



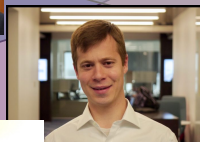
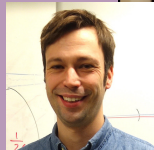
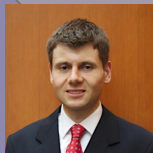
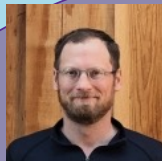
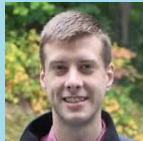
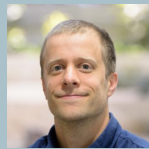
November 15, 2021

# SIMULATION & SYSTEMS RESEARCH AT THE Q-NEXT CENTER

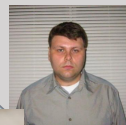
**Martin Suchara**  
Thrust Lead

# THE QUANTUM SIMULATION & SYSTEMS PRINCIPAL INVESTIGATORS

## Modeling & Optimization of Systems

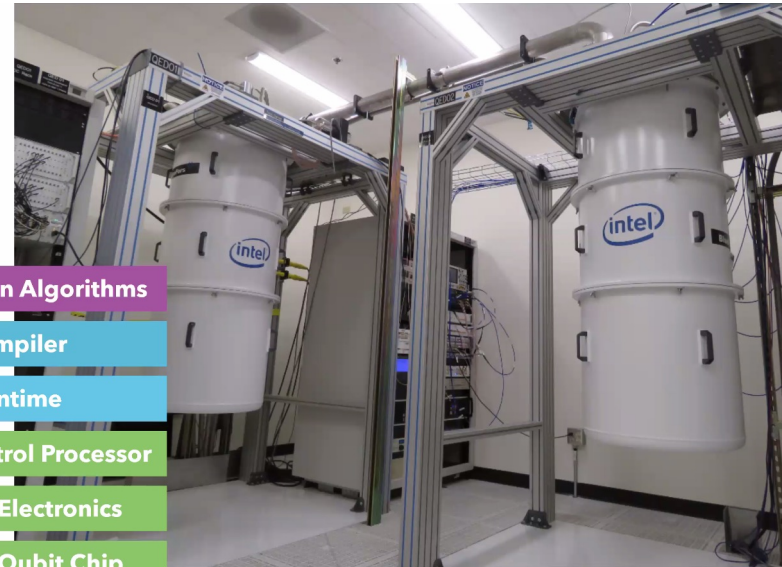


## Material Simulations on Quantum Computers



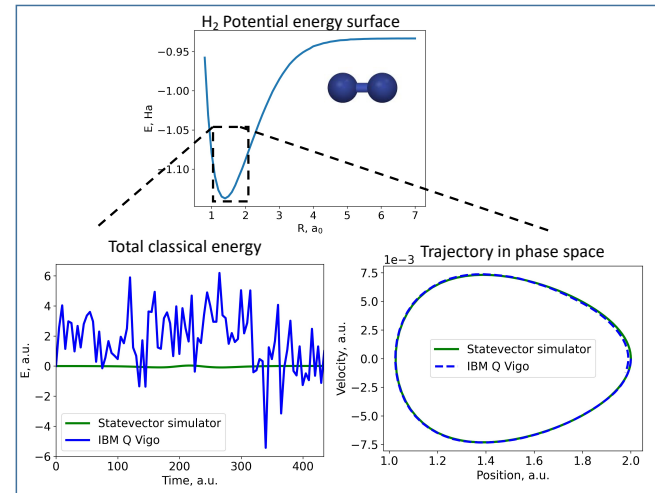
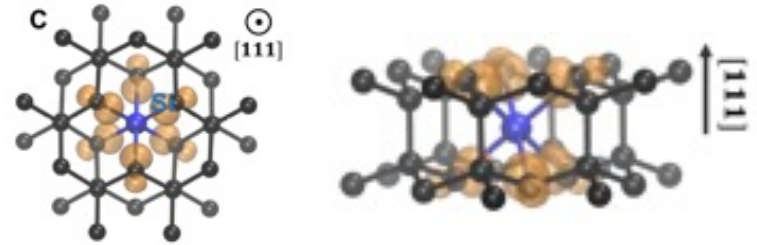
# PROJECT FOCUS AREA 1: MULTI-QUBIT SYSTEM ENGINEERING

- We perform full-stack quantum system research that spans qubit control, pulse-engineering techniques that optimize gate fidelity, and systems architecture research
- Our scientists are collaborating with Intel and ColdQuanta on development of fully-functional silicon spin qubit and neutral atom testbeds
- Open quantum system simulations will allow studying and addressing noise in these systems



# PROJECT FOCUS AREA 2: MATERIAL SIMULATIONS ON QUANTUM COMPUTERS

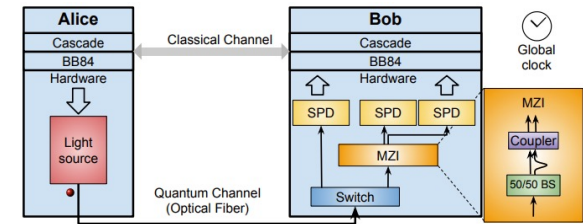
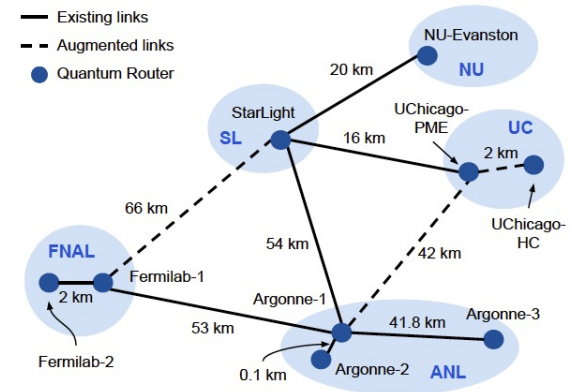
- We are building a comprehensive toolbox that allows first-principles electronic structure calculations of the Q-NEXT center materials
- The toolbox will be used to study color centers and defects in SiC, develop theories to model phonons, and study spin-dynamics
- Research combines the use of quantum computers and classical supercomputers, and leverages our quantum algorithms and compilers research





# PROJECT FOCUS AREA 3: ENTANGLEMENT IN COMMUNICATION, COMPUTING AND SENSING

- We introduced the first US-based quantum network simulator and plan to use it to help develop and standardize the future quantum internet
- We also study modularized quantum computing architectures, quantum compilers and quantum algorithms that exploit entanglement
- Finally, we design new sensing protocols for metrologically useful entanglement in arrays of solid-state and atomic qubits

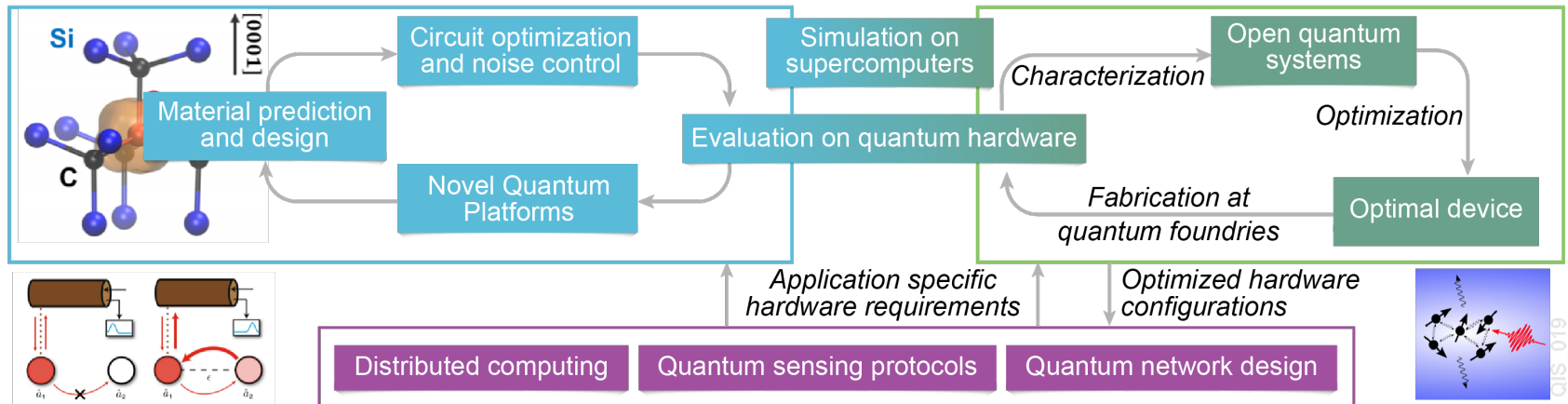




# THRUST INTEGRATION AND COLLABORATIVE USE OF FACILITIES

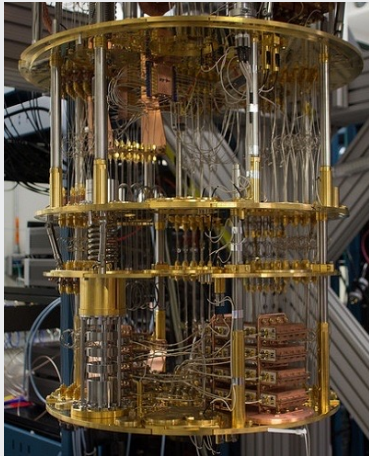
# PROJECT INTEGRATION AND INTERSECTIONS WITH OTHER THRUSTS

- Material and device models (with the Materials & Integration and Quantum Foundries thrusts)
- Simulators and protocols for long-distance communication (with the Quantum Communication thrust)
- Sensing across length and frequency scales (with the Quantum Sensing thrust)



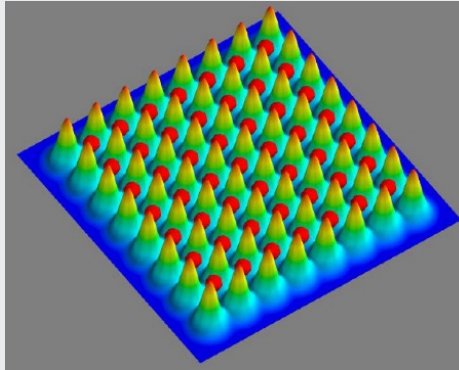
# PLANNED USE OF QUANTUM TESTBEDS AT Q-NEXT

IBM Q



Superconductors  
65 qubits  
 $F_1=0.999$ ,  $F_2=0.98$

ColdQuanta



Neutral atoms  
121 qubits  
 $F_1=0.991$ ,  $F_2=0.95$

Intel Testbed



Silicon spin qubits  
27+ qubits  
 $F_1=0.9996$ ,  $F_2=0.98$



# QUANTUM SIMULATORS AND COMPUTING FACILITIES



- High-performance computers and quantum simulators at Argonne
- Contact me to learn about available open-source simulators and facility access



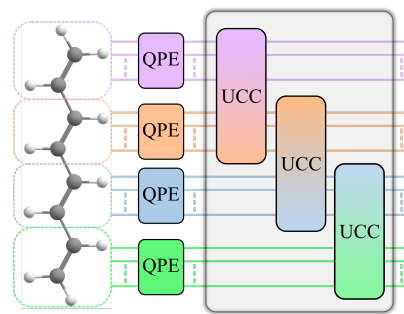
# SCIENTIFIC HIGHLIGHTS

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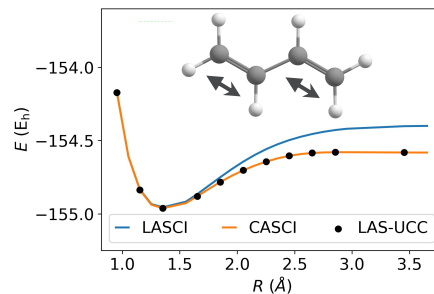
## Localized Active Space Methods for Quantum Chemistry Calculations on Quantum Computers

- A favorably scaling fragmentation-based approach was designed to obtain wave functions for strongly correlated compounds
- Demonstrates that chemically guided algorithms can significantly push the limits on the size of systems that can be simulated on quantum devices

➤ Matthew Otten, Matthew R. Hermes, Riddhish Pandharkar, Yuri Alexeev, Stephen Gray, and Laura Gagliardi, Manuscript In Preparation



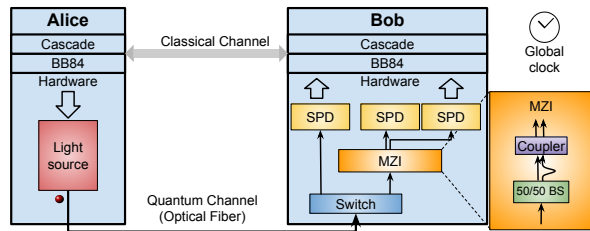
LAS-UCC circuit separated into unentangled QPE fragments and “2-local” inter-fragment correlations added with UCC



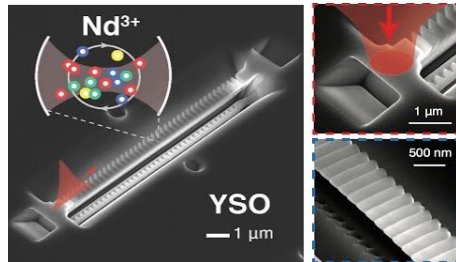
Energies for concerted bond breaking in butadiene calculated with CASCI/LASCi (complete/localized active space configuration interaction), and LAS-UCC

# SCIENTIFIC HIGHLIGHTS

## Progress in Development of a Simulator of Quantum Network Communication (SeQUeNCe)



Optical components in a simple 2-node setup.



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

- We are building a comprehensive network simulator that allows simulating long-distance quantum interconnects at the photon-level, including modeling the behavior of memories and repeaters
- The simulator will allow performance evaluations of technologies developed at Q-NEXT and serve as a protocol testbed

- X. Wu, A. Kolar, J. Chung, D. Jin, T. Zhong, R. Kettimuthu and M. Suchara. "SeQUeNCe: A Customizable Discrete-Event Simulator of Quantum Networks." Quantum Science and Technology, 2021
- Available on GitHub at <https://github.com/sequence-toolbox>





# Q-NEXT

NEXT GENERATION QUANTUM  
SCIENCE AND ENGINEERING