Overview of ORNL Quantum Computing Capabilities and Interests

Presented at the
Quantum Testbed Stakeholder Workshop

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Washington, DC
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ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE
National Laboratory

Outline

- Laboratory strategy and history in QC
- LDRD investments in quantum computing
- Relevant ORNL capabilities and partnerships
- ORNL testbed facility model

Laboratory Strategy and History

ORNL Quantum computing materials and interfaces strategy

Opportunity

- Integrate core competencies in materials, modeling, and isotopes to establish a broad R&D effort in quantum computing
- Create S&T base to drive computing beyond exascale and into quantum computing

ORNL assets

- Expertise in quantum information science and quantum computing
- Unique resources for materials characterization
- Strengths in first principles theory, modeling, and simulation for quantum materials
- National User Facilities: CNMS, OLCF, SNS

Strategy

- Develop tools necessary to characterize and design high-fidelity physical qubits
- Explore methods to interface qubits to traditional computers
- Develop a multi-qubit research test bed
- Research methods to program multi-qubit systems
- Foster multiagency ties to secure long-term funding

Outcome
Cross-cutting R&D portfolio establishing ORNL as a national leader in quantum computing

Quantum computing in context

In the sciences

1980s–1990s
A curious idea; first quantum algorithms

2000s
Proof-of-principle demonstrations
Initial QC hardware
Error correction and control theory

2010s
Focus on practicality and improving quality and control
Circuit synthesis

Current status
Qubit fragility presents tremendous challenges
Attempt to broaden suite of applications

At ORNL: Internal (LDRD) and programmatic support

2000–present:
Photonic quantum communications
Pioneering studies of photon entanglement
State-of-the-art photon sources for QI applications
Integrated photonic circuits for QI processing
Quantum communications to secure power grid

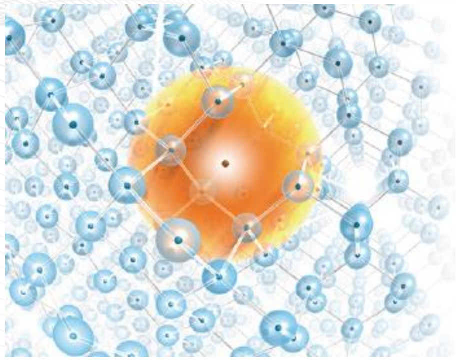
2008–present: Quantum computing
Modeling and simulation of noise and error in quantum circuits
Quantum hardware description language
High-performance computing with quantum accelerators

2011–present: Quantum sensing
Sub-shot-noise detection
Plasmonic sensors for chem/bio detection

Scientific motivator: "…potential ability to realize full control of large-scale quantum coherent systems…"
BESAC: Challenges at the Frontiers of Matter and Energy, 2015

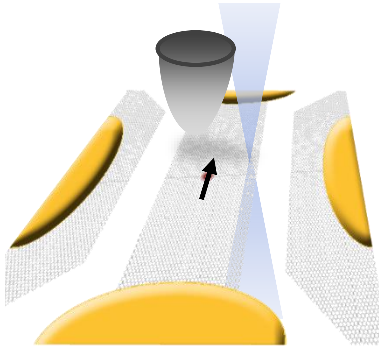
LDRD investments in QC

Current Quantum Computing LDRD: $6M of investments (FY16-18)

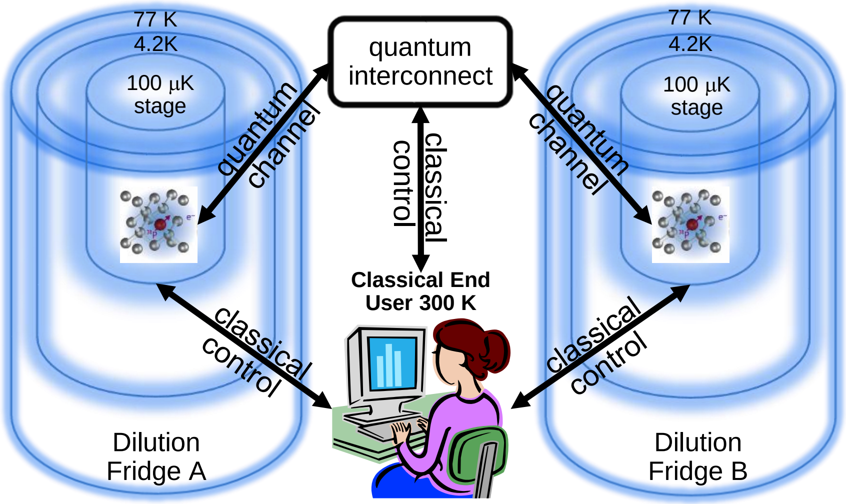


P donor in Si
(Humble, Lupini)

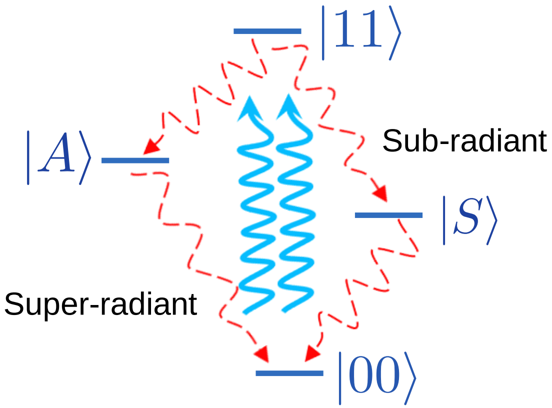
Qubit operations
Heat dissipation
(Peters)



Graphene Qubit
(Jesse)

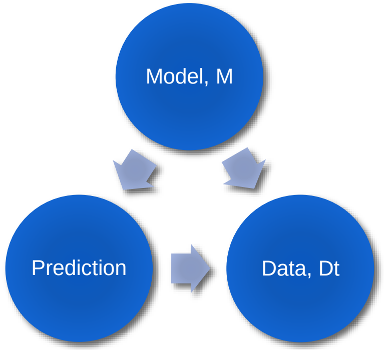


Quantum/Classical Interfaces (Lougovski)

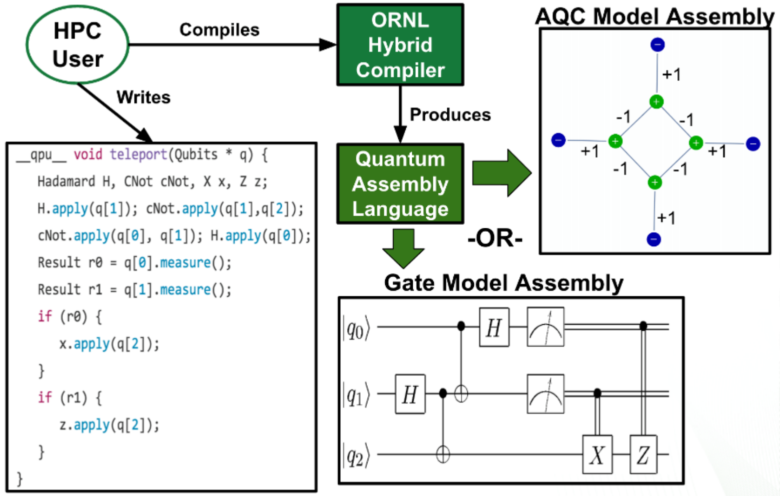


$$|S\rangle = |01\rangle + |10\rangle$$
$$|A\rangle = |01\rangle - |10\rangle$$

Dissipative QC (Evans)



Qubit fidelity modeling
(Bennink)



Qubit Compiler
(McCaskey)

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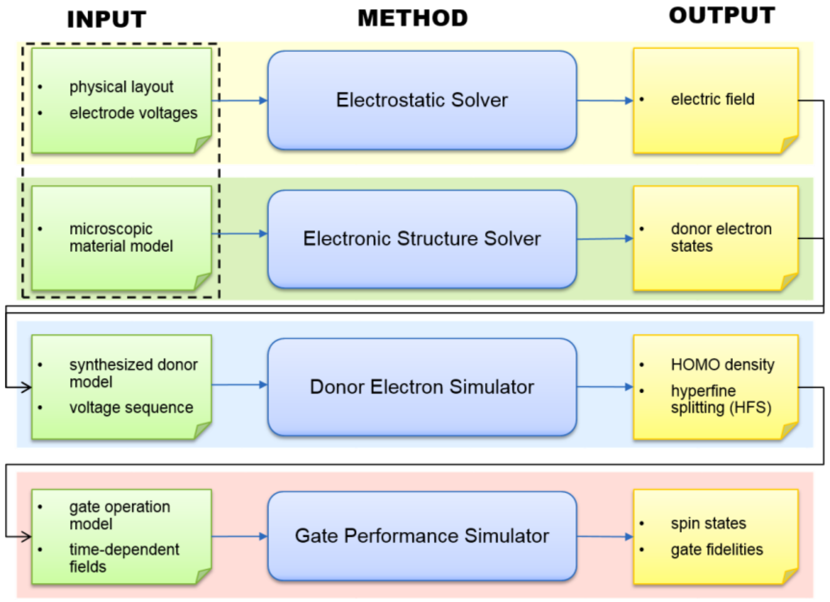
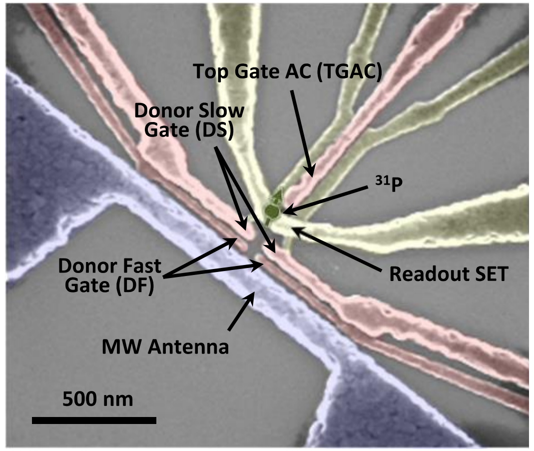
Quantum Device Modeling and Simulation

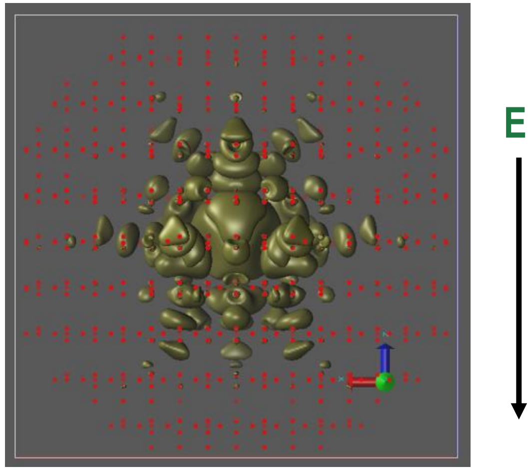
- **Few-qubit systems are within reach of exact, high-fidelity modeling and simulation**
  - We can compare model expectations to experimental observations, qubit behaviors
- **Modeling and simulation provide a means of testbed design verification and device validation**



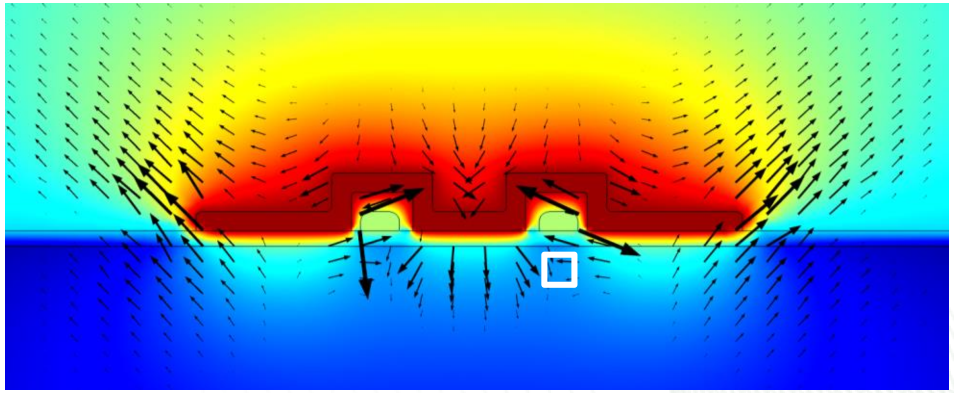
Computational Workflow for Verifying Qubit Design (Humble et al. 2016)



Photograph of P-doped silicon donor device from UNSW (Laucht et al. 2015)

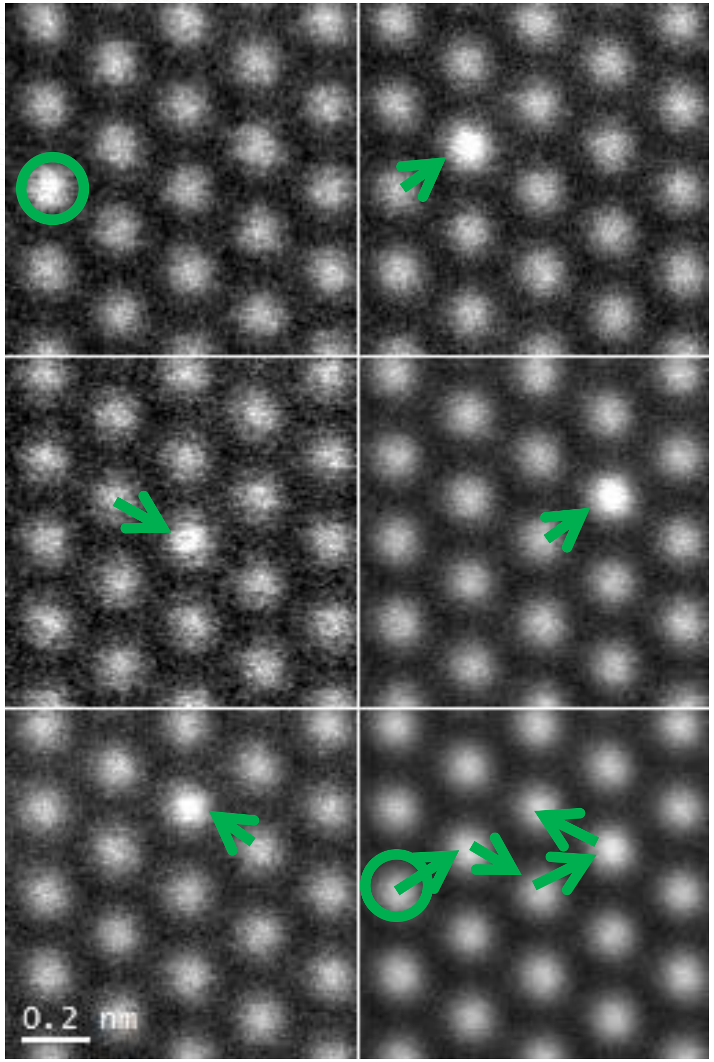


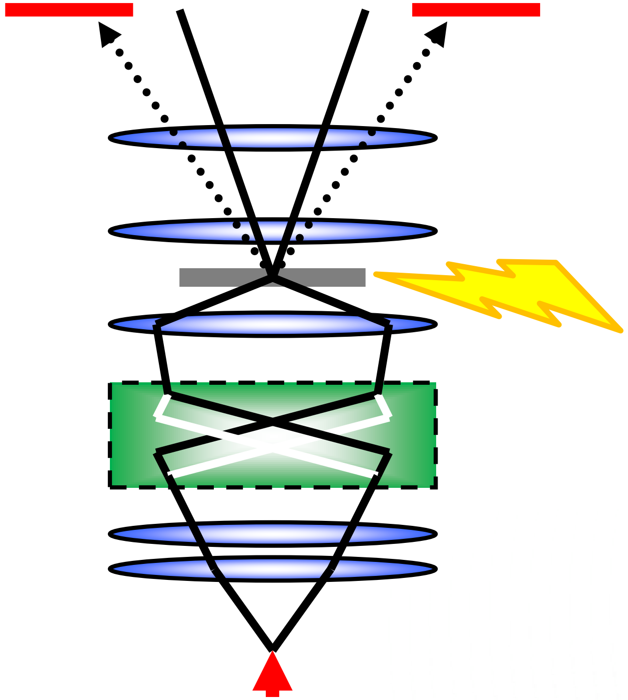
HOMO spin density of Si:P using DFT (Jakowski et al, 2016)



Low-temperature EM potential calculations with field arrows for UNSW device (Curtis et al. 2016)

Scanning Transmission Electron Microscopy





EELS
Electrical properties at atomic resolution

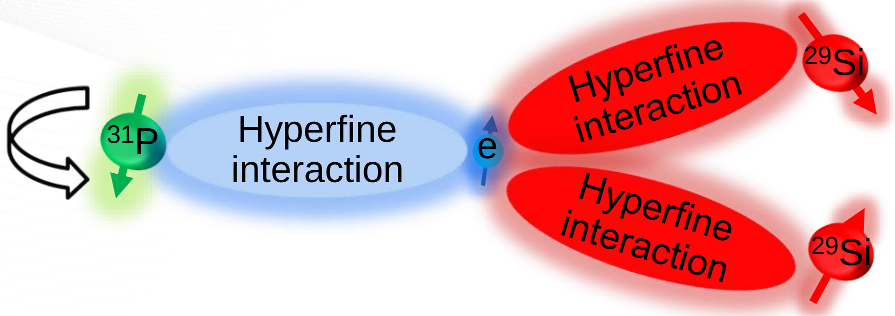
Z-Contrast Imaging
Image and analyze single dopant atoms

Cathodoluminescence
Probe the quantum state of complex systems at high spatial resolution

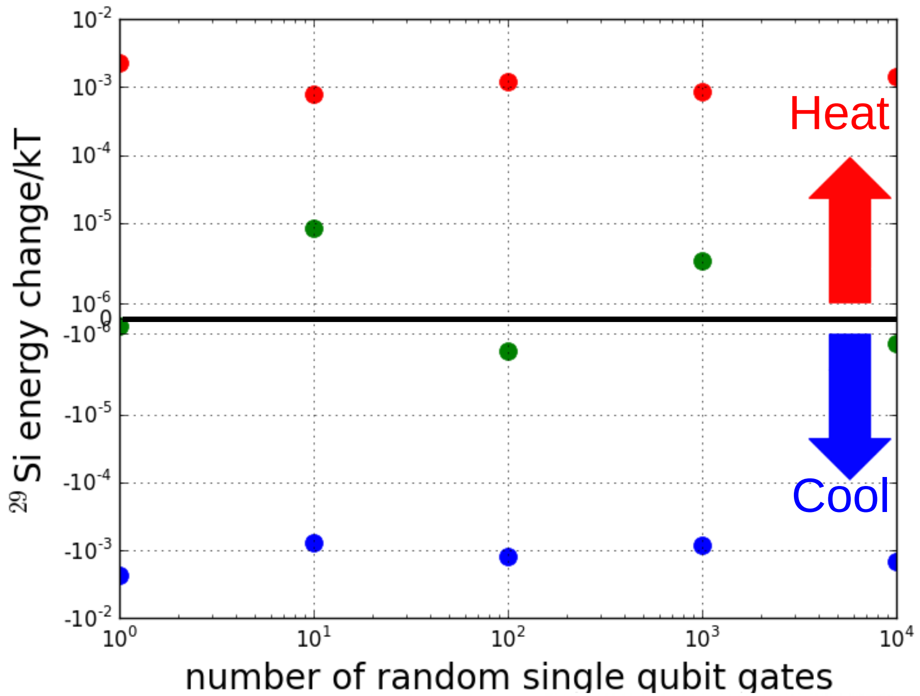
High-Energy Beam
Able to manipulate samples at atomic scale

5 consecutive positions of a single Bi in Si dopant moving under electron-beam irradiation. The final panel that shows the sum of all 50 frames, and arrows indicate the steps between positions.

Qubit Operations & Heat Dissipation



Qubit operations (gates) couple to the substrate!

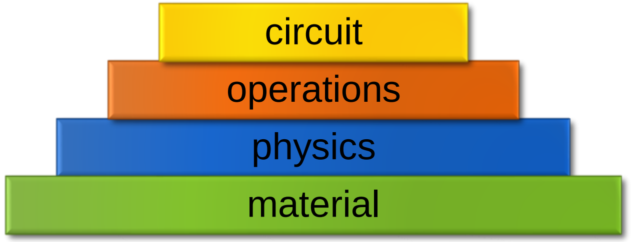


- Developed Hamiltonian simulations for ~10 spin qubits
- Unexpected discovery: gates can ***cool*** or ***heat*** Silicon (Si) quantum computers depending on random ^{29}Si location
- Results indicate heating is not a problem for near term testbeds but may need to be considered for large processors

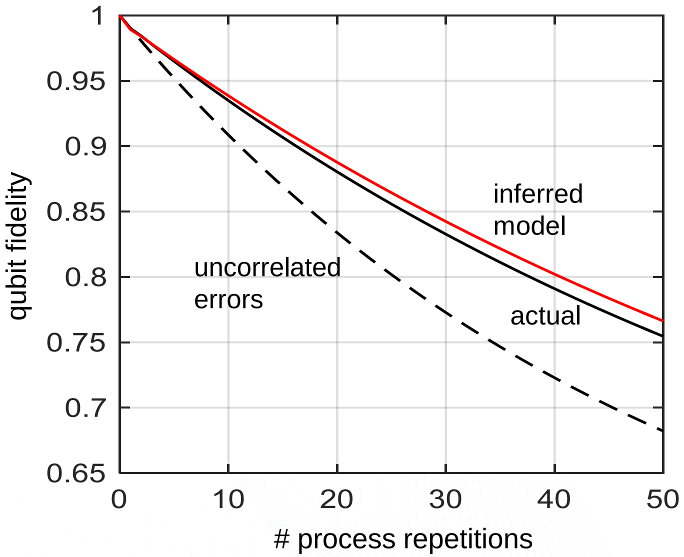
P. Lougovski & N. A. Peters *in preparation* (2017).

Advanced Characterization Theory

Problem
- Qubit operations must be characterized accurately to predict reliability of quantum computations
- Established methods do not characterize correlated noise and control drift

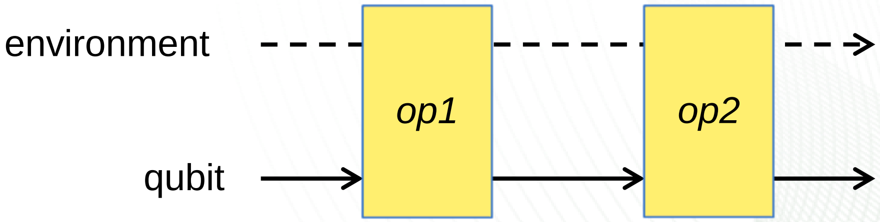


Approach
- Infer operational model solely from operation data
- Model dimension is free parameter



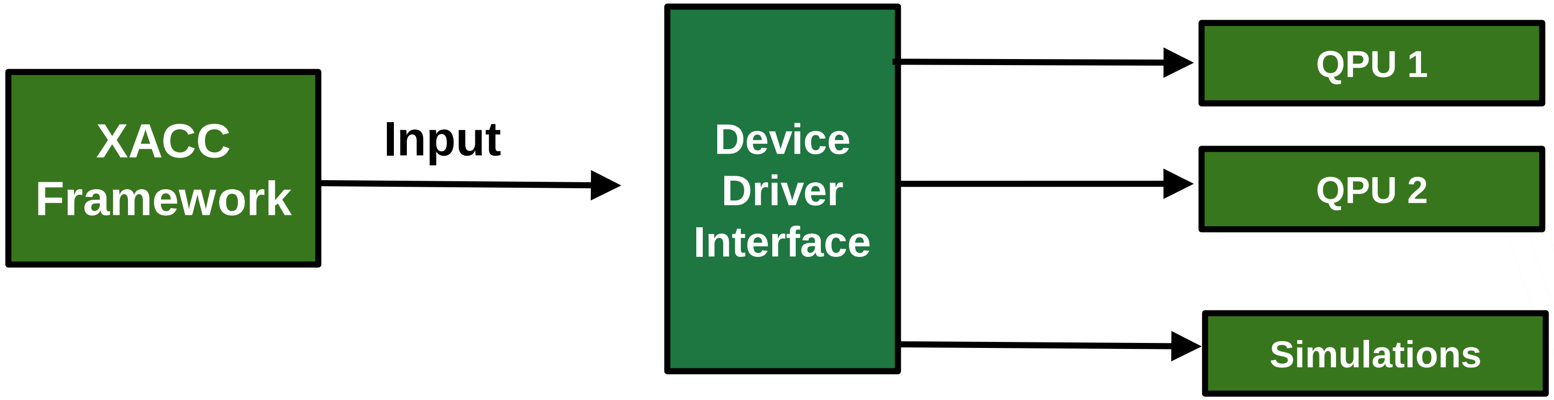
Status (15 months)
- Formally determined necessary and sufficient experiments for complete device characterization
- Devised theory & software to fully characterize a quantum process (dynamical dimension, parameters)

Next Steps
- Extend method to multiple operations
- Uncertainty quantification
- Adaptive/optimal characterization



Quantum Acceleration in Scientific High Performance Computing

- **We use a modular programming framework to enable quantum acceleration within existing HPC applications,**
  - Open source code https://github.com/ORNL-QCI/xacc
- **A programming framework that is language and device agnostic**
  - Users write **kernels** using Scaffold, Quipper, ProjectQ, etc.
  - The XACC framework manages the run-time and kernel execution
  - The framework enables integration with quantum processing units (IBM, D-Wave) as well as numerical simulator backends



A quantum kernel definition

```
// Quantum Kernel executing teleportation of
// qubit state to another.
const std::string src("__qpu__ teleport (qbit& qreg) {\n"
                      "   // Initialize qubit to 1\n"
                      "   X(qreg[0]);\n"
                      "   H(qreg[1]);\n"
                      "   CNOT(qreg[1],qreg[2]);\n"
                      "   CNOT(qreg[0],qreg[1]);\n"
                      "   H(qreg[0]);\n"
                      "   cbit c1 = MeasZ(qreg[0]);\n"
                      "   cbit c2 = MeasZ(qreg[1]);\n"
                      "   if(c1 == 1) Z(qreg[2]);\n"
                      "   if(c2 == 1) X(qreg[2]);\n"
                      "}\n");
```

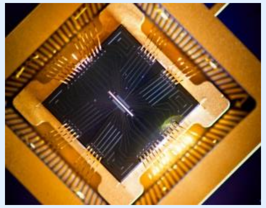
```
int main (int argc, char** argv) {
    // Create a reference to the IBM5Qubit Accelerator
    auto ibm_qpu = std::make_shared<IBM5Qubit>();
    // Allocate some qubits, give them a unique identifier...
    auto qbits = ibm_qpu->allocate("qreg", {0,1,2});
    // Construct a new Program
    xacc::Program quantumProgram(ibm_qpu, src);
    // Build the program
    quantumProgram.build("--compiler scaffold --writeIR teleport.xir");
    // Retrieve the constructed kernel
    auto teleport = quantumProgram.getKernel("teleport");
    // Execute the kernel!
    teleport(qbits);
    // Get the execution result
    qbits->printState(std::cout);
}
```

Example API usage

Quantum Interconnect for Dissimilar Matter Qubits

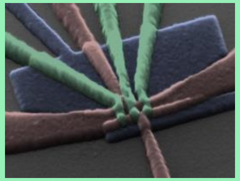
Qubit Testbed

Trapped Ions



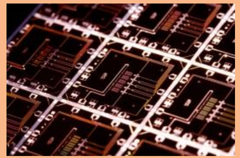
jqi.umd.edu/news/future-ion-traps

Silicon



10.1126/science.aal2469

Superconducting



doi:10.1038/nature13171

Quantum Interconnect via Spectrally-Encoded Photonic Qubits

J.M.Lukens & P.Lougovski, Optica **4**(1), 8-16 (2017)

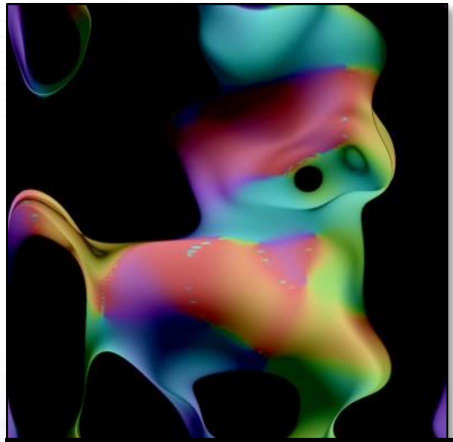
Advantages of Spectral Interconnect:

- Uses off the shelf telecom equipment
- Deployable over existing fiber networks
- Matches dissimilar matter qubits
- Frequency multiplexing enables scalability
- Interferometric stability (single spatial mode operations)
- Reconfigurable without changing hardware
- Provides arbitrary matter qubit connectivity

Relevant ORNL capabilities and partnerships

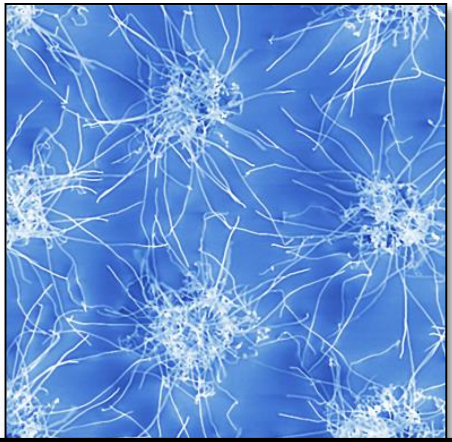
Center for Nanophase Materials Sciences provides capabilities for qubit research

Synthesis



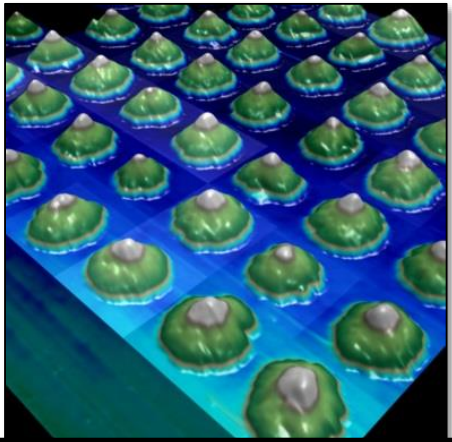
2D, precision synthesis, selective deuteration

Nanofabrication



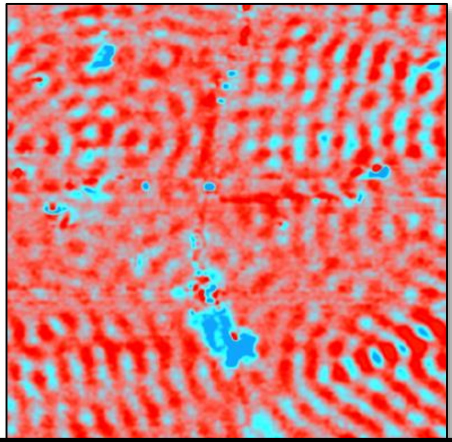
Direct-write, microfluidics, cleanroom

Advanced microscopy



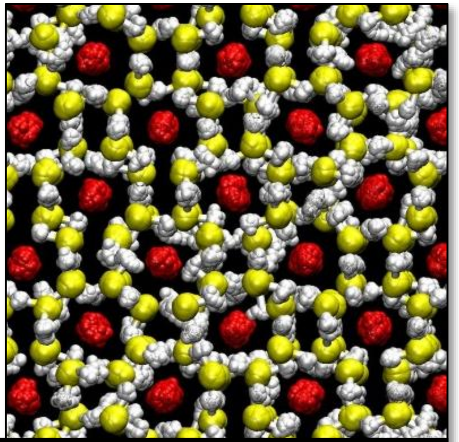
AFM (a CNMS specialty), STM, aberration-corrected TEM/STEM, atom probe tomography

Functional characterization



Laser spectroscopy, transport, magnetism, electromechanics

Theory and modeling

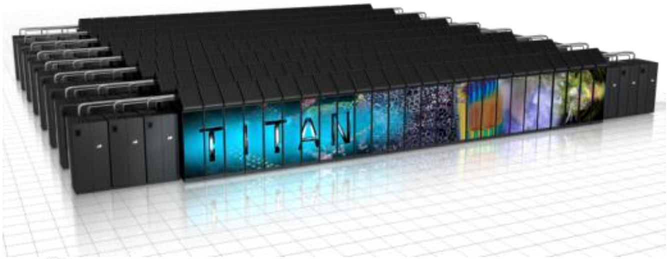


Nanomaterials Theory Institute; gateway to leadership-class high-performance computing

Oak Ridge National Laboratory

Oak Ridge Leadership Computing Facility (OLCF) is one of the world’s most powerful computing facilities

- Provide world’s most powerful open resources for scalable computing and simulation, data and analytics, and infrastructure for science
- Deliver leading-edge science relevant to missions of DOE and key federal and state agencies
- Attract the brightest talent and partnerships from all over the world
- Invest in cross-cutting partnerships with industry
- Summit will replace Titan as the OLCF’s leadership supercomputer



Titan

Peak performance	27 PF/s
Memory	710 TB
Disk bandwidth	240 GB/s
Square feet	5,000
Power	8.8 MW

Gaea

Peak performance	1.1 PF/s
Memory	240 TB
Disk bandwidth	104 GB/s
Square feet	1,600
Power	2.2 MW

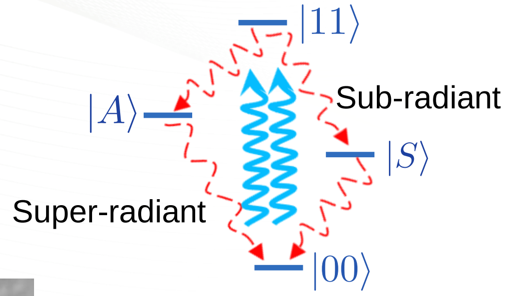
Beacon

Peak performance	210 TF/s
Memory	12 TB
Disk bandwidth	56 GB/s

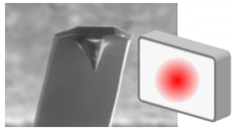
Eos

Peak performance	240.9 TF/s
Memory	47 TB
Disk bandwidth	30 GB/s

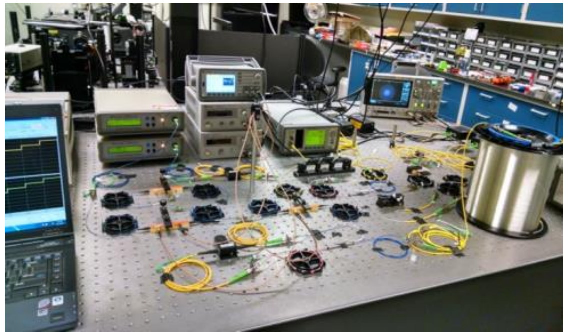
The Quantum Information Science Group supports research and development in a variety of quantum technologies



Optical Pumping



QUANTUM
INFORMATION SCIENCE
OAK RIDGE NATIONAL LABORATORY



Quantum Sensing

- Compressive Quantum Imaging
- Quantum Plasmonic Sensors
- Ultra-sensitive MEMS Displacement
- Standoff Spectroscopy
- Opto-mechanical Force Microscopy

Quantum Computing

- Circuit Model Simulations
- Analog Digital Quantum Simulations
- Physical Qubits Modeling
- Quantum Characterization, Verification and Validation

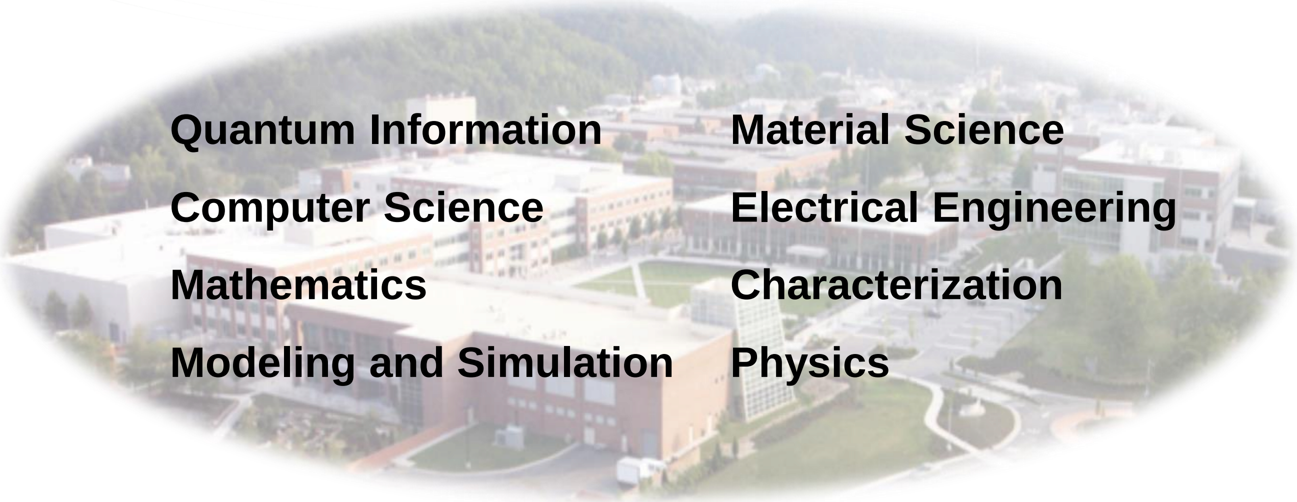
Quantum Communication

- Quantum Networks
- Quantum Key Distribution
- Quantum Secret Sharing
- Quantum Random Number Generators

More information:
https://www.ornl.gov/division/csed/quantum-information
Contact: gricew@ornl.gov

The Quantum Computing Institute provides lab-wide integration of our unique capabilities and partnerships

- **ORNL interaction point for resources in quantum computing**
  - *Our mission is to foster collaborations and partnerships in developing quantum computing for scientific applications of next generation computing systems*
- **The QCI leverages expertise across ORNL:**



Quantum Information	**Material Science**
Computer Science	**Electrical Engineering**
Mathematics	**Characterization**
Modeling and Simulation	**Physics**

- **Focused Research, Community Outreach, Partnerships, User Support, Facilities**
- **40+ staff and associates working on collaborative research**

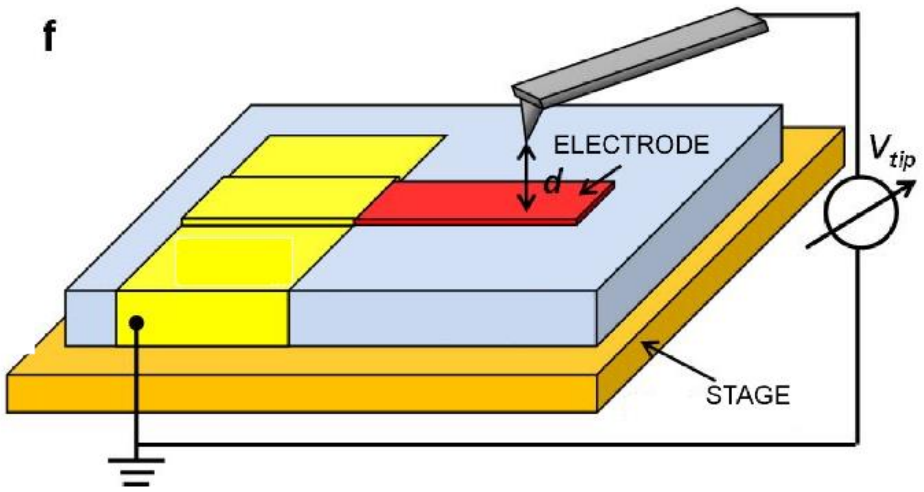
More information available at quantum.ornl.gov

Our partnership network leverages expertise from academia, industry, and government

IBM
Georgia Tech
University of Virginia
The University of Tennessee UT
Virginia Tech
APL Johns Hopkins Applied Physics Laboratory
MIT Lincoln Laboratory
Georgia Tech Research Institute
University of Toronto
Illinois University of Illinois at Urbana-Champaign
Purdue University
Sandia National Laboratories
NASA
ARL
Texas The University of Texas at Austin
Vanderbilt University
University of Nebraska Lincoln
D-Wave
GE Global Research
Qubitekk
Pacific Northwest National Laboratory Proudly Operated by Battelle Since 1965
Naval Air Systems Command
OU The University of Oklahoma
Lockheed Martin
جامعة خليفة Khalifa University
Raytheon BBN Technologies
WKU
SIU Southern Illinois University Carbondale
QxBranch
Applied Communication Sciences
NC State University
Universidad del País Vasco Euskal Herriko Unibertsitatea
IDQ
Florida State University 1851
Schola Genevensis 1559
Oak Ridge National Laboratory

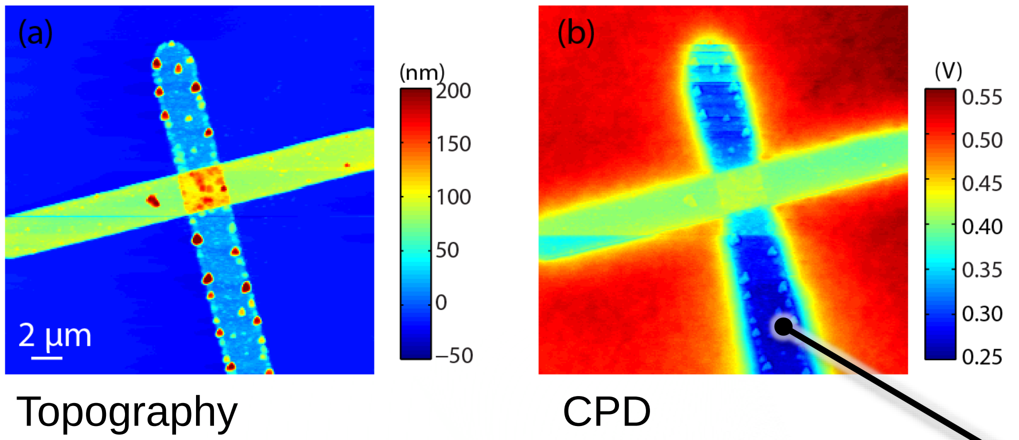
Kelvin probe force microscopy with MIT Lincoln Laboratory

Understanding anomalous heating of ion-trap qubits using Kelvin probe force microscopy (KPFM) and X-ray photoelectron spectroscopy



Kelvin probe AFM: DC/AC biased probe detects electrostatic forces on a sample surface, mapping work function on a surface with nanometer precision

Understanding surface contamination of superconducting qubits: Standard AFM and KPFM imaging on model Au/Si sample

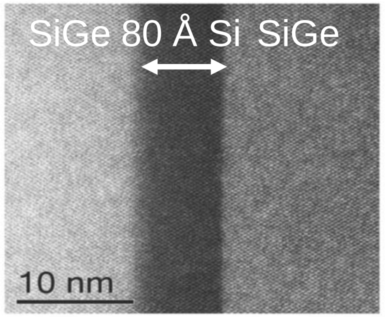


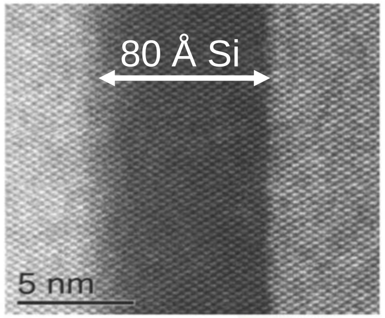
Small blue dots: Distortions in work function map may be due to localized distortions in the electric field caused by residual contaminants (both distortions and contaminants may be detectible using this technique)

L. Collins et al., "Multifrequency spectrum analysis using fully digital G-mode-Kelvin probe force microscopy," ***Nanotechnol.*** In press

Partnerships: Interfacial optimization for improved qubit devices

Understand electrostatically gated quantum dot structures in SiGe/Si/SiGe heterostructures



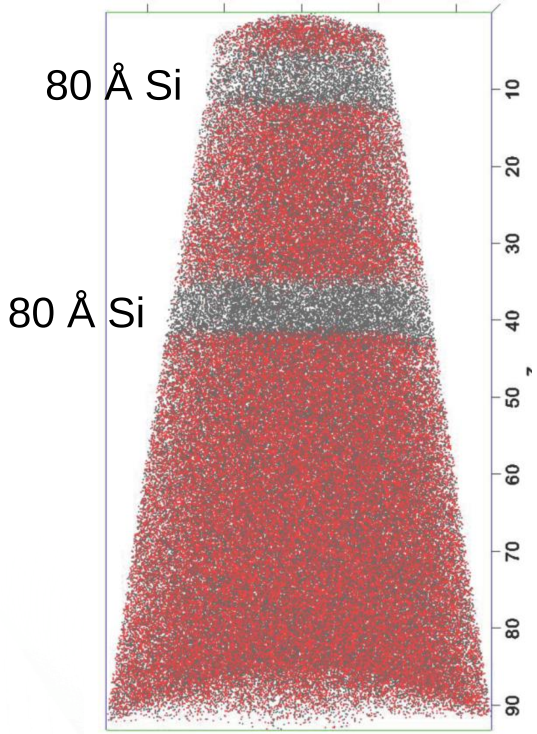


Z-contrast STEM images of 80 Å Si well reveal an atomically "sharp" Si/SiGe interface and a "10 Å diffuse" Si/SiGe interface

Collaboration to investigate SiGe/Si/SiGe interfacial structures and chemistries at the sub-Å level

Partner grows SiGe/Si/SiGe via chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) under various deposition conditions

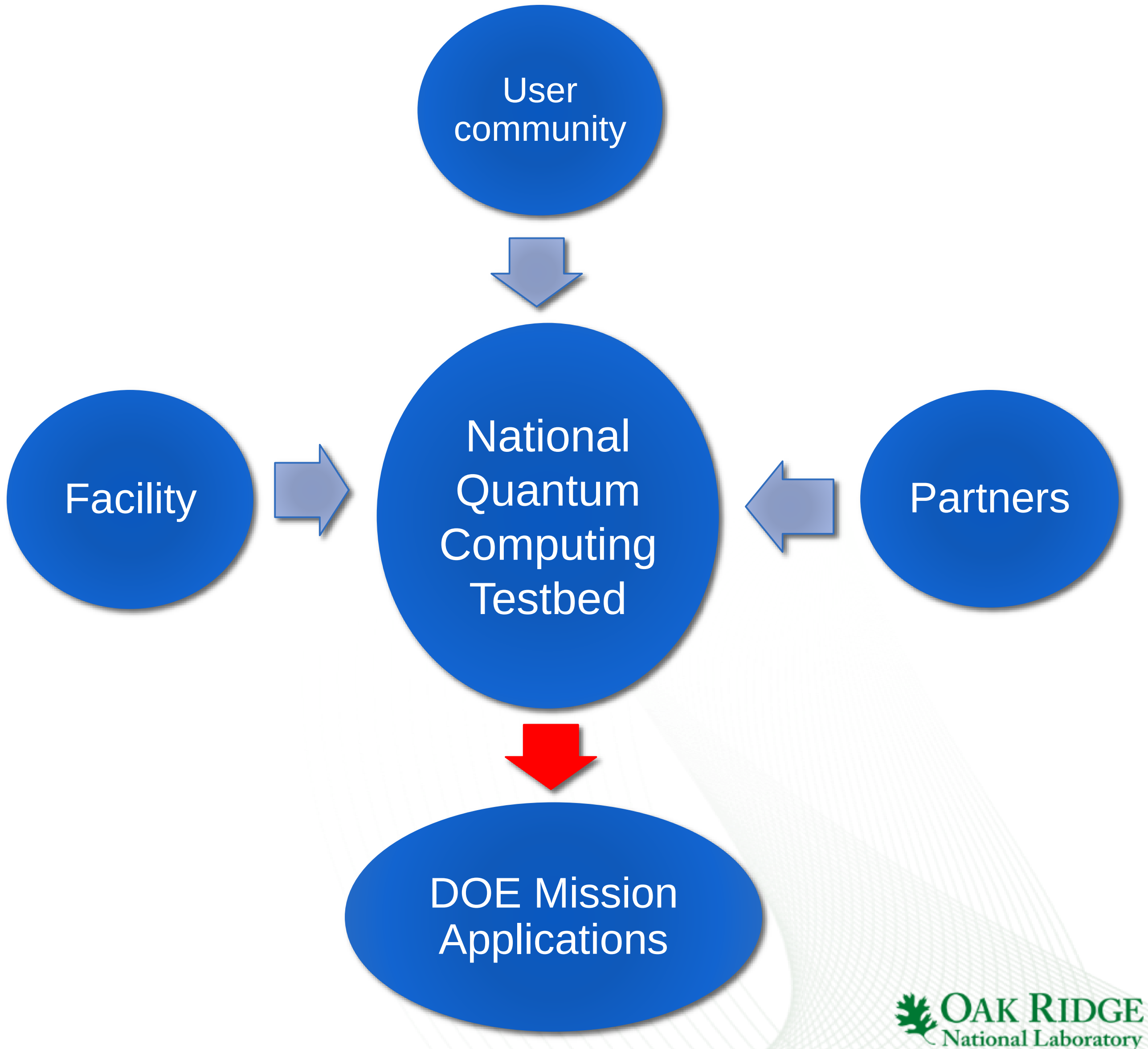
ORNL optimizes CVD and MBE processing variables and reliably produces high-fidelity interfaces through application of expertise in aberration-corrected Z-contrast STEM imaging, electron energy loss spectroscopy, and atom probe tomography to provide the single-atom-level understanding of defects, interfacial steps/terraces, chemistry, composition, and structural thermal stability



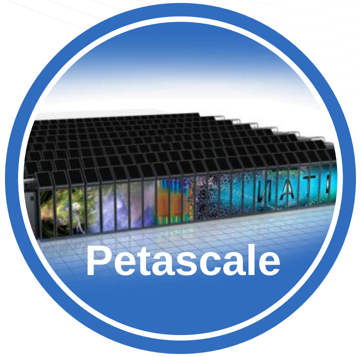
Atom probe tomography map of a double-Si-well heterostructure (Si: grey; Ge: red)

A Vision for the ASCR National Quantum Computing Testbed

- **A user community dedicated to research, development, and deployment of new devices**
  - Scientific use case research
  - Software and programming development
  - Hardware deployment and integration
  - Training and career development
- **A facility for collaboration and partnership**
  - A venue for quantum co-design
  - A platform for testing common standards
  - An experiment in quantum computing practice
- **A national resource for advanced computing research for DOE missions**



The Path to Quantum Computing



- Quantum Computing will accelerate research solving DOE mission problems after exascale
- A quantum computing testbed will require the interdisciplinary scientific workforce that a large multipurpose Lab provides
- ORNL operates open user facilities for the Office of Science with well over 3,200 users per year
- ORNL maintains extensive collaborations with universities, industry and other Labs in QC and QIS
- We are excited and vested in making Quantum Computing a reality!