

National QIS Research Centers: Mission and Activities

FESAC Meeting
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NQISRC Directors

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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

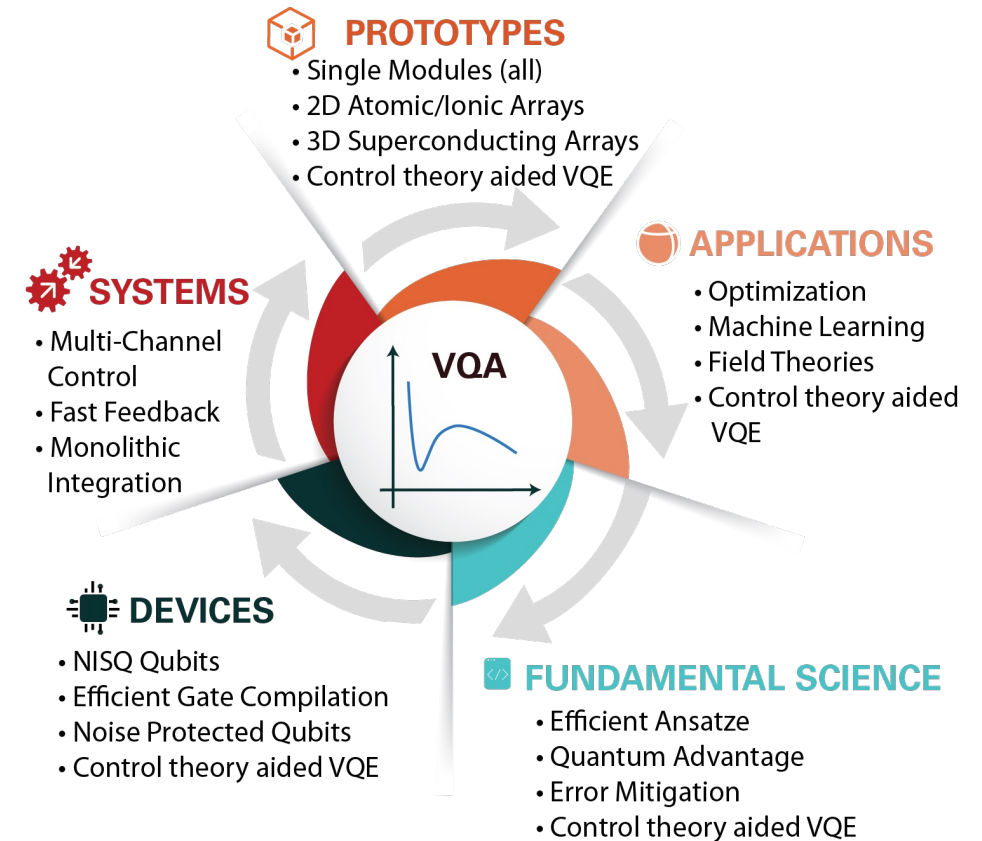
Fundamental Science is basic research that underpins discoveries and exploration to deliver long-term innovation.

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



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.



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

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

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.



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.

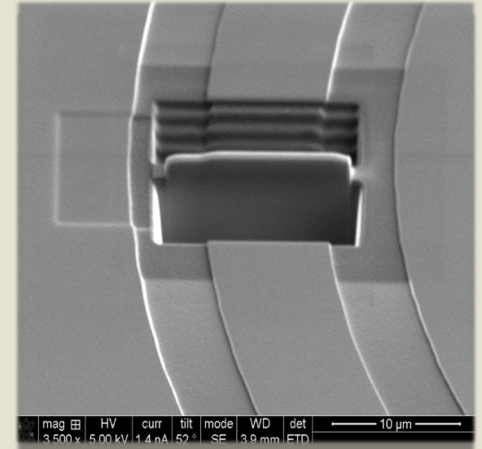
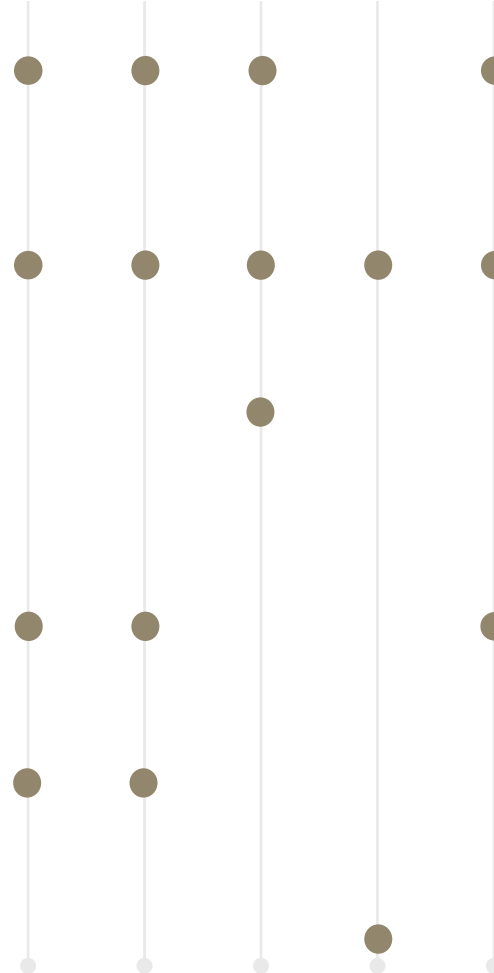
Advanced Materials for Quantum Tech


Characterization

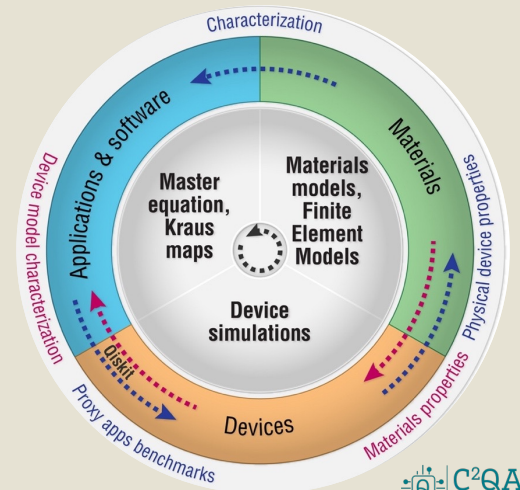
- Materials discovery programs to mitigate the key limiting mechanisms of coherence in semiconductor qubits, and superconducting radio-frequency cavities and qubits
- Device modeling, characterization, and simulation, targeting > 10x performance improvement
- Systems-level materials optimization for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

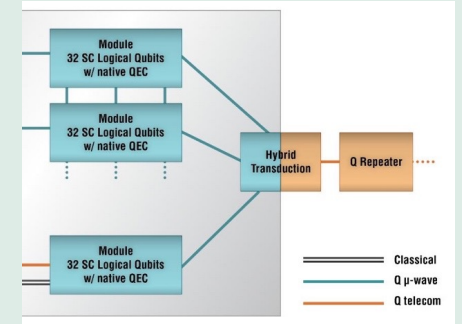
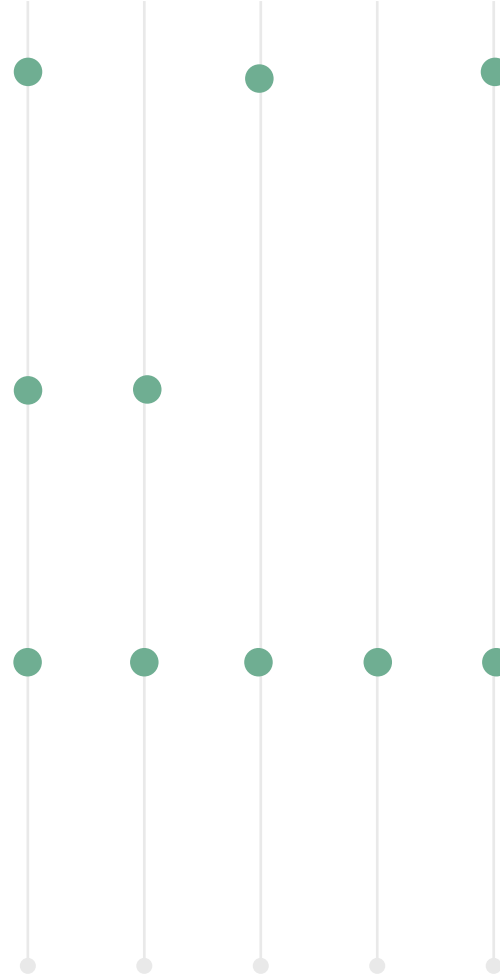


Advanced materials analysis of qubit fragments - FIB-SEM cross section shown. 

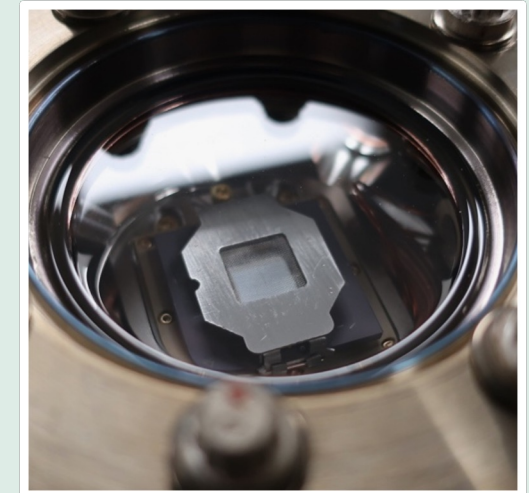


Computing: Programmable Quantum Systems

- 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



Microwave-optical interconnect

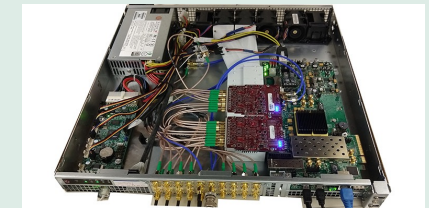
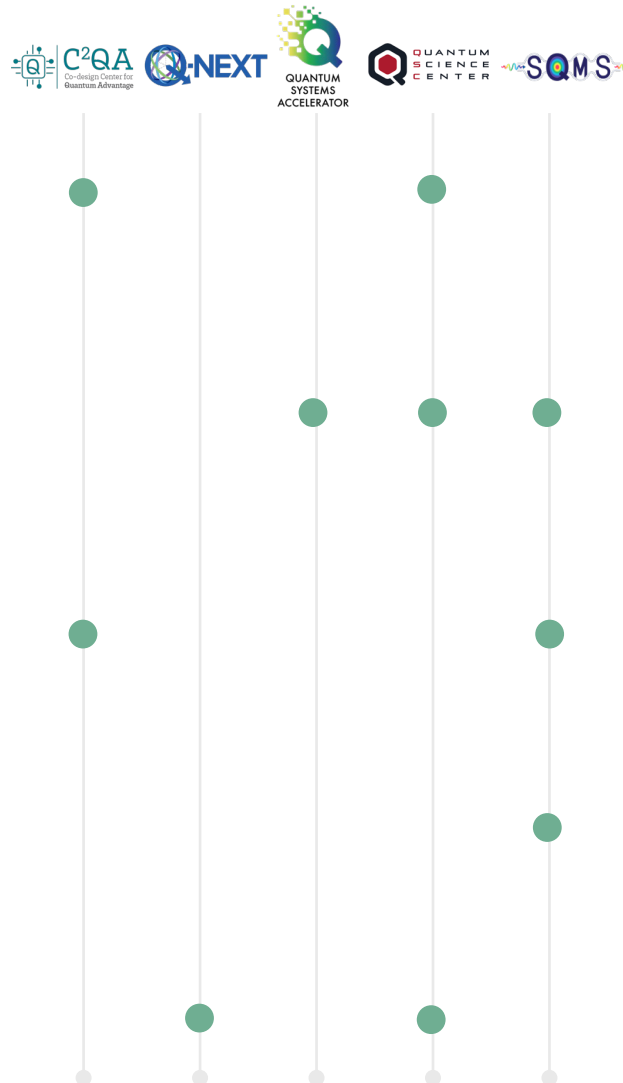


Cryo-cooled ion trap device



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



QubiC system – modular FPGA-based controls

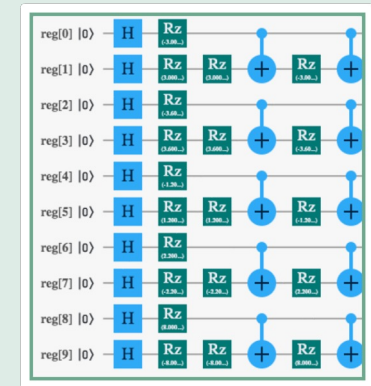
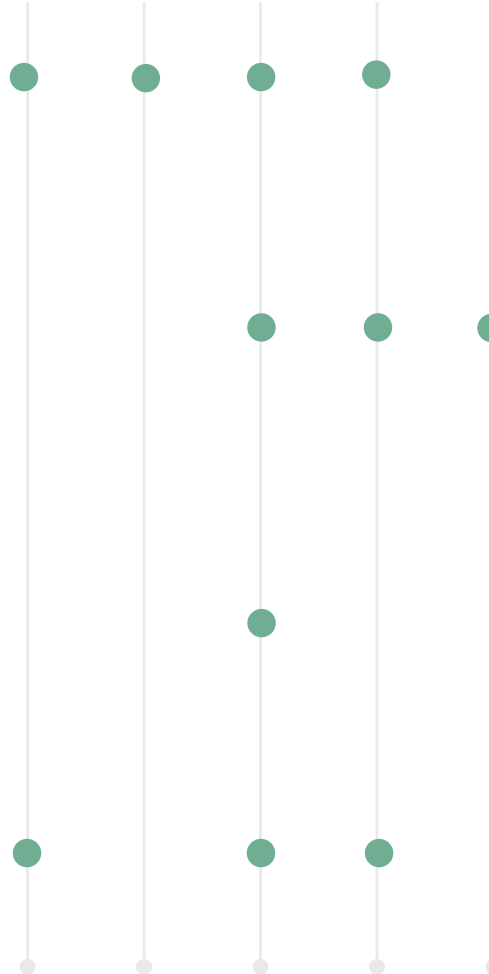


Integration of high-quality cavities with qubits

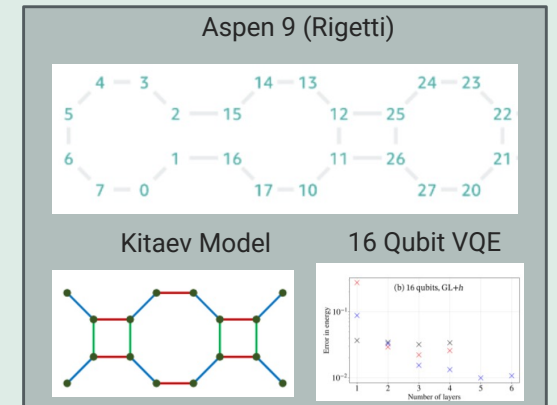


Computing: Algorithms and Applications

- 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



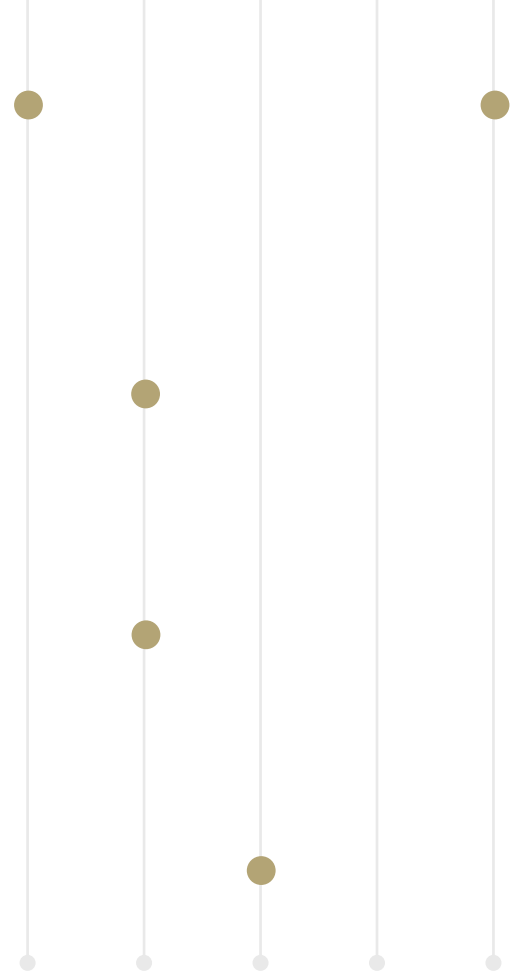
A quantum circuit used for validating quantum devices



Efficient quantum simulations with geometric compatible hardware

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

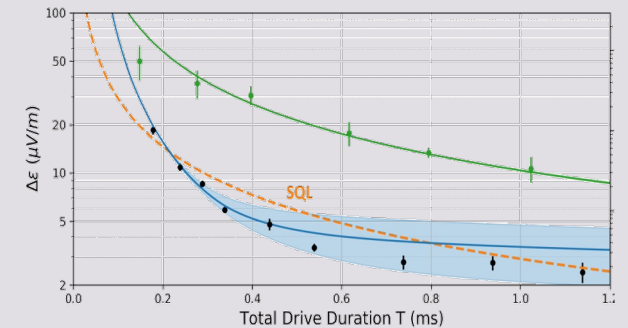
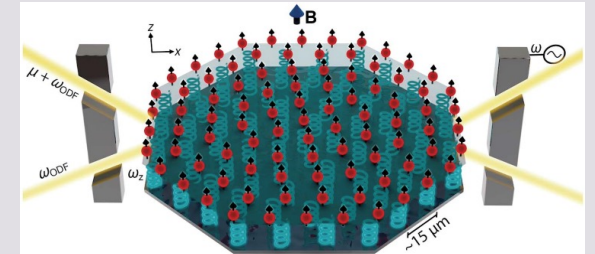
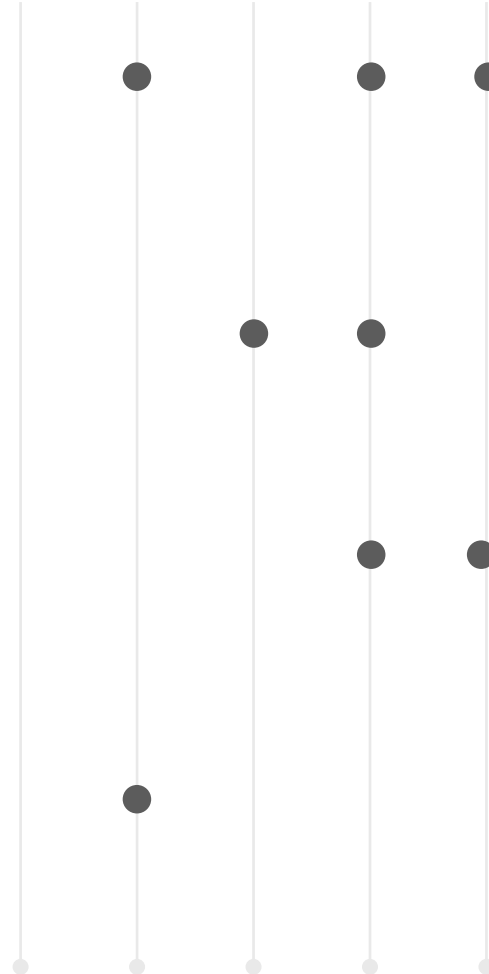
Quantum memory and repeater prototypes

Modular photonic interconnect switch for ion trap

High-Performance Instruments and Sensors



- 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

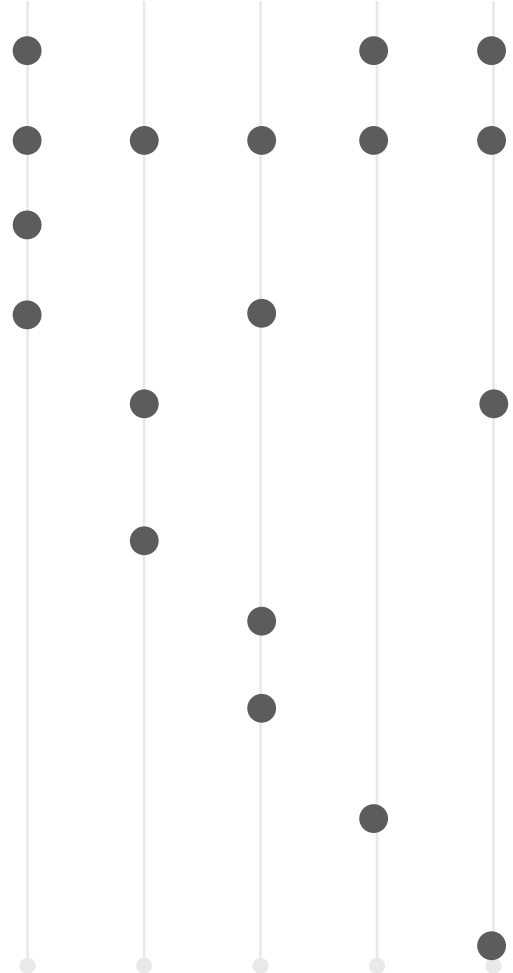


Sensor based on Beryllium ions and electric field sensitivity as function of sensor drive duration



Next Generation of the Quantum Workforce

- 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



Carolyn B. Parker Fellowship



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



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.



- 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 C²QA
- The Centers collaborated for future cross-promotion of Center workforce and student programs

Management

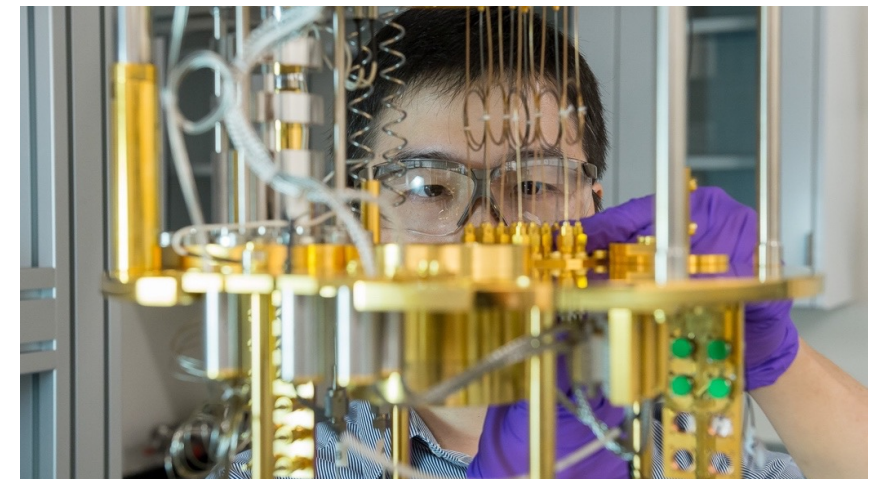
- Operations leadership from each Center meet regularly to share best practices in Center management and risk mitigation
- The Centers are building communities of practice focused on cybersecurity and EH&S

Communications / Outreach

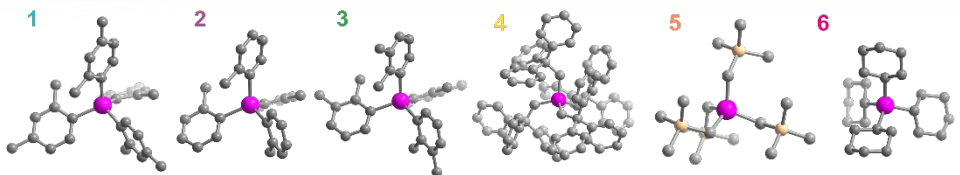
- A cross-Center communications team collaborates on the development of materials to communicate our goals and progress
- An NQISRC Panel was accepted to participate in the 2022 AAAS Annual Meeting



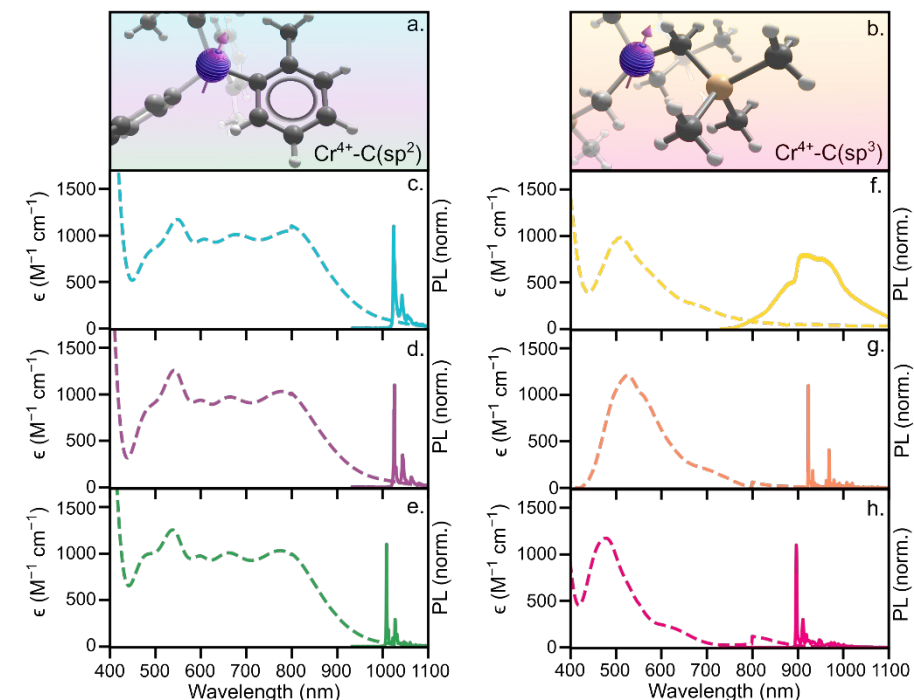
NQISRC Panel at QIS Career Fair hosted by  C²QA Co-design Center for Quantum Advantage



Chemically-Tunable Emission in Molecular Color Centers



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

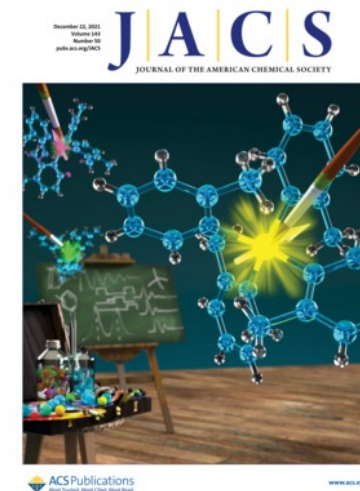
Chemical synthesis enables tunable, controllable, predictable synthesis of units for quantum information science. Controlled modulation of chemical ligands enables predictable shifts in zero-field splitting and optical emission in a series of molecular color centers.

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. Laurenza *et al.* Journal of the American Chemical Society. <https://pubs.acs.org/doi/10.1021/jacs.1c10145>

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

Accomplishment

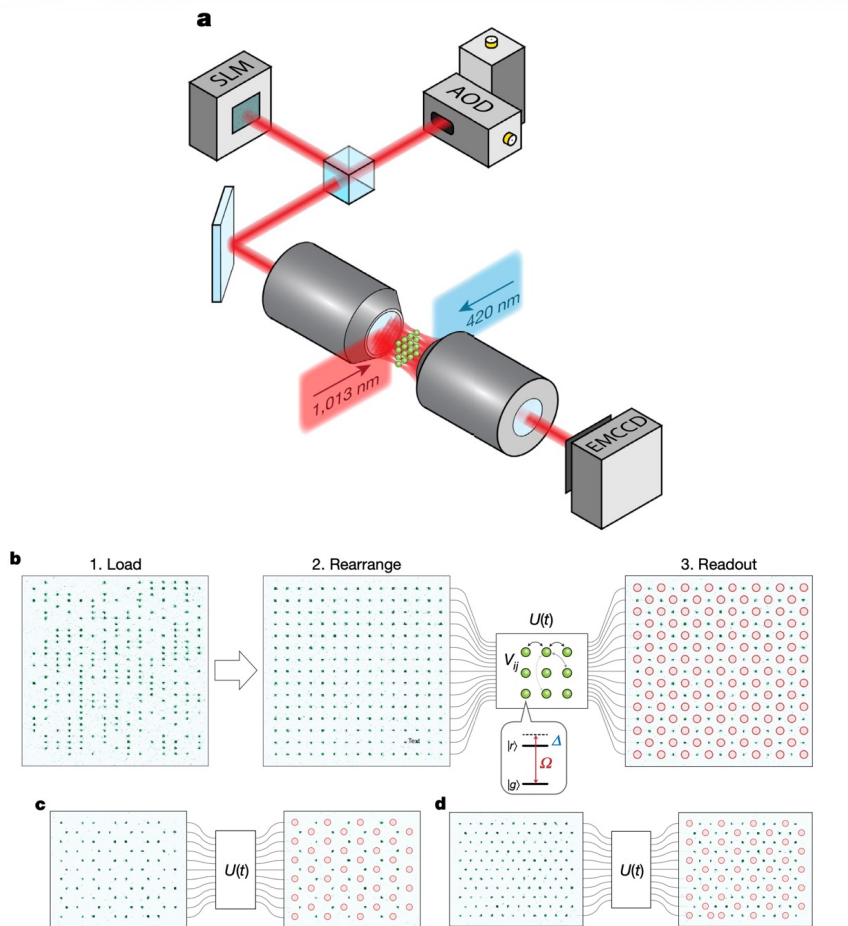
Studied quantum phases of a spin system using a programmable quantum simulator based on a two-dimensional array of neutral atoms in Rydberg states.

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.



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)

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.

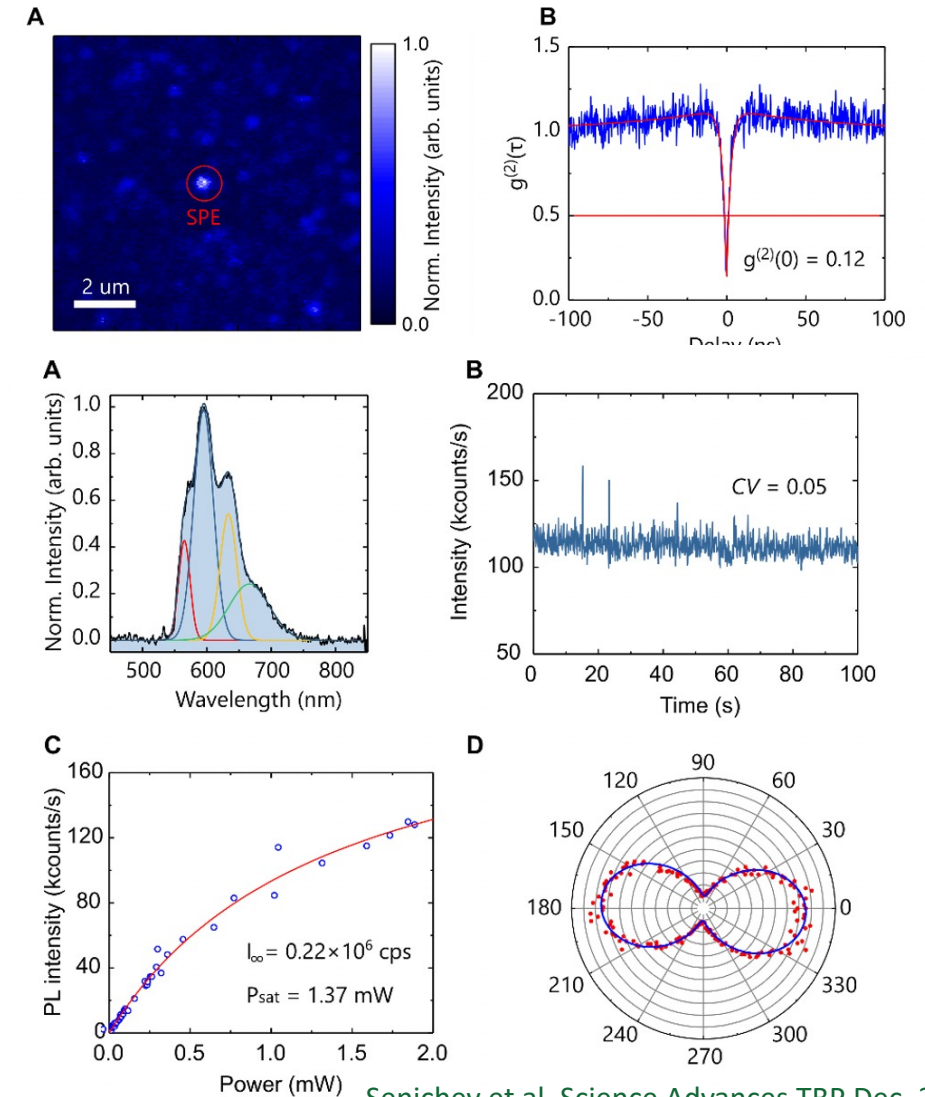
Significance and Impact

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

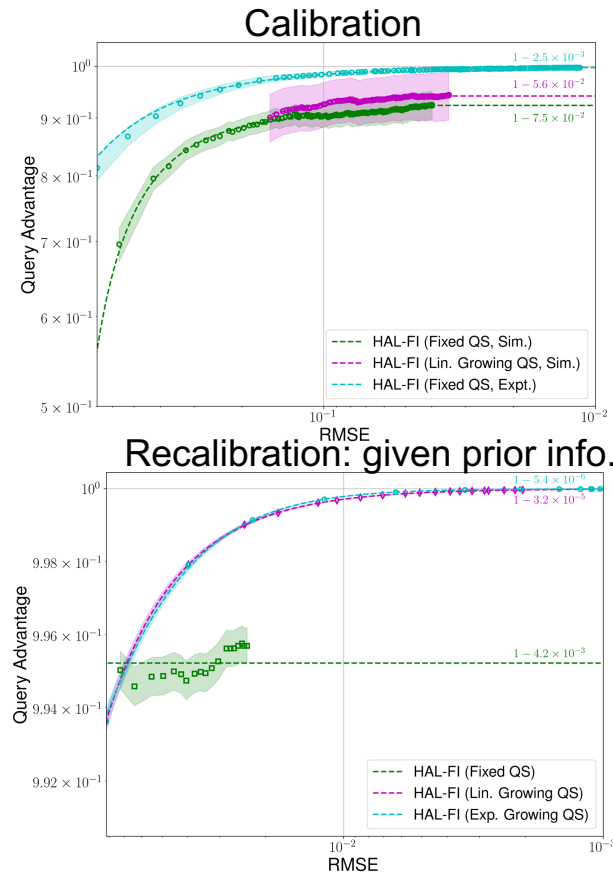
To be published in Science Advances (abj0627) in Dec. 2021; invention disclosure: 2001-SHAV-69443 (Purdue)



Senichev et al. Science Advances TBP Dec. 2021

Active Learning of Quantum System Hamiltonians Yields Query Advantage

Query advantage of HAL-FI over standard methods



Authors: A. Dutt, E. Pednault, C. Wu, S. Sheldon, J. Smolin, L. Bishop, I. Chuang.

Work was performed at: MIT and IBM T.J. Watson
arXiv: 2112.14553

Scientific Achievement

Introduces the active learning algorithm HAL-FI for Hamiltonian learning that reduces resource requirements by multiple orders of magnitude

Significance and Impact

Hamiltonian learning is a routine commonly carried out during calibration which is currently resource intensive and must be made practical on large-scale quantum systems.

Using HAL-FI, Hamiltonian learning can be performed much faster and be regularly carried out for quantum system characterization, and quantum control during calibration

Details

- Hamiltonian learning is accomplished by the experimentalist through queries to the quantum system
- HAL-FI uses active learning to take advantage of an experimentalist's ability to continuously interact with the quantum system and make queries based on information collected from previous calibrations or during learning
- In learning the two-qubit cross-resonance Hamiltonian on a 20-qubit IBM Quantum device, HAL-FI achieves up to 99.8% reduction in queries over standard methods and 99.1% reduction over non-adaptive algorithms

Discovery of Niobium Nano-hydride Precipitates in Superconducting Transmon Qubits

Scientific achievement

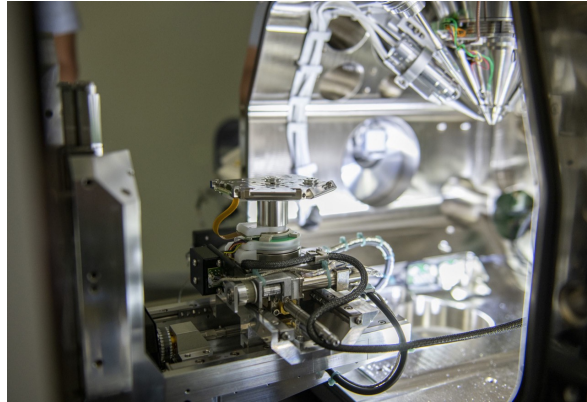
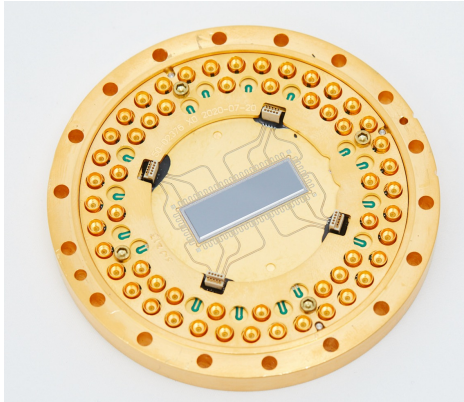
First ever performed cryogenic microscopy studies of superconducting qubits lead to the discovery of the presence of hydride precipitates in the Rigetti Computing and other transmon qubit devices

Significance and Impact

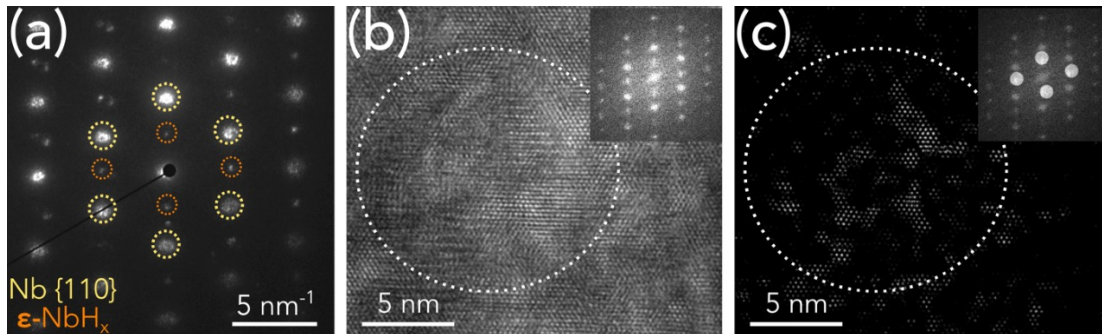
Niobium nano-hydrides are poorly superconducting phases that can cause qubit device performance limitations and degradation over time and with subsequent cooldowns

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



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

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 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