

# National QIS Research Centers: Mission and Activities

BESAC Meeting  
December 6, 2021

## NQISRC Directors

David Awschalom - Q-NEXT

David Dean - QSC

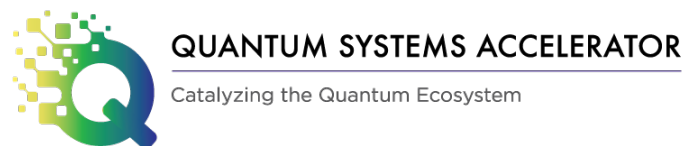
Anna Grassellino - SQMS

Andrew Houck - C<sup>2</sup>QA

Irfan Siddiqi - QSA

## Slide Coordinator:

Christopher Spitzer, Assoc. Dir. for Ops, QSA



# 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

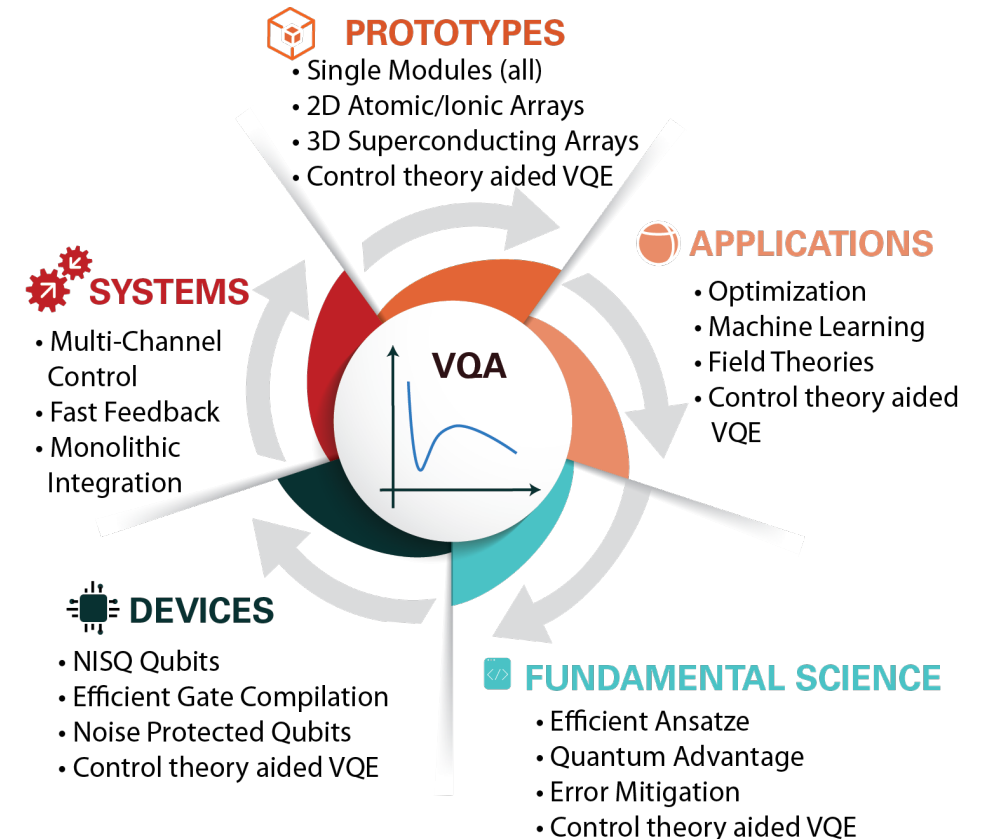
**Fundamental Science** is basic research that underpins discoveries and exploration to deliver long-term innovation.

**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*

C<sup>2</sup>QA 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 manipulating and distributing entangled states of matter. Its mission is to deliver quantum interconnects, communications links, networks of sensors, simulation testbeds, and a national resource for pristine materials for devices.



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.

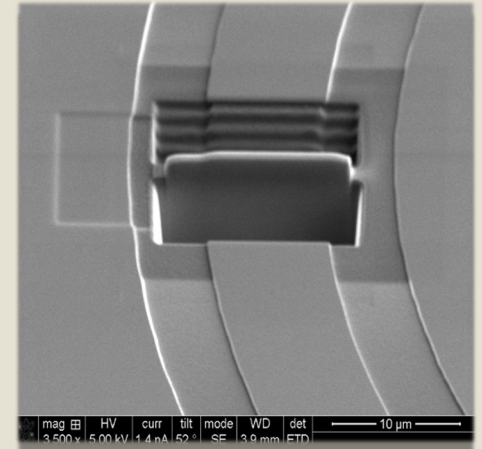
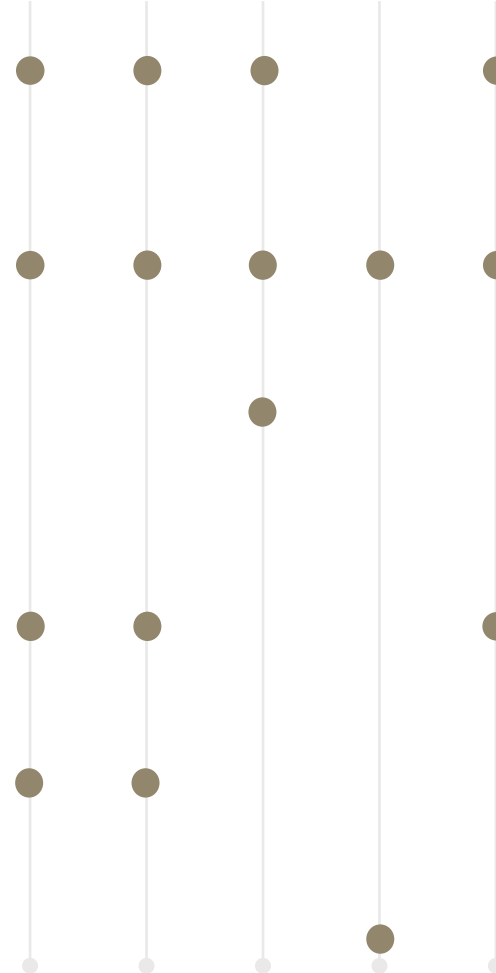
# Advanced Materials for Quantum Tech


## Characterization

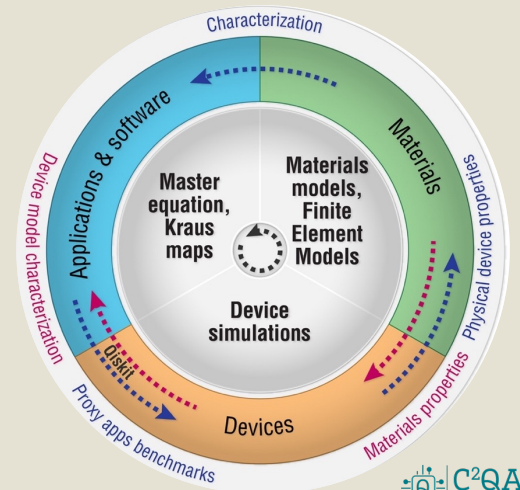
- Materials discovery programs to mitigate the key limiting mechanisms of coherence in semiconductor qubits, and superconducting radio-frequency cavities and qubits
- Device modeling, characterization, and simulation, targeting > 10x performance improvement
- Systems-level materials optimization for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

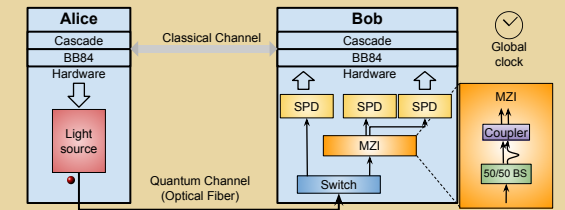
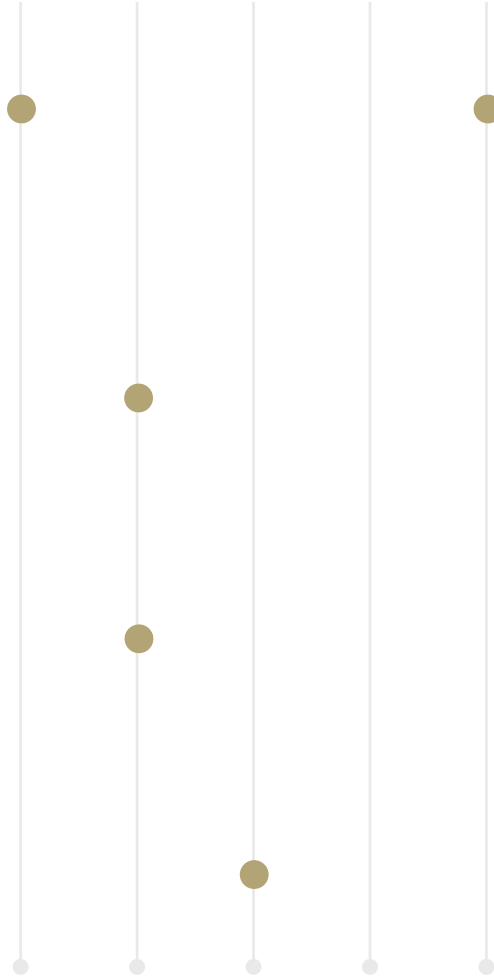


Advanced materials analysis of qubit fragments - FIB-SEM cross section shown. 

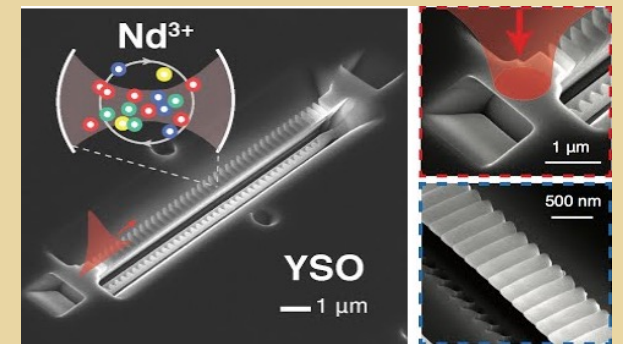


# Entanglement Distribution Networks

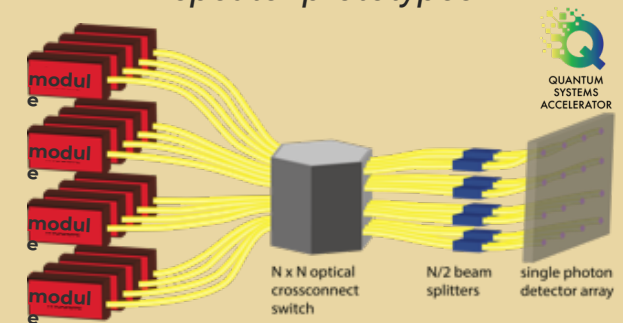
- Superconducting circuit QED memories and clusters linked by microwave-to-optical quantum communication
- Quantum interconnects development and communication links demonstration
- Comprehensive network simulator for long-distance quantum interconnects, memories, and repeater nodes.
- Modular photonics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



Optical components in 2-node setup



Quantum memory and repeater prototypes



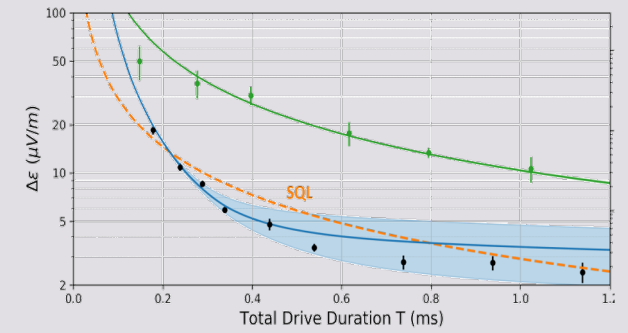
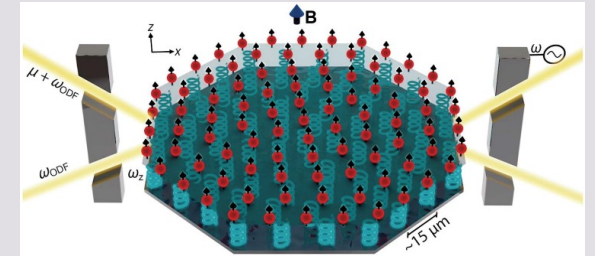
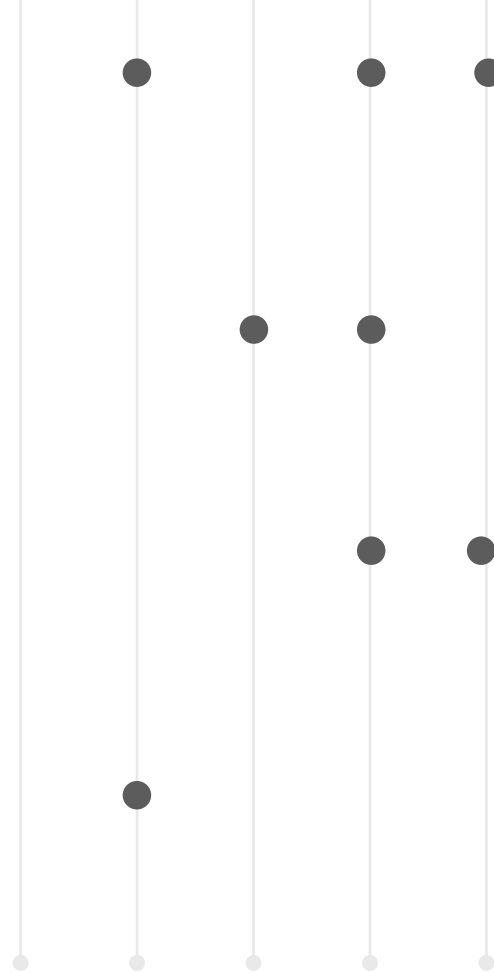
Modular photonic interconnect switch for ion trap



# 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

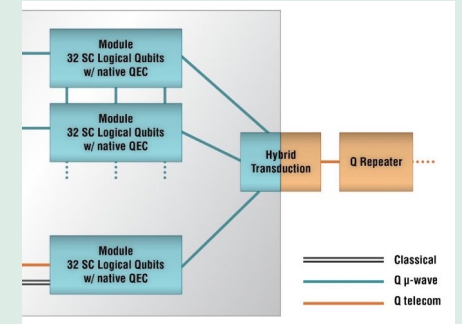
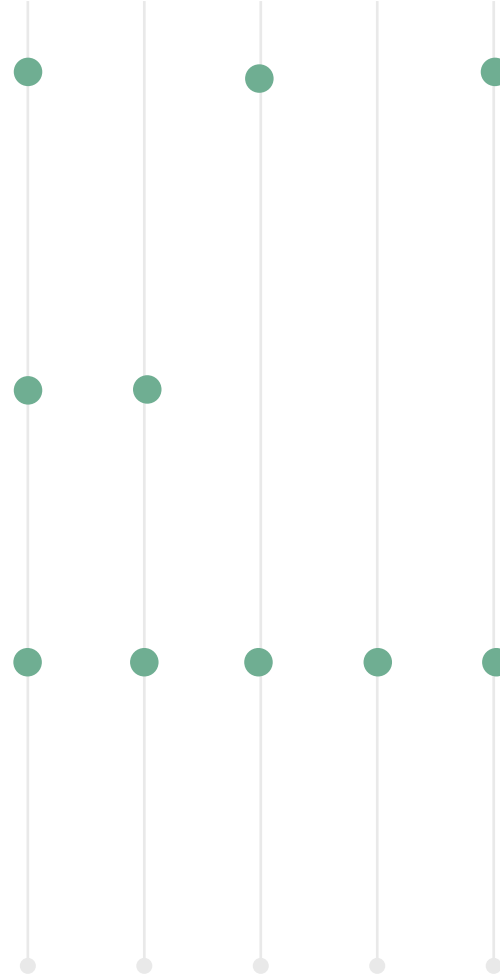


*Sensor based on Beryllium ions and electric field sensitivity as function of sensor drive duration*

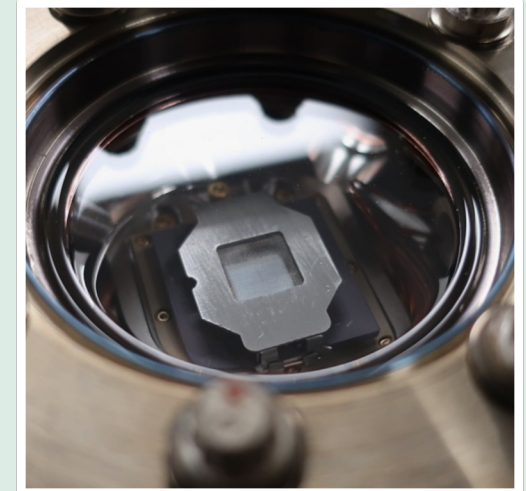


# Computing: Programmable Quantum Systems

- 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*



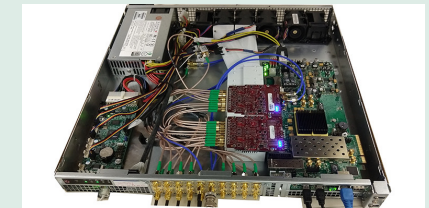
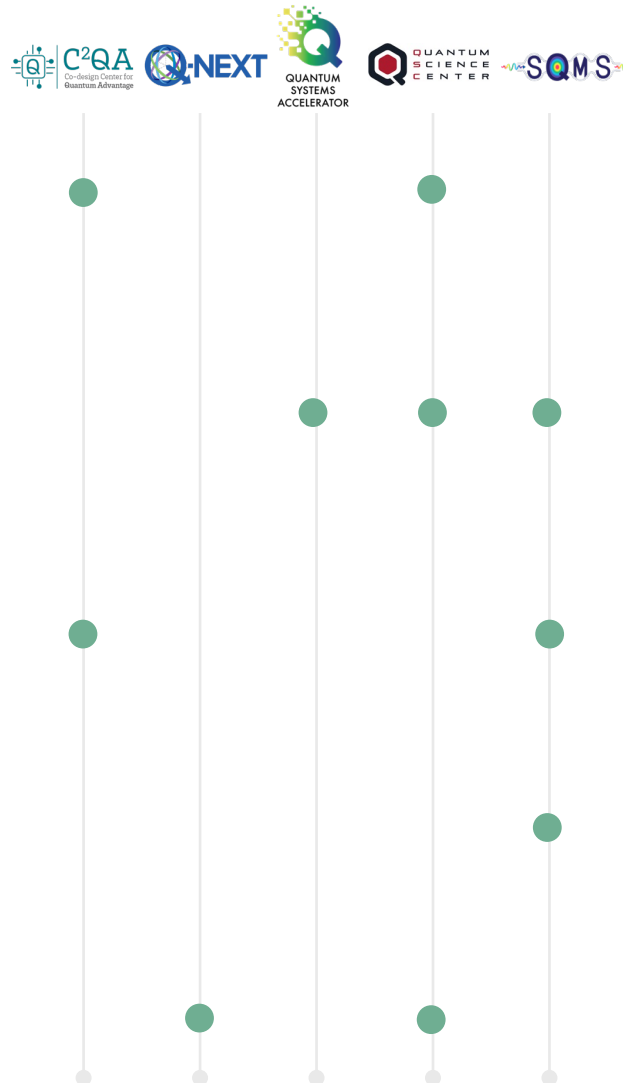
*Cryo-cooled ion trap device*





# 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*

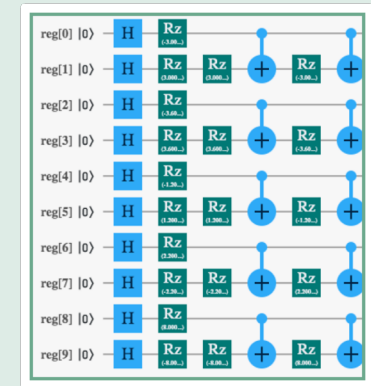
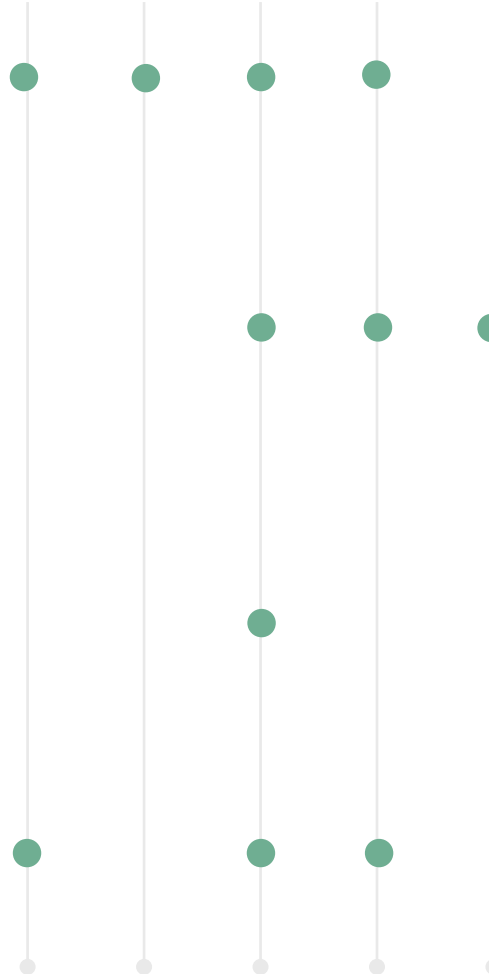


*Integration of high-quality cavities with qubits*

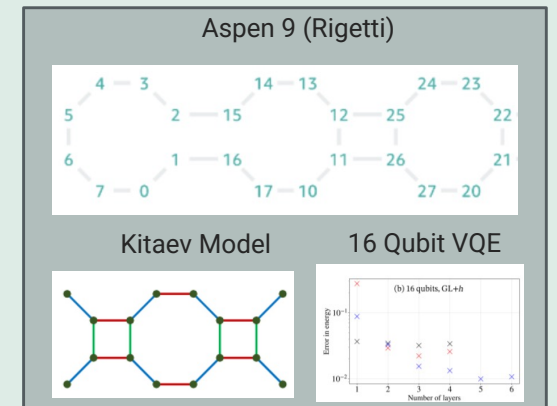


# Computing: Algorithms and Applications

- 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



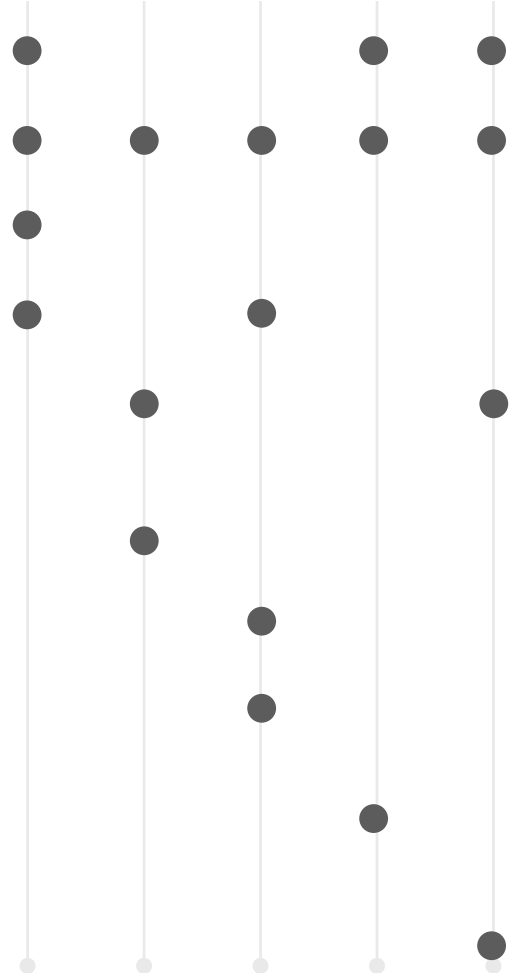
*A quantum circuit used for validating quantum devices*



*Efficient quantum simulations with geometric compatible hardware*

# 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

- Held a workshop to identify technical areas for coordination, and synergies between the centers
- Developed plans for cross-Center topical workshops exchange of technical information

## Instrumentation and Facilities

- Coordination for a workshop to include virtual tours of the light sources and other user facilities, a discussion of access procedures, and introductions to facility experts

## Workforce

- All Centers participated in a QIS Career Fair organized by C<sup>2</sup>QA
- Cross-promotion of Center workforce and student programs

## Management

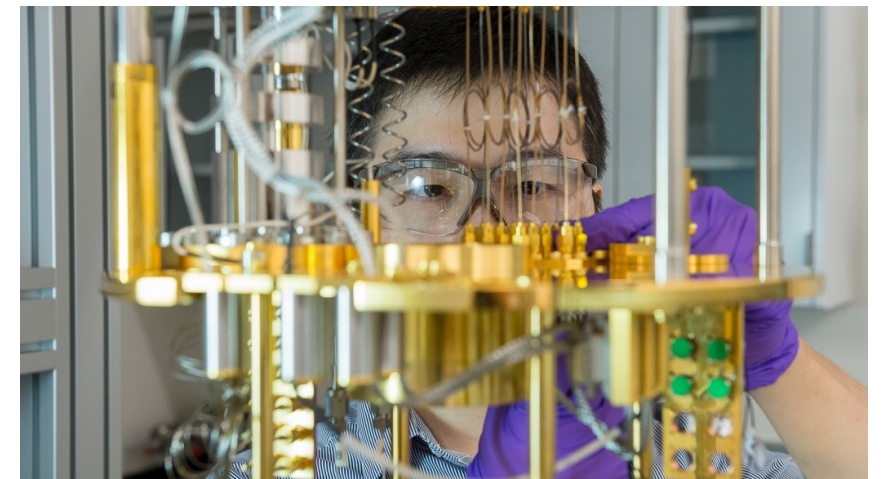
- Created a cross-Center operations group to share best practices in Center management and risk mitigation
- Developed plans for communities of practice in security and EH&S

## Communications / Outreach

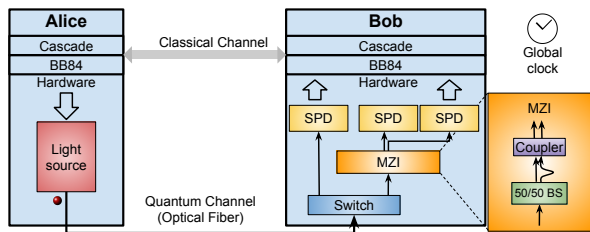
- Formed a coordinating group across Centers and development of joint materials
- NQISRC Panel accepted in the 2022 AAAS Annual Meeting



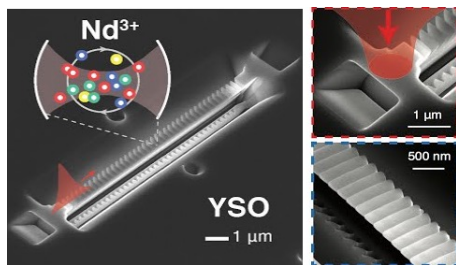
NQISRC Panel at QIS Career Fair hosted by  C<sup>2</sup>QA Co-design Center for Quantum Advantage



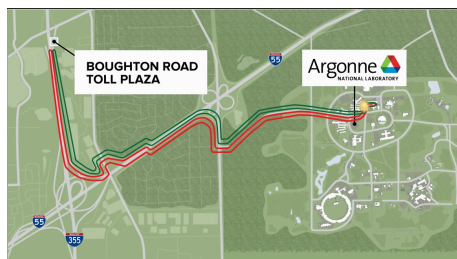
# Development of a comprehensive quantum network simulator



Optical components in a simple 2-node setup.



Q-NEXT quantum memory and repeater prototypes will be evaluated.



Simulations complement real-world experiments.

## Scientific Achievement

Q-NEXT is building a comprehensive network simulator (“SeQUeNCe”) that allows simulation of long-distance quantum interconnects at the photon-level with high accuracy, including modeling the behavior of quantum memories and repeater nodes. Q-NEXT research takes a co-design approach by linking system performance of repeater-enabled links with device-level properties.

## Significance and Impact

The simulator will allow performance evaluations of a broad range of Q-NEXT science and technology, and will provide a testbed for development of new protocols.

## Details

- We constructed models of elementary optical components (light sources, SPDCs, detectors, atomic memories) and implemented simple quantum network protocols (entanglement management, resource reservation, QKD).
- We built a prototype of the modularized discrete event simulator that includes a scheduler and an entanglement manager. We validated our models by simulating existing QKD and teleportation experiments and the behavior of a metropolitan network.
- SeQUeNCe is available for download at GitHub: <https://github.com/sequence-toolbox>
- X. Wu, A. Kolar, J. Chung, D. Jin, T. Zhong, R. Kettimuthu and M. Suchara. 2021. “SeQUeNCe: a customizable discrete-event simulator of quantum networks.” *Quantum Science and Technology*, 2021. <https://doi.org/10.1088/2058-9565/ac22f6>.
- M.K. Singh, L. Jiang, D.D. Awschalom, S. Guha, *IEEE Trans. on Quant. Eng.* V2, 4102909 (2021).

# Quantum phases of matter on a 256-atom programmable quantum simulator

## Accomplishment

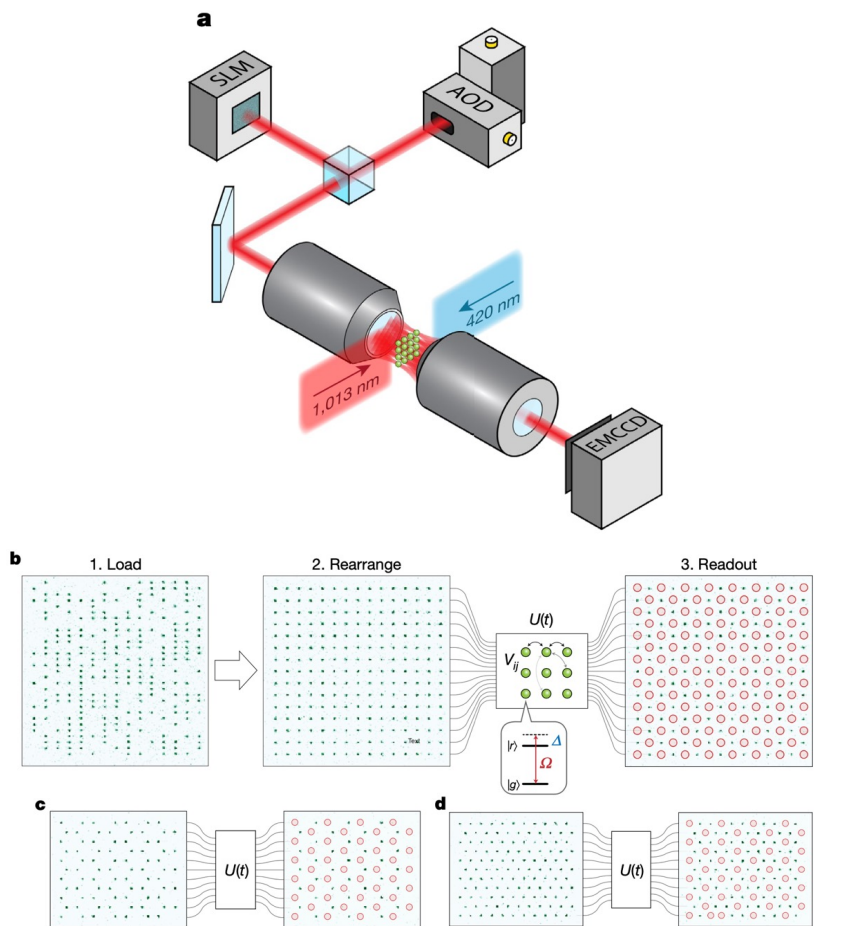
Studied quantum phases of a spin system using a programmable quantum simulator based on a two-dimensional array of neutral atoms in Rydberg states.

## 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)



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science

Work was performed at Harvard University, the University of Innsbruck, UC Berkeley, and MIT



QUANTUM SYSTEMS ACCELERATOR  
Catalyzing the Quantum Ecosystem



# 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.

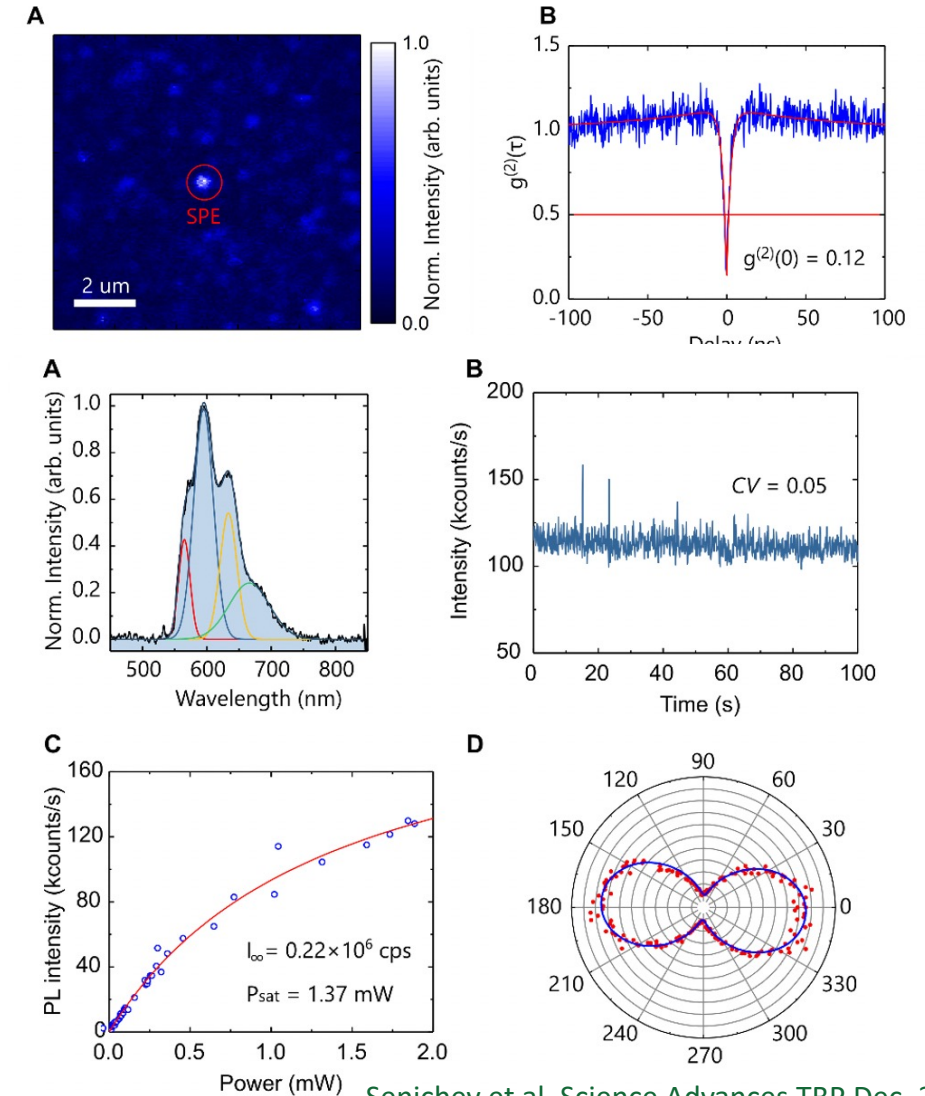
## Significance and Impact

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

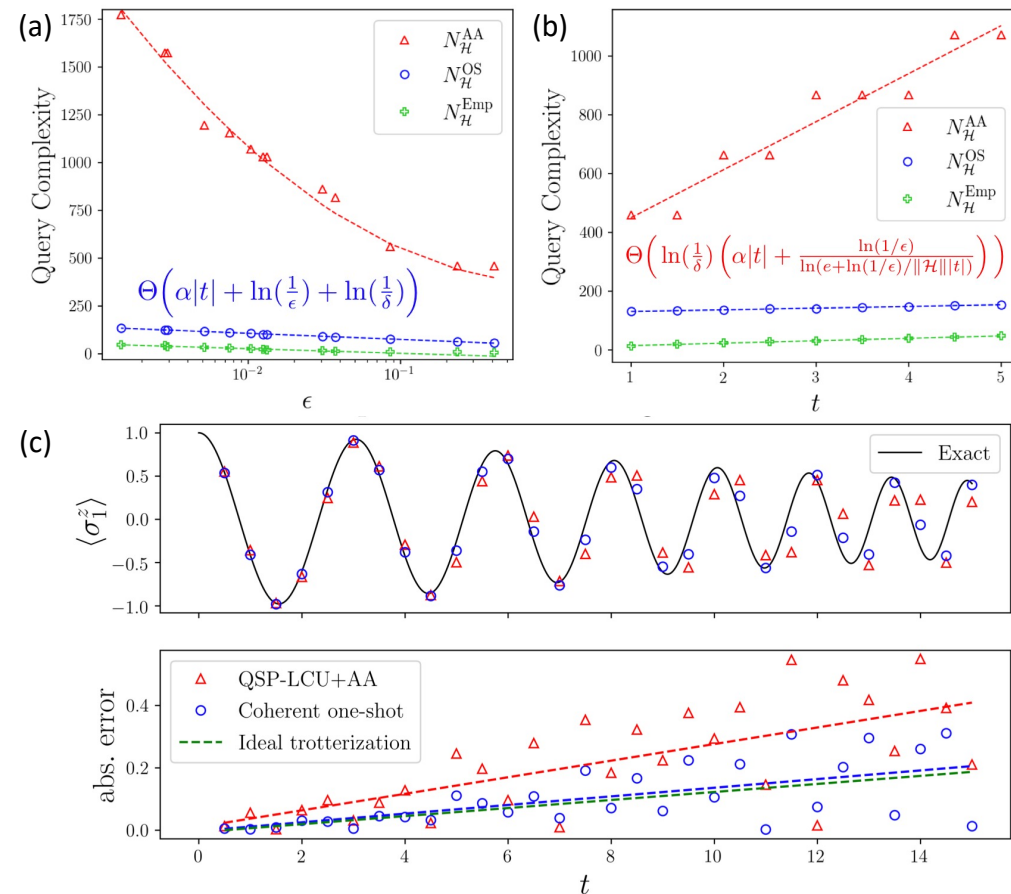
- Fabricated by HDPCVD and subsequent rapid thermal annealing
- SPEs are bright ( $>10^5$  counts/s), stable, linearly polarized
- High-purity single-photon emission with  $g^{(2)}(0) < 0.2$  without background correction or spectral filtering
- SPEs exhibit PL peaks at virtually the same wavelengths – 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

# C<sup>2</sup>QA Highlight - 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  $\epsilon$  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

## Scientific achievement

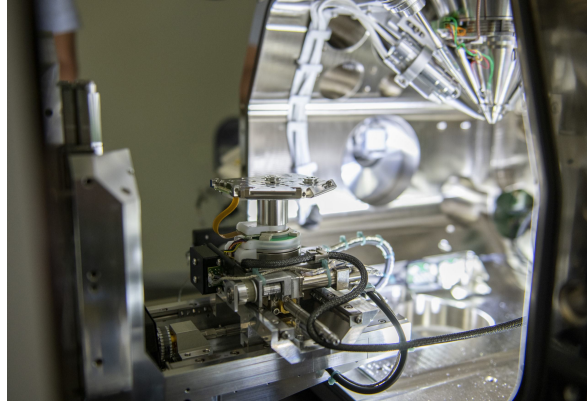
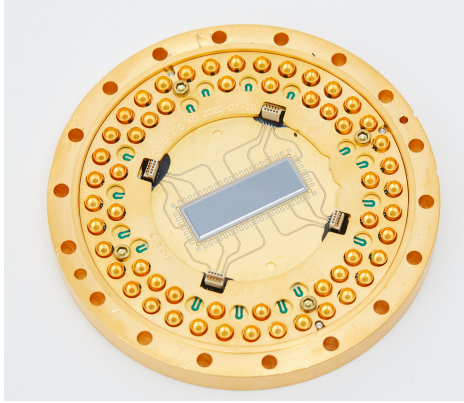
First ever performed cryogenic microscopy studies of superconducting qubits lead to the discovery of the presence of hydride precipitates in the Rigetti Computing and other transmon qubit devices

## Significance and Impact

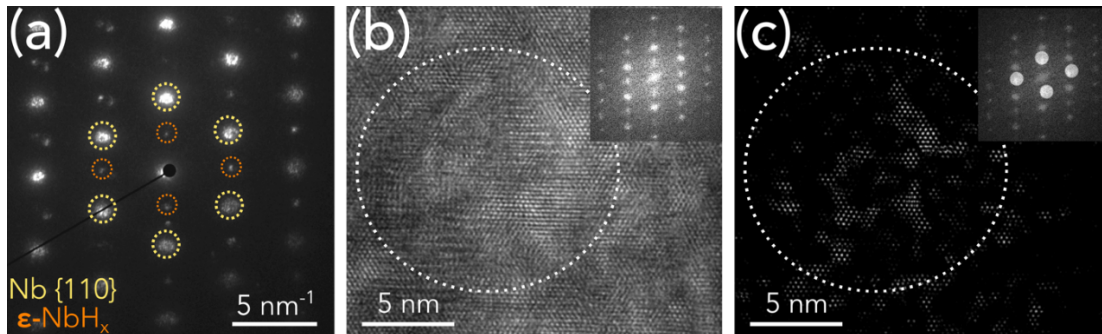
Niobium nano-hydrides are poorly superconducting phases that can cause qubit device performance limitations and degradation over time and with subsequent cooldowns

## 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
- Cross-Center workshop on algorithms and co-design approaches



## Instrumentation and Facilities

- Workshops 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<sup>2</sup>QA, to provide pathways into QIS
- Second meeting of Chief Diversity Officers for continued exchange of best practices and resources for QIS DEI
- Coordinated QIS summer school