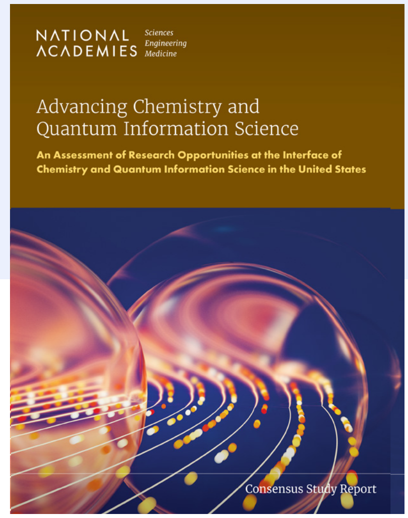
NATIONAL ACADEMIES *Sciences Engineering Medicine*

**Consensus Study Report**
**Highlights**




# Advancing Chemistry and Quantum Information Science

## An Assessment of Research Opportunities at the Interface of Chemistry and Quantum Information Science in the United States

The field of quantum information science (QIS) investigates how to use quantum behavior—essentially the most fundamental laws of physics—to encode, sense, process, and transmit information. The field has witnessed a dramatic rise in scientific research activities over the past decade as excitement has grown about its potential. QIS has already led to significant advancements in atomic clocks, atom interferometers, optical magnetometers, atomic electric field sensors, and quantum optical effects.

While the physics community has led the way in exploring quantum properties, chemistry offers new pathways to move beyond the current limits of QIS. For example, creating well-designed molecular quantum bits, or qubits, that can approach the quantum limits will open a new class of memory storage that could revolutionize computing, strengthen encryption, and enhance quantum sensing, among other applications. In turn, QIS holds the potential to enable extraordinary discoveries in chemistry that could, for example, facilitate new drug and material design and sustainable energy production.

Recognizing the possibility that QIS could lead to disruptive technologies—with the potential to create groundbreaking products and new industries—federal agencies across the U.S. government have made a coordinated effort to accelerate quantum research and development. The National Quantum Initiative Act, signed into law in 2018, emphasized the need to maintain research that stimulates transformative and fundamental scientific discoveries—an approach that puts "science first." This report, conducted at the request of the Department of Energy (DOE) and National Science Foundation (NSF) provides recommendations on how to facilitate and support research at the intersection of chemistry and QIS.

### FUNDAMENTAL RESEARCH AREAS AND PRIORITIES

To support sustained U.S. leadership in science and innovation, a robust QIS research enterprise is needed. Considering the "science first" sentiment of the National Quantum Initiative, fundamental scientific research in chemistry and its implications on future QIS applications and vice versa is needed. DOE and NSF should support fundamental research to advance the field of quantum information science using chemistry-based approaches, which include experimental and theoretical studies, prioritizing the following three areas of research: 1) design and synthesis of molecular qubit systems; 2) measurement

## BOX 1. THREE FUNDAMENTAL RESEARCH AREAS TO ADVANCE QIS

1. **Design and Synthesis of Molecular Qubit Systems**
   *Key Problem: Current Knowledge of Designing Molecular Qubits Is Limited and Will Need to Be Enhanced to Drive New Developments for QIS Applications*
   Qubits are the counterpart of the binary digit or bit of classical computing. Atomic control promises a new class of designs capable of functioning as sensors tuned for specific environments or analytes, as nodes that emit at desired frequencies for quantum optical networking, and as innovative new topologies for quantum computing. Synthetic molecular chemistry offers a unique tool kit of unparalleled control over structure, scalability, and quantum-scale interactions, and is poised to accelerate the development of bottom-up quantum technologies. This molecular approach spans every component of synthetic chemistry, from organic systems, to inorganic molecules, to extended solids comprised of molecules.

2. **Measurement and Control of Molecular Quantum Systems**
   *Key Problem: New Measurement Approaches and Techniques Are Needed for Deep Study of Chemical Systems*
   To further understanding of QIS, chemists are playing a large role in the development of novel measurements—for example, employing entangled photons to prepare entangled electron spins that can be probed using magnetic resonance measurements. Chemists are also developing novel approaches for the use of spin and spin transduction, which could be a fruitful avenue for QIS imaging and sensing applications. Utilizing both magnetic and optical approaches, chemists are advancing QIS ideas with real materials and molecules beyond the atomic systems in the gas phase used in most physics applications.

3. **Experimental and Computational Approaches for Scaling Qubit Design and Function**
   *Key Problem: Scaling up Robust Qubit Architectures Is a Major Challenge in Developing Next-Generation Quantum Systems That Requires Advances in Experiments and Classical and Quantum Computation.*
   The primary obstacle limiting the accelerated development of quantum computers and quantum algorithms is having access to robust qubit architectures capable of being scaled up and retaining their function. To address the scalability challenge, computational theorists will need to simulate electronic structures of proposed qubit designs reliably to a high degree of accuracy. This level of prediction will expedite the qubit discovery phase and provide further insight into mechanisms limiting scalability and function.

and control of molecular quantum systems; and 3) experimental and computational approaches for scaling qubit design and function (see Box 1).

### QIS Advantages for Chemistry

Even as chemistry can advance QIS, the potential for using quantum computing to solve chemistry problems is equally exciting. Currently, these types of problems are elusive and need to be identified. DOE, NSF, and other funding agencies, both public and private, should develop initiatives to support multidisciplinary research in quantum information science to address how quantum-accelerated calculations could solve chemistry problems. In connection with these initiatives, the research community should establish a set of standards for how to evaluate quantum advantage in specific chemistry use cases.

## SUPPORTING SCIENTIFIC PROGRESS THROUGH COLLABORATION, FACILITIES, AND DATA

Progress in advancing the research priorities identified in the report will require identifying the collaborations needed across chemistry, biochemistry, material science, physics, engineering, and information science; identifying needs and opportunities for infrastructure, instrumentation, and tools; and evaluating access to data.

### Collaboration Across Disciplines

In chemistry, interdisciplinary activities between researchers from various sub-disciplines have led to the development of novel solutions to chemistry challenges with applications in medicine, energy, cosmetics, agriculture, and other industries. Collaborations in QIS are also essential because the field involves diverse topics ranging from quantum mechanics to information processing. Collaborations in QIS have historically involved physicists, engineers, and computer scientists, which have ultimately led to more efficient use of resources and accelerated scientific progress. DOE and NSF should support cross-disciplinary activities that support collaborations at the interface of QIS and chemistry to expedite discoveries and development in this emerging field.

### Access to Facilities, Centers, and Instrumentation

For the United States to maintain a global competitive edge in the growing research areas at the interface between chemistry and QIS, national user facilities must remain at the cutting edge, which includes continual renewal of instrumentation. This applies not only to the major infrastructure (e.g., magnets and beamlines) but perhaps more importantly to the user end-stations (e.g., mid-scale instruments). DOE and NSF should support the development of new instrumentation and techniques for the unique needs at the interface of chemistry and quantum information science. Broader access to laboratory-scale and mid-scale instrumentation is needed for the field to progress.

### Access to Data and Database Development

Equally valuable to QIS and chemistry research are the products not only of software but of experiments—in other words, data. In the case of QIS applications, both theoretical and experimental data are invaluable not only for validating one another but for facilitating mutual method development. Because the amount of QIS-specific data is only expected to grow, the community will need to establish a well-structured database with clear guidelines in the near future. FAIR—Findability, Accessibility, Interoperability, and Reusability—standards that emphasize properly labeling and determining the reusability of data would serve as baselines to be applied wherever possible to ensure professional data management and stewardship. DOE and NSF should establish open-access, centralized databases that include quantum information science (QIS)-relevant data to enhance predictions and expedite new discoveries.

## BUILDING AND STRENGTHENING THE QIS WORKFORCE

Like any major modern scientific pursuit, the journey to new discoveries and developments is undoubtedly a powerful human experience that is often shared in a collaborative setting—hence DOE, NSF, and DOD's efforts to establish multidisciplinary research centers. To achieve broader access and inspire the next generation of quantum information scientists, chemistry education and outreach initiatives can be improved across various levels of workforce training and development by expanding to include nontraditional technical candidates across the country. DOE, NSF, and other U.S. federal agencies should support efforts to create a more diverse and inclusive chemical QIS workforce.

### QIS and Chemistry Education Development

Tasking K-12 educators with the additional expectation to create specialized curricula and concepts (e.g., quantum chemistry, quantum mechanics, and quantum algorithms) is a significant obstacle. Initiatives around the nation aimed at creating resources for educators will alleviate this extra burden and help sustain workforce development for emerging fields such as QIS. Some universities in the United States are offering a minor degree, master's degree, or certificate in quantum information science and engineering (QISE), however chemistry-related courses are limited in these degree pathways.

### Barriers to Entry into QIS and Chemistry

Building and strengthening the QIS workforce requires addressing barriers that exist to enter the field, both for students and trained chemists. As part of this effort, understanding the motivation behind "why" an individual would want to join the field will further the industry's understanding of how to reach a broader base and identify ways to encourage students to consider pursuing QIS as a viable career option. The report provides recommended actions to help lower the barriers to entry in both the classroom and industry to broaden the pool of diverse researchers and candidates in the QIS and chemistry workforce.

### Development of a Diverse, Quantum-Capable Workforce

Workforce demands for QIS in chemistry are rapidly expanding. At the same time, industrial corporations recognize that the field lacks diversity, both in the current workforce and new entrants. Because the research activities at the interface of chemistry and QIS are just beginning to blossom, a unique opportunity exists in this emerging field to create a more diverse, equitable, and inclusive workforce. The report identifies a number of actions to increase diversity that could be undertaken by various entities involved in programmatic development at colleges and universities; in job advertising; and in professional development for employees at national laboratories, academic institutions, and industry.


#### COMMITTEE ON IDENTIFYING OPPORTUNITIES AT THE INTERFACE OF CHEMISTRY AND QUANTUM INFORMATION SCIENCE

**Theodore G. Goodson, III (Chair)**, University of Michigan; **David D. Awschalom**, University of Chicago; **Ryan J. Babbush**, Google, LLC; **Lawrence W. Cheuk**, Princeton University; **Scott K. Cushing**, California Institute of Technology; **Natia L. Frank**, University of Nevada, Reno; **Danna E. Freedman**, Massachusetts Institute of Technology; **Sinéad M. Griffin**, Lawrence Berkeley National Laboratory; **Stephen O. Hill**, Florida State University; **Hongbin Liu**, Microsoft Quantum; **Marilu Perez Garcia**, Ames Laboratory; **Brenda M. Rubenstein**, Brown University; **Eric J. Schelter**, University of Pennsylvania; **Michael R. Wasielewski**, Northwestern University-Evanston; and **Damian Watkins**, Aperio Global.

#### STUDY STAFF

**Linda Nhon**, Study Director; **Andrew Bremer**, Program Officer; **Ayanna Lynch**, Research Assistant; and **Kayanna Wymbs**, Program Assistant.



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