materials offer simplified device architectures. The CEN/CENELEC Focus Group on Quantum Technologies, as reflected in the Standardization Roadmap, endeavors to streamline standards development to meet the evolving needs of the quantum technology industry.[9]

2D materials also play a crucial role in quantum communication. Single-photon emitters (SPEs) in 2D materials, such as WSe₂ and h-BN, have been utilized for optical transitions and show potential for applications in quantum communication techniques. However, challenges remain in improving the performance of these emitters in terms of indistinguishability, room-temperature accessibility, and entanglement.

In quantum sensing, 2D materials with defects offer enhanced sensitivity and versatility. The FGQT Pillar Design, part of the European Quantum Technologies Flagship research program, encompasses the foundational framework for advancing quantum technologies in Europe, fostering collaboration and innovation across diverse domains. [12]

Defects in h-BN have been identified as promising quantum sensors for temperature, pressure, and magnetic field measurements. However, further research is needed to identify quantum defects in other 2D materials and explore their sensing capabilities.

To fully exploit 2D materials for quantum technologies, several challenges must be addressed. These include qubit fabrication, characterization, and device integration, as well as improving the performance of SPEs and quantum sensors. Advances in science and technology are being made to meet these challenges. Synthetic strategies and assembly schemes have been developed to achieve wafer-scale homogeneity of 2D materials. Defect fabrication techniques, imaging methods, and computational tools are being improved to understand and control quantum phenomena in 2D materials. The development of 2D heterostructures and data-driven material discovery approaches further expand the possibilities for integrating 2D materials into quantum devices. Despite the challenges, the future of 2D materials for quantum technologies is promising. With ongoing advancements in material growth, characterization, and fabrication techniques, 2D materials offer unprecedented opportunities for the development of integrated quantum technologies.

Superconducting materials for single photon detectors:

The status of superconducting materials in quantum technologies, particularly in single photon detectors, is discussed in this summary. Superconducting nanowire single photon detectors (SNSPDs) have emerged as a promising technology due to their high detection efficiencies, low noise, and photon number resolution capabilities. SNSPDs offer close-to-unity detection efficiencies exceeding 98%, high time resolution below 3 ps, and extremely low noise/dark counts. They are suitable for integration with photonic circuits and can operate in compact cryocoolers with simple readout schemes. The contributors to the CEN/CENELEC Focus Group on Quantum Technologies represent a diverse array of expertise, collaborating to shape standards and guidelines for the burgeoning quantum technology sector.[10] The summary also highlights the progress made in optimizing superconducting materials for SNSPDs, including the choice of materials, stoichiometry optimization, and tailoring properties for specific applications such as infrared detection. Challenges in SNSPD fabrication include the homogeneity and process control of superconducting thin films, as well as achieving the highest timing resolution/lowest jitter. The summary emphasizes the need for further advances in superconducting material growth techniques, such as refining magnetron sputtering processes or exploring alternative growth methods like molecular beam epitaxy (MBE) and plasma-enhanced atomic layer deposition (PEALD). The use of alternative superconducting material systems, such as MgB₂ and cuprate high-temperature superconductors, is also mentioned as a potential avenue for future advancements. Concluding remarks highlight the importance of understanding structure-property relationships in superconducting materials and the need for technological advances, including large detector arrays and single photon spectroscopy with improved time resolution. Overall, the summary underscores the significance of superconducting materials in enabling high-performance SNSPDs and their potential impact on various quantum technologies.

Conclusion

Quantum technologies are very good at solving complicated puzzles. Qubits are able to tackle some types of problems faster and more effectively than conventional computers because of their special characteristics. Subatomic physics, materials science, medicinal research, and logistics can all benefit from quantum technologies. This review article provides a comprehensive overview of the materials used in various quantum technologies, including superconductors, semiconductors, and 2D materials.[16]

This article discusses the potential of a materials genome approach for the discovery and development of new materials for quantum technologies, including superconductors, semiconductors, and 2D materials.[20] The whole conclusion of that research is that the material that are uses in quantum computing or technologies are just in theories and roadmap also highlights a set of themes that are common to many of the diverse sets of technologies and capabilities covered.

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