National QIS Research Centers: Mission and Activities

ASCAC Meeting
March 29, 2022

NQISRC Directors
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C^{2}QA Co-design Center for Quantum Advantage

Q-NEXT NEXT GENERATION QUANTUM SCIENCE AND ENGINEERING

QUANTUM SCIENCE CENTER

QUANTUM SYSTEMS ACCELERATOR Catalyzing the Quantum Ecosystem

SQMS SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

NQISRC Overview

The first large-scale QIS effort that crosses the technical breadth of Office of Science.

- Effort established in 2020, under the National Quantum Initiative Act passed in 2018.
- Five Centers launched in Fall 2020, each led by a National Laboratory and representing a partnership of labs, universities, and industry.
  - ❖ Total funding: $575 million over 5 years, subject to appropriations
- The Centers take distinct yet complementary approaches to tackle major cross-cutting challenges in areas of significant national impact.
- Significant leveraging of DOE investments in user facilities and other resources.
- The Centers play a central role in stewardship of the QIS ecosystem, including broad industry engagement and support for the development of a diverse and inclusive workforce.
- Coordination across the Centers is maintained by an Executive Council.

Advanced materials for quantum technologies

Entanglement distribution networks

High-performance instruments and sensors

Full-stack quantum computation

The NQISRC research portfolio tiles the space of emerging quantum technologies.

Integrating Across the QIS Innovation Chain

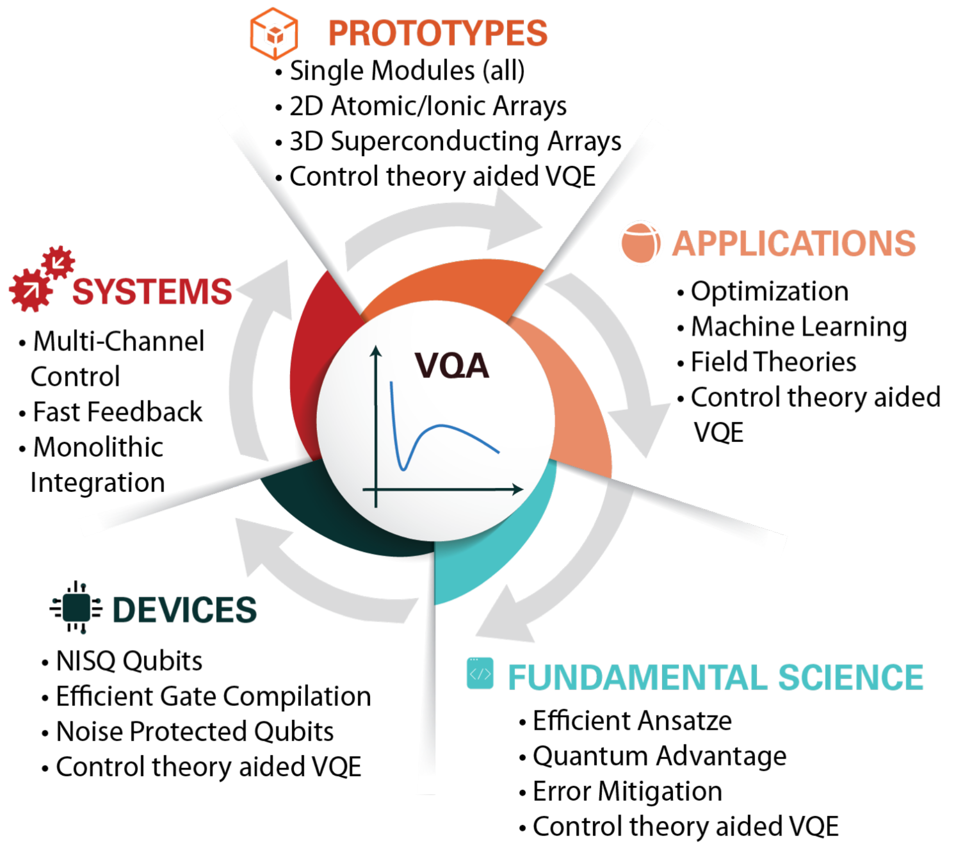
Fundamental Science is basic research that underpins discoveries and exploration to deliver long-term innovation.

Devices research applies science to build new paradigms and methods for next-gen quantum technologies.

Systems integrate solutions into practical settings that apply to US economic competitiveness and security.

Prototypes offer a first look at use-driven development with feedback to improved solution development.

Applications represent solutions of best practice that accelerate the impact of quantum technology.



Co-design cycle for variational quantum algorithms

Center-Scale Efforts to Tackle Key QIS Challenges

C²QA — Co-design Center for Quantum Advantage	Co-design Center for Quantum Advantage *Lead Lab: BNL*	C²QA aims to overcome the limitations of NISQ computer systems to achieve quantum advantage for scientific applications using superconducting microwave circuits, and hybrid superconducting/optical devices for quantum communication.
Q-NEXT	Next Generation Quantum Science and Engineering *Lead Lab: ANL*	Q-NEXT focuses on the science of controlling and distributing entangled states of matter. Its goals are to deliver quantum interconnected communications links, networks of ultra-precise sensors, novel simulation testbeds, and a national resource for pristine quantum materials.
Quantum Systems Accelerator	Quantum Systems Accelerator *Lead Lab: LBNL*	QSA pairs advanced quantum prototypes — based on neutral atoms, trapped ions, and superconducting circuits — with algorithms specifically designed for imperfect hardware to demonstrate optimal applications computing, materials science, and fundamental physics.
QUANTUM SCIENCE CENTER	Quantum Science Center *Lead Lab: ORNL*	QSC designs materials that enable topological quantum computing; implementing new quantum sensors to characterize topological states and detect dark matter; and designing quantum algorithms and simulations of quantum materials, chemistry, and quantum field theories.
SQMS	Superconducting Quantum Materials and Systems Center *Lead Lab: FNAL*	SQMS seeks transformational advances in the major cross-cutting challenge of understanding and eliminating the decoherence mechanisms in superconducting 2D and 3D devices, with the goal of enabling construction and deployment of superior systems for computing and sensing.

Advanced Materials for Quantum Tech

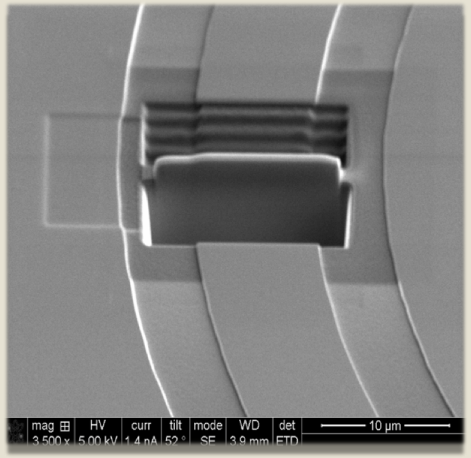
Characterization

- Materials discovery programs to mitigate the key limiting mechanisms of coherence in semiconductor qubits, and superconducting radio-frequency cavities and qubits
- Device modeling, characterization, and simulation, targeting > 10x performance improvement
- Systems-level materials optimization for high-coherence devices

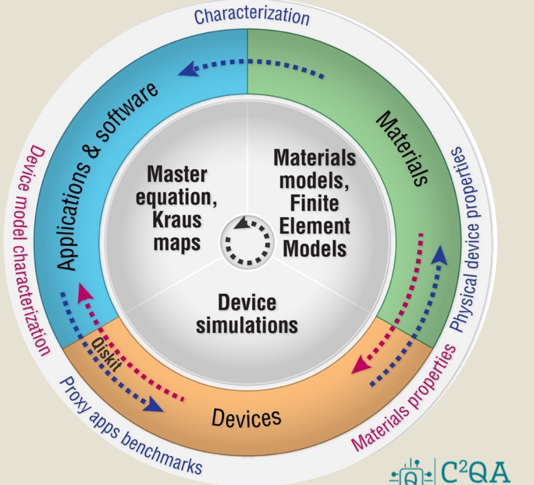
Synthesis

- Quantum facilities to provide a source of semiconductor and superconducting materials
- Guidelines for designing and screening new quantum defects and defect-host systems
- New topological materials to protect quantum information

	C2QA	Q-NEXT	Quantum Systems Accelerator	Quantum Science Center	SQMS
Materials discovery programs	●	●	●		●
Device modeling, characterization, and simulation	●	●	●	●	●
Systems-level materials optimization			●		
Quantum facilities	●	●			●
Guidelines for designing and screening	●	●			
New topological materials				●	



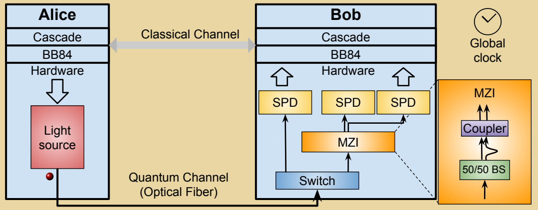
Advanced materials analysis of qubit fragments - FIB-SEM cross section shown. SQMS



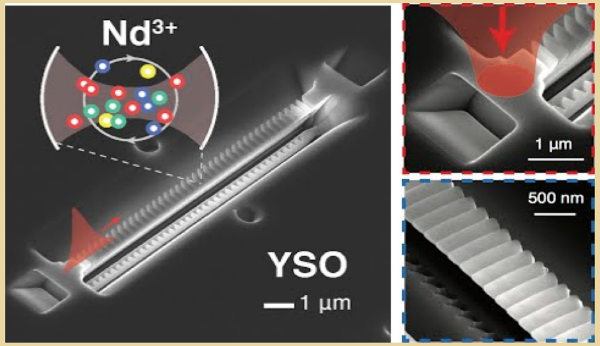
C2QA Co-design Center for Quantum Advantage

Entanglement Distribution Networks

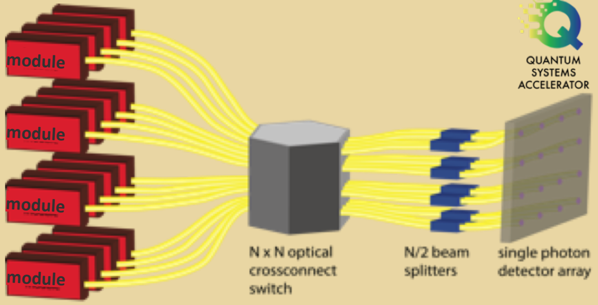
- Superconducting circuit QED memories and clusters linked by microwave-to-optical quantum communication
- Quantum interconnects development and communication links demonstration
- Comprehensive network simulator for long-distance quantum interconnects, memories, and repeater nodes.
- Modular photonics for ion trap computing interconnects



Model optical components in a communication network



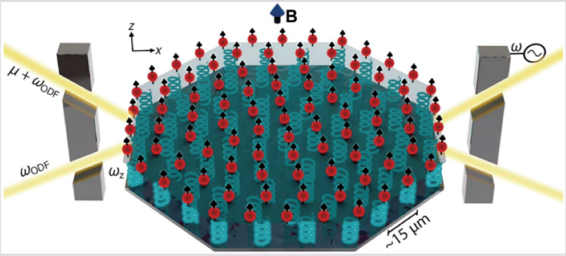
Quantum memory and repeater prototypes

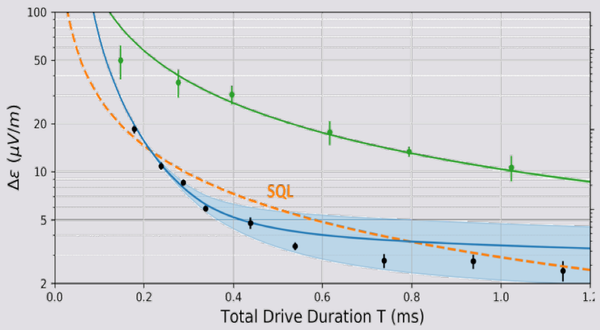


Modular photonic interconnect switch for ion trap

High-Performance Instruments and Sensors

	C2QA	Q-NEXT	Quantum Systems Accelerator	Quantum Science Center	SQMS
New quantum sensors based on superconducting technology		●		●	●
New quantum sensors based on many-body entanglement in highly-correlated systems			●	●	
New quantum sensor designs based on advanced materials to detect dark matter and topological quasiparticles				●	●
Precision quantum sensor network development and demonstration		●			

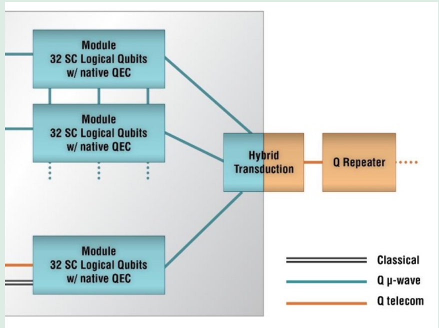




Sensor based on Beryllium ions and electric field sensitivity as function of sensor drive duration

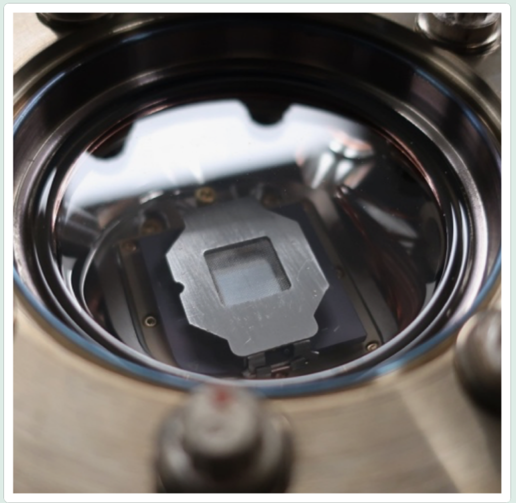
Computing: Programmable Quantum Systems

	C²QA	Q-NEXT	Quantum Systems Accelerator	Quantum Science Center	SQMS
Novel hybrid discrete-variable superconducting qubits and continuous-variable microwave oscillator modular architectures.	●		●		●
Superconducting circuit QED modules linked by microwave-to-optical interconnects	●	●			
Next-gen prototypes for semiconductor, superconducting, trapped ion, neutral atom, and photonic systems	●	●	●	●	●



C²QA Co-design Center for Quantum Advantage

Microwave-optical interconnect

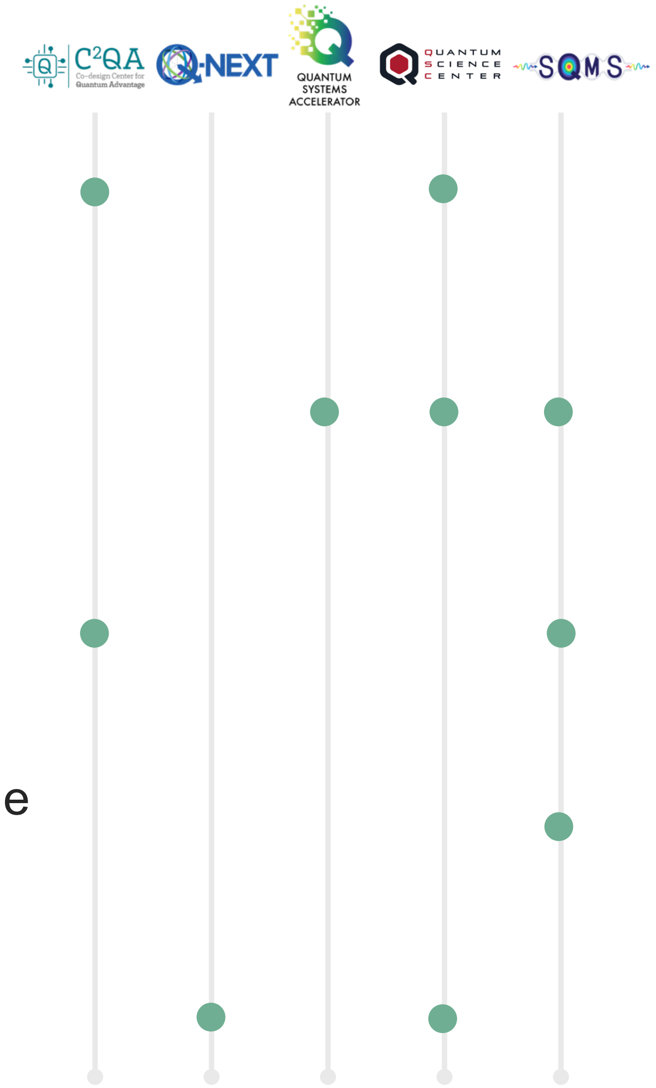


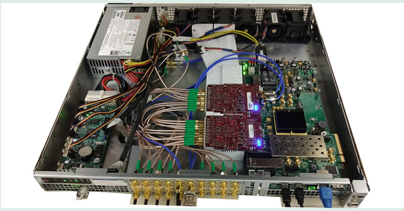
Cryo-cooled ion trap device

Quantum Science Center

Computing: Integrated Quantum Engineering

- Hardware-efficient quantum error mitigation, communication, and remote entanglement
- Extensible cryo-electronic and integrated optical/microwave controls
- Integration of high-quality cavities with qubits
- Construction of record-size dilution fridge, capable of hosting thousands of qubits
- New solid state quantum computing platforms





QUANTUM SYSTEMS ACCELERATOR

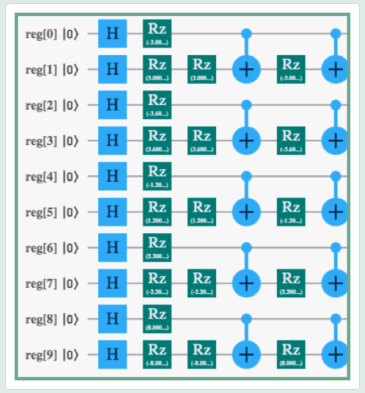
QubiC system – modular FPGA-based controls

Integration of high-quality cavities with qubits

SQMS

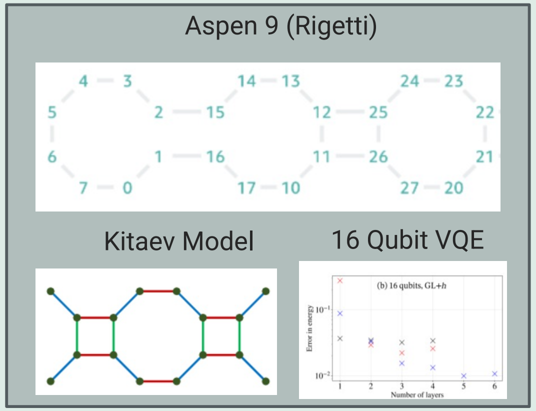
Computing: Algorithms and Applications

	C2QA	Q-NEXT	Quantum Systems Accelerator	Quantum Science Center	SQMS
Platform-aware simulation, emulation, and optimization	●	●	●	●	
Hardware-optimized simulations for HEP, NP, quantum chemistry, strongly-correlated matter, and materials			●	●	●
Extensible benchmarks and protocols for cross-platform validation and verification			●		
Noise mitigation and efficient fault resilience on near-term hardware	●		●	●	



QUANTUM SCIENCE CENTER

A quantum circuit used for validating quantum devices



SQMS

Efficient quantum simulations with geometric compatible hardware

Next Generation of the Quantum Workforce

	C²QA	Q-NEXT	Quantum Systems Accelerator	Quantum Science Center	SQMS
QIS topical summer school program	●			●	●
Internships through DOE SULI and other mechanisms	●	●	●	●	●
Software and science applications journal club	●				
K-12 Teacher Training	●		●		
Partnering program for students and industry or national lab advisors		●			●
Participation in the Open Quantum Initiative		●			
Pilot national lab apprenticeship program			●		
Lead annual Chief Diversity Officer meeting for DEI best practices in QIS training and recruitment			●		
Dedicated QIS GEM and HBCU programs				●	
Carolyn B. Parker fellowship for under-represented minorities					●

Q-NEXT

Carolyn B. Parker Fellowship

SQMS

Engagement with Industry Partners

The NQISRCs broadly engage with industry partners to accelerate the deployment of quantum-enabled technologies, bringing the benefits of Center research to the public.

- Technical exchange and alignment with industry needs facilities through QED-C TACs
- Creation of roadmaps and standard for quantum technology
- Expedited technology transfer, including novel mechanisms for practical commercialization such as patent pooling
- Development of national databases that incorporate processes, metrology, and testing data

OUR PARTNERS

Ames Laboratory
Applied Materials
Argonne National Laboratory
Boeing
Brookhaven National Laboratory
California Institute of Technology
City College of New York
ColdQuanta
Colorado School of Mines
Columbia University
Cornell University
Duke University
Fermilab
General Atomics
Goldman Sachs
Harvard University
Howard University
HRL Laboratories
IBM
Illinois Institute of Technology
INFN (Istituto Nazionale di Fisica Nucleare)
Intel
Janis
Johns Hopkins University
Keysight Technologies
Lawrence Berkeley National Laboratory
Lockheed Martin
Los Alamos National Laboratory
Massachusetts Institute of Technology
Microsoft
MIT Lincoln Laboratory
Montana State University
NASA-Ames Research Center
National Institute of Standards and Technology
Northwestern University
Oak Ridge National Laboratory
Pacific Northwest National Laboratory
Pennsylvania State University
Princeton University
Purdue University
Quantum Opus
Rigetti Computing
Rutgers University
Sandia National Laboratories
SLAC National Accelerator Laboratory
Stanford University
Stony Brook University
SUNY Polytechnic Institute
Temple University
Thomas Jefferson National Accelerator Facility
Tufts University
Unitary Fund
Università degli Studi di Padova
Université de Sherbrooke
University of Arizona
University of California, Berkeley
University of California, Santa Barbara
University of Chicago
University of Colorado Boulder
University of Illinois at Urbana-Champaign
University of Maryland
University of Massachusetts at Amherst
University of New Mexico
University of Pittsburgh
University of Southern California
University of Tennessee, Knoxville
University of Texas at Austin
University of Washington
University of Wisconsin–Madison
Virginia Tech
Yale University

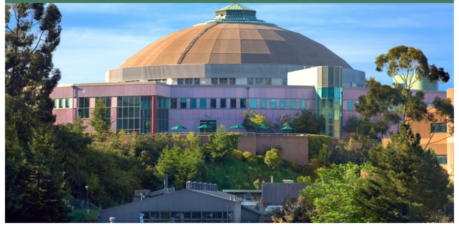
Forging Connectivity Across the Ecosystem

The NQISRCs create new synergies between DOE programs by leveraging world-class facilities including light sources, high performance computing facilities, foundries, and nanoscience centers.

BNL National Synchrotron Light Source II

FNAL SRF Foundry

LBNL Advanced Light Source



Sandia Center for Integrated Nanotechnologies

Argonne Solid State Materials Foundry

Argonne Advanced Photon Source

LBNL Molecular Foundry

SLAC Superconducting Materials Foundry

- Cross-Center workshops and other activities introduce QIS-relevant capabilities of the facilities to the researcher community
- The Centers share anticipated needs of the QIS community with facility experts to guide the development of new capabilities

Capabilities available for QIS include:

- Hard and soft X-ray light sources to probe atomic and electronic structure – significant benefit from upcoming light source upgrades at APS and ALS.
- Class-10, 100, and 1000 cleanrooms for device fabrication
- Advanced lithographic, etching, and deposition tools
- Optical, electron, and scanning probe microscopy technologies
- Nanostructure characterization tools
- Theory and simulation resources

Joint Center Accomplishments – Year 1

Technical Coordination
- Center technical leadership participated in a workshop to identify synergies and areas for coordination and collaboration between the NQISRCs
- The Centers developed plans for joint topical workshops and for the exchange and sharing of technical information to accelerate our scientific progress

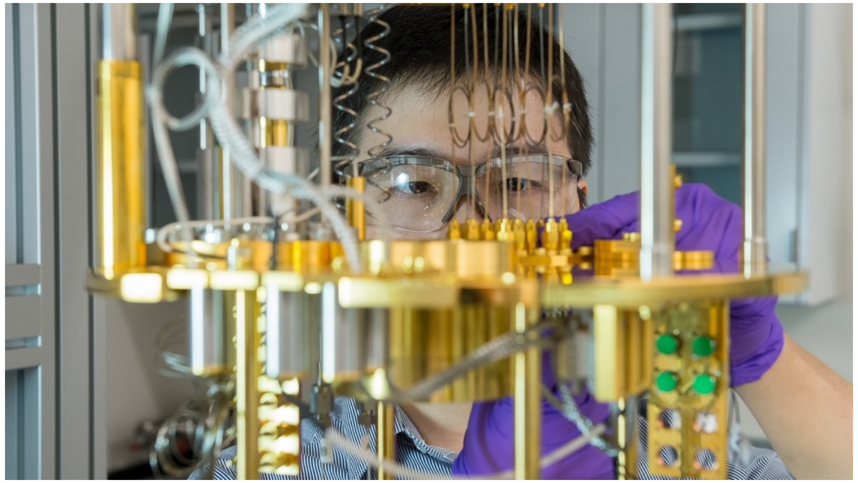
Instrumentation and Facilities
- Each Center contributed to a joint workshop on the applicability of the National Science User Facilities for QIS research. The workshop included virtual tours of the user facilities, a discussion of access procedures, and introductions to facility experts

Workforce
- All Centers participated in a QIS Career Fair organized by C^2QA
- The Centers collaborated for future cross-promotion of Center workforce and student programs

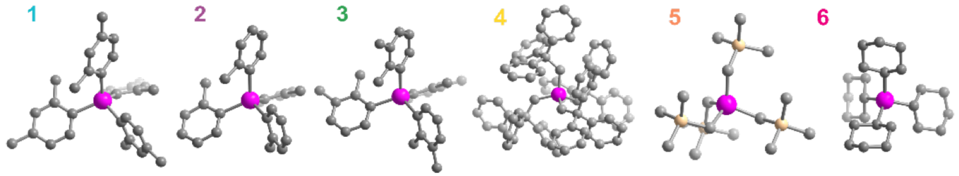
Management
- Operations leadership from each Center meet regularly to share best practices in Center management and risk mitigation
- The Centers are building communities of practice focused on cybersecurity and EH&S

Communications / Outreach
- A cross-Center communications team collaborates on the development of materials to communicate our goals and progress
- An NQISRC Panel was accepted to participate in the 2022 AAAS Annual Meeting

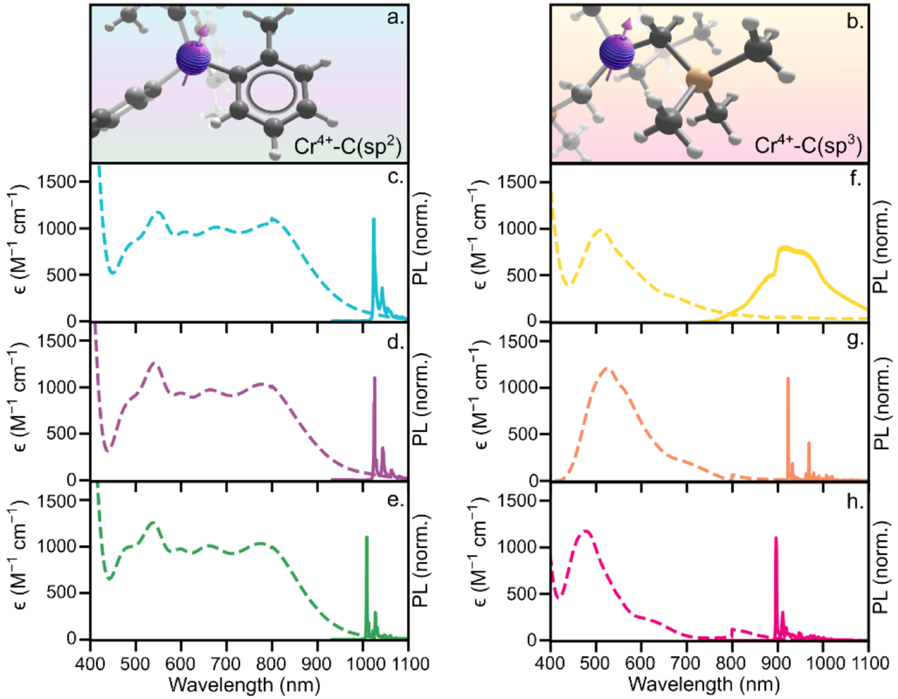
NQISRC Panel at QIS Career Fair hosted by C2QA



Chemically-Tunable Emission in Molecular Color Centers



Molecular structures of Cr(2,4-dimethylphenyl)$_4$ (**1**), Cr(*o*-tolyl)$_4$ (**2**), Cr(2,3-dimethylphenyl)$_4$ (**3**), Cr(2,2,2-triphenylethyl)$_4$ (**4**), Cr((trimethylsilyl)methyl)$_4$ (**5**), and Cr(cyclohexyl)$_4$ (**6**).



Variation in metal-ligand bonding between **1-3** (a) and **4-6** (b). Room temperature UV-Vis-NIR spectra (dashed lines) and 4 K PL spectra (solid lines) of **1** (c), **2** (d), **3** (e), **4** (f), **5** (g), and **6** (h).

Scientific Achievement

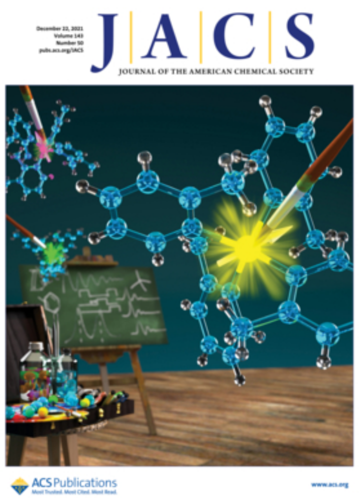
Chemical synthesis enables tunable, controllable, predicable synthesis of units for quantum information science. Controlled modulation of chemical ligands enables predictable shifts in zero-field splitting and optical emission in a series of molecular color centers.

Significance and Impact

The ability to rationally target color centers with specific properties such as emission frequency will enable directed design of qubits towards specific sensing and communications applications.

Details

- We synthesized two classes of tetrahedral Cr^{4+}-based compounds, wherein substantial differences in metal-ligand bonding interactions in each class directly influence emission energies and zero-field splitting.
- Modulating spin delocalization onto the ligand provides a handle to control the emission energies.
- The variation in ground state spin structure suggests that molecular symmetry could be used to introduce clock-like transitions at zero field.



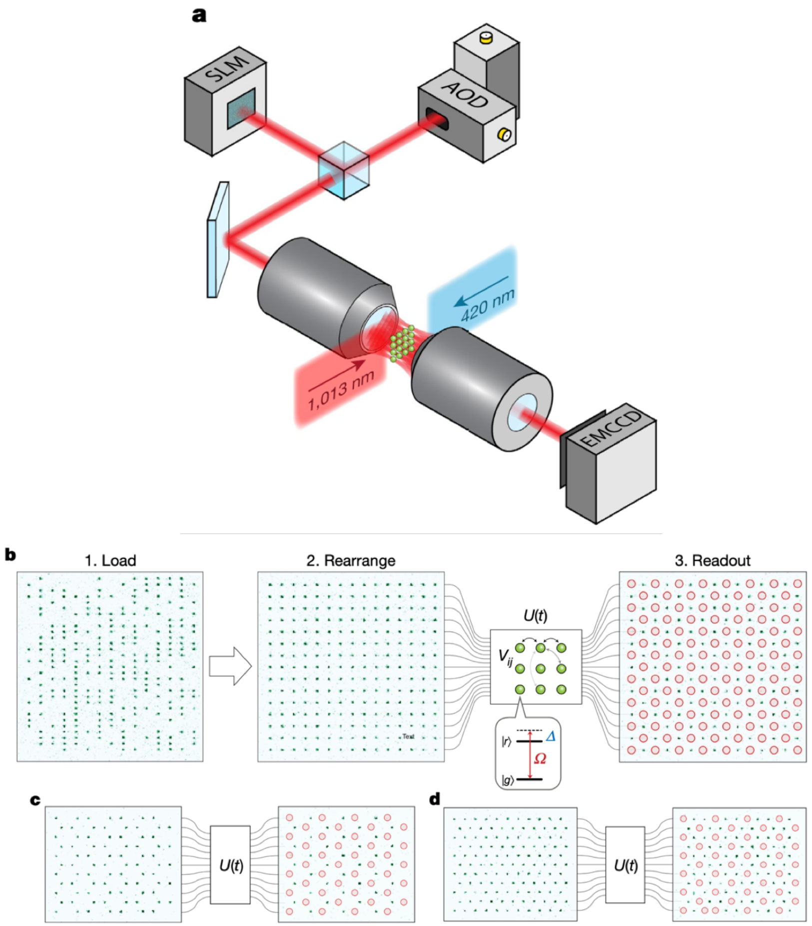
D. W. Laorenza *et al*. Journal of the American Chemical Society. https://pubs.acs.org/doi/10.1021/jacs.1c10145

U.S. DEPARTMENT OF ENERGY | Office of Science

Work was performed at Northwestern University, University of Chicago, Columbia University, and Massachusetts Institute of Technology

Q-NEXT

Quantum Phases of Matter on a 256-Atom Programmable Quantum Simulator



a) The experimental platform with a 2D array of optical tweezer traps. b-d) The sequence of loading and rearranging atoms to simulate a two-dimensional spin model.

S. Ebadi, et. al., *Nature* **595**, 227-232 (2021)

Accomplishment

Studied quantum phases of a spin system using a programmable quantum simulator based on a two-dimensional array of neutral atoms in Rydberg states.

Significance and Impact

Demonstrates a new tool for investigations of complex matter, including exotic quantum phases and non-equilibrium dynamics.

Details

– Simulated quantum phases and phase transitions which had not been previously observed in a (2 + 1)-dimensional Ising spin model.

– Implemented the simulation on arrays of 64 to 256 neutral atoms with tunable interactions, using optical tweezer traps.

– Created a platform also suitable for quantum information processing and implementation of hardware-efficient quantum algorithms.

Discovery of Room-Temperature, Single-Photon Emitters in SiN

Scientific Achievement

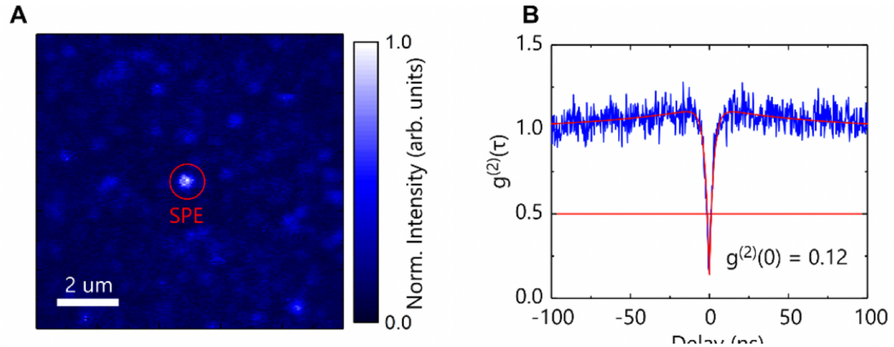
Purdue researchers report on the first-time observation of room-temperature, single-photon emitters in silicon nitride (SiN) films grown on silicon dioxide substrates obtained by careful selection of the growth conditions for low auto-fluorescing SiN.

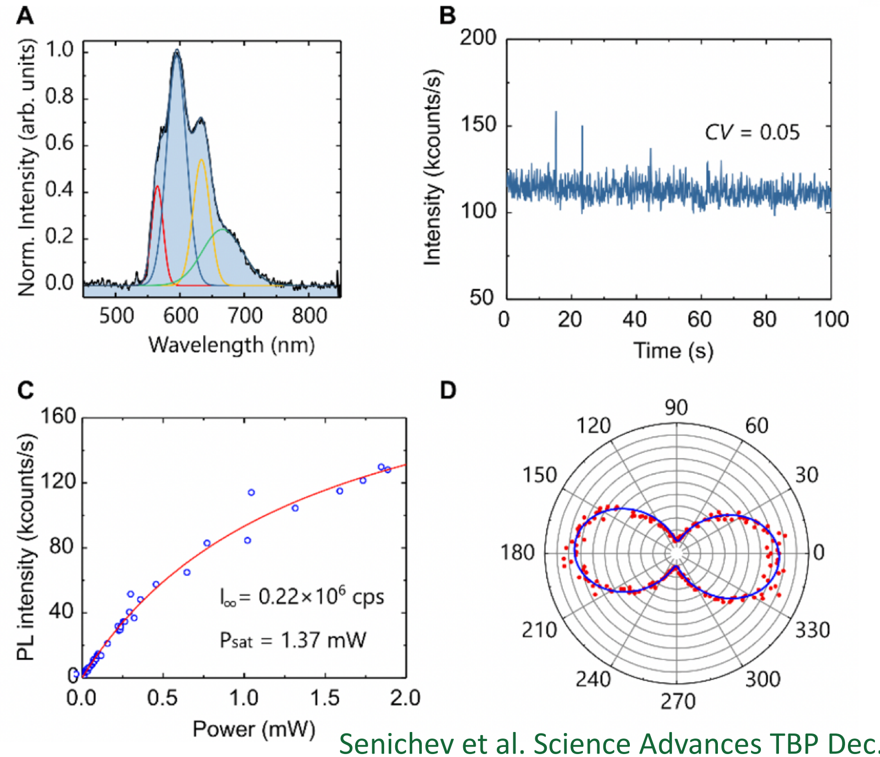
Significance and Impact

Single-photon emitters in SiN have the potential to enable direct, scalable, and low-loss integration of quantum light sources with the well-established photonic, on-chip platform.

Research Details

- Fabricated by HDPCVD and subsequent rapid thermal annealing
- SPEs are bright (>10^5 counts/s), stable, linearly polarized
- High-purity single-photon emission with $g^{(2)}(0)<0.2$ without background correction or spectral filtering
- SPEs exhibit PL peaks at virtually the same wavelengths – emission comes from a particular type of defect center
- On-chip sources of single photon emission, such quantum emitters in SiN, have the potential to enable broad applications in quantum communication, computing, and simulations

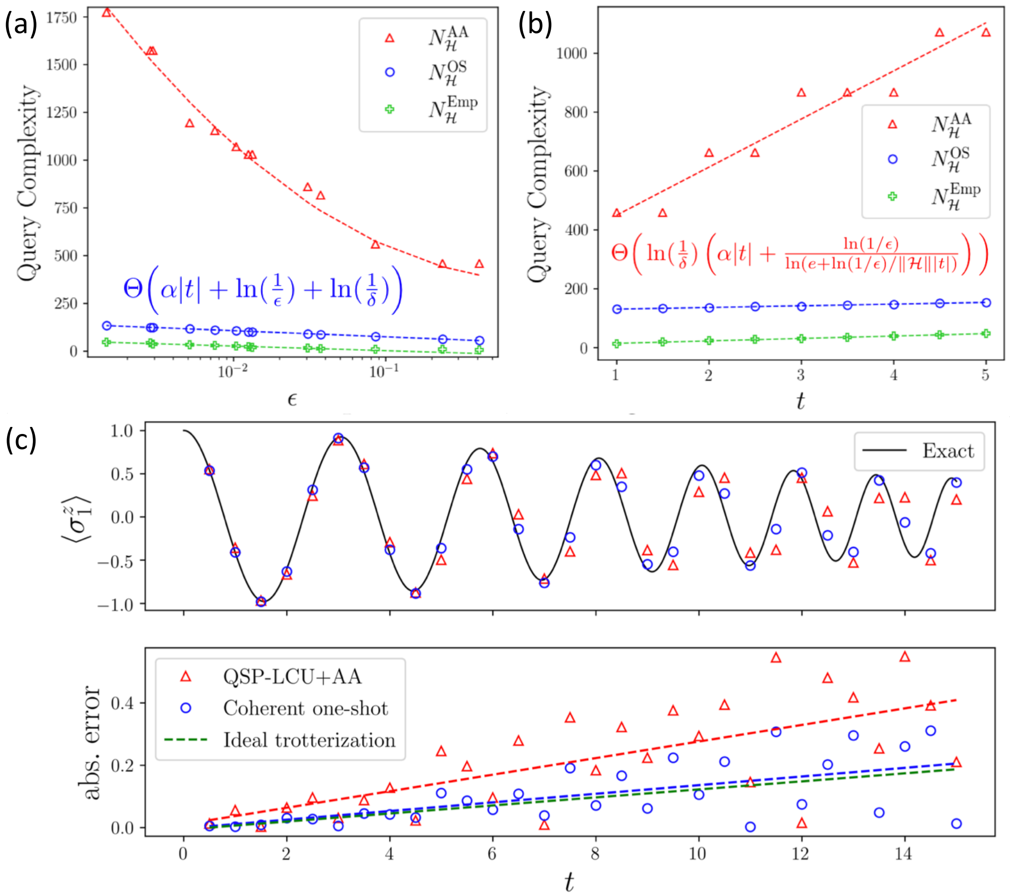




To be published in Science Advances (abj0627) in Dec. 2021; invention disclosure: 2001-SHAV-69443 (Purdue)

Senichev et al. Science Advances TBP Dec. 2021

Efficient Fully-Coherent Hamiltonian Simulation



Comparison of the theoretical query complexity of LCU+amplitude amplification (AA, red), our algorithm (OS, blue), and empirical bound (Emp, green) a) vs. error ϵ and b) vs. simulation time t; c) Hamiltonian simulation of a time-dependent Heisenberg model.

J. M. Martyn, Y. Liu, Z. E. Chin, I. L. Chuang. arXiv:2110.11327 (2021)

Work performed at Massachusetts Institute of Technology.

Scientific Achievement

We develop an efficient and fully-coherent Hamiltonian simulation quantum algorithm that succeeds with an arbitrarily high success probability with near optimal query complexity.

Significance and Impact

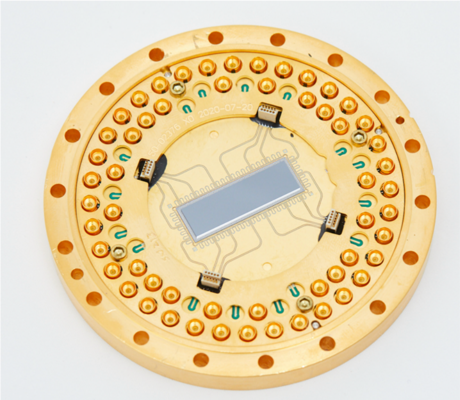
Significant query complexity improvement compared to previous algorithms; the ability to be fully-coherent allows concatenation into larger and more powerful quantum algorithms.

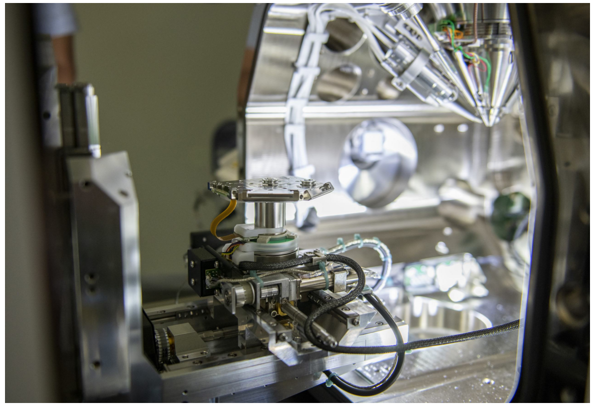
Details

– Design polynomial approximation to the complex exponential function and apply an affine transformation to the Hamiltonian.

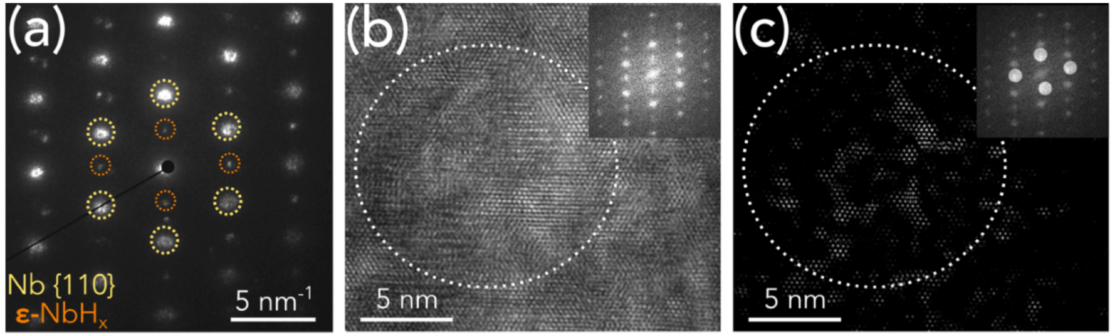
– Query complexity being a sum of linear in time, logarithmic in inverse error, logarithmic in inverse failure probability.

Discovery of Niobium Nano-hydride Precipitates in Superconducting Transmon Qubits





Lamellas of superconducting qubits from real Rigetti Computing processors are dissected via FIB-SEM at FNAL and studied for the first time via cryo-TEM



Cryogenic TEM, electron diffraction images of Rigetti 2D qubits , revealing the presence of hydrides precipitates in the niobium film at T=100K

Scientific achievement

First ever performed cryogenic microscopy studies of superconducting qubits lead to the discovery of the presence of hydride precipitates in the Rigetti Computing and other transmon qubit devices

Significance and Impact

Niobium nano-hydrides are poorly superconducting phases that can cause qubit device performance limitations and degradation over time and with subsequent cooldowns

Details

– Cryogenic AFM, electron diffraction and high-resolution transmission electron microscopy (TEM) analyses are performed on the Nb films at room temperature and cryogenic temperature (106 K)

– The results suggest the existence of two possible types of Nb hydride domains in Nb grains: (i) ~5 nm-sized Nb hydride domain with irregular shapes; (ii) 10s~100 of nm-sized distinct Nb hydride domains

– Pathways to mitigate the formation of the Nb hydrides are under study

J. Lee, Z. Sung, A. Murthy, M. Reagor, A. Grassellino, and A. Romanenko; https://arxiv.org/pdf/2108.10385.pdf

Work was performed at Fermi National Accelerator Laboratory material science lab and NUANCE user facility

Joint Center Plans: Next Steps

Coordination in Technical Areas

- Develop database of quantum materials characteristics, including standards development
- Technical roadmaps to drive innovation
- Cross-center workshops (eg. algorithms and co-design approaches)
- Open all-hands meetings

Instrumentation and Facilities

- Activities for existing researchers on the application of user facilities to QIS
- Identification and promotion of additional resources, including testbeds and characterization tools

Ecosystem Stewardship

- Second annual career fair, hosted by C^2QA, to provide pathways into QIS
- Chief Diversity Officers to continue exchange of best practices and resources for QIS DEI
- Coordinated QIS summer school planned for 2023
- Coordinated workforce development and communications activities