Lawrence Berkeley National Laboratory Quantum Computing Capabilities & Interests

Irfan Siddiqi, ***Materials Science Division (MSD)***
Jonathan Carter, ***Computational Research Division (CRD)***

Quantum Testbed Stakeholder Workshop
Hosted by the Advanced Scientific Computing Research Program
February 14 – 16, 2016

BERKELEY LAB

U.S. DEPARTMENT OF ENERGY

Office of Science

LBNL Capabilities and Interests Summary

Advanced & Impactful Computing

- National Energy Research Scientific Computing (NERSC) Facility
- Quantum Computation
- Post-Moore Digital
- Special-purpose computing (e.g. Neuromorphic)

Creative Interdisciplinary Partnerships

- Cross-division & UC Berkeley
- *CAMERA*: Math & Light Source Data
- ***AQuES*** (Adv. Quantum Enabled Simulation): Computer Science, Engineering, Molecular Foundry, Chemical Sciences, & Materials Science

Core Capabilities in Quantum Computation

- **Existing quantum computing hardware based on trapped ions, cold atoms, & superconducting circuits** with well defined pathways for expansion
- Expertise in applied quantum algorithms, verification & validation, coherent measurement, feedback & control, multi-layer modular software stacks, & high-level user interfaces
- Fabrication of nanoscale integrated circuits
- Complex digital, low frequency, microwave, & optical engineering resources
- Management expertise in successful multi-user computational & experimental facilities

Quantum Computing Hardware : Summary

Hartmut Häffner
Materials Science Division
Trapped Ions

Dan Stamper-Kurn
Materials Science Division
Ultracold Atoms

Irfan Siddiqi
Materials Science Division
Superconducting Circuits

Coupled Electronic/Nuclear Systems

- Chemical energies
- Reaction dynamics
- Charge transport

Quantum Ising, Bose-Hubbard, Spin-Boson

- Ising-like magnets
- Superfluidity
- Electron-phonon interactions

Fermi Hubbard at fractional doping

- Photosynthesis
- Superconductivity
- Spin liquids
- Solar water splitting

Synthetic gauge fields, Relativistic theories

- Topological Materials
- QCD
- QFT
- Gravity

Quantum Computing Hardware : Summary

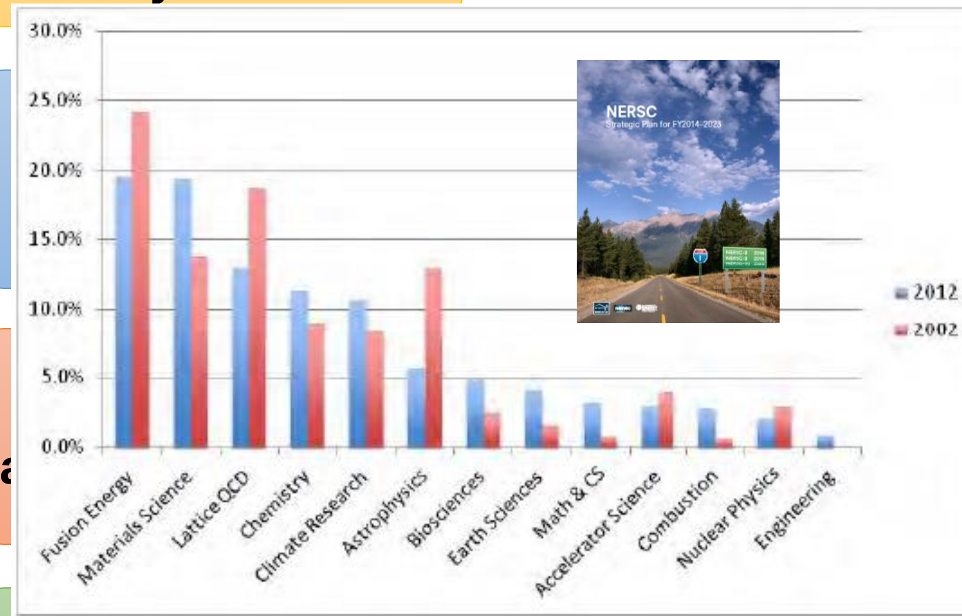
Hartmut Häffner
Materials Science Division
Trapped Ions

Dan Stamper-Kurn
Materials Science Division
Ultracold Atoms

Irfan Siddiqi
Materials Science Division
Superconducting Circuits

Coupled Electronic/Nuclear Systems

- Chemical energies
- Reaction dynamics
- Charge transport

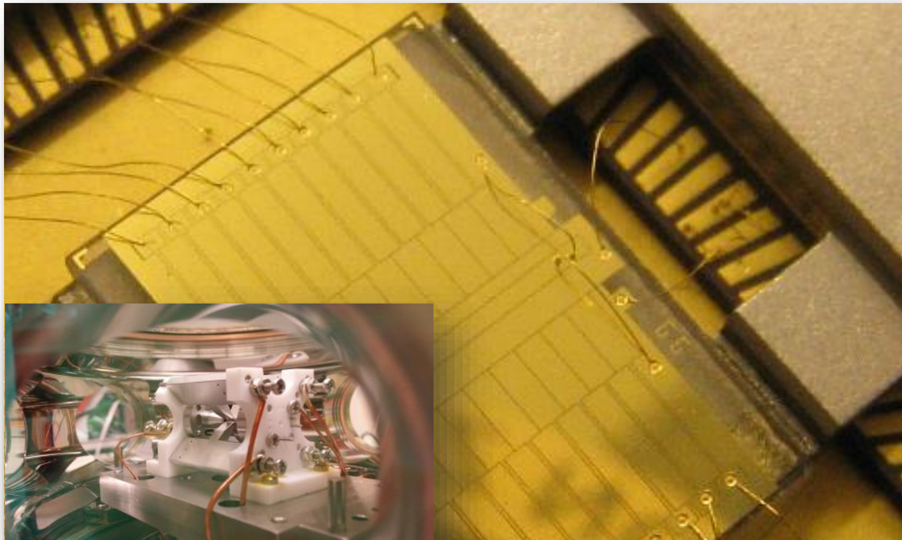


- Topological Materials

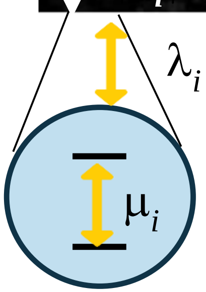
Synthetic gauge fields, Relativistic theories

- QCD
- QFT
- Gravity

Quantum Computing Hardware : Trapped Ions



- Identical ions (1-100)
- Individual control
- Long-range interaction
- Long coherence times
- Highly coordinated graphs
- Full characterization

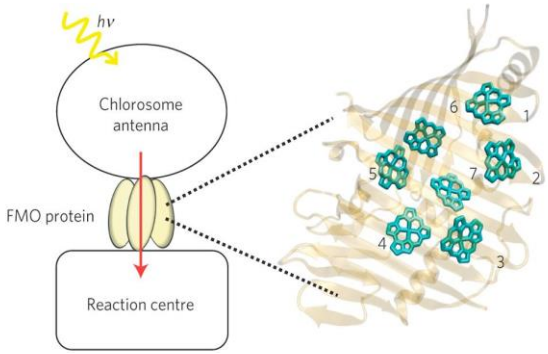


$$H = \hbar \sum \Delta_{\text{ion}} \sigma_i^z + \hbar \sum \omega_{\text{r},i} a_i^\dagger a_i + \sum t_{ij} \left(a_i^\dagger a_j + a_i a_j^\dagger \right) + \sum \lambda_i \sigma_i^x (a_i + a_i^\dagger) + \sum \mu_i \sigma_i^y .$$

Quantum Computing Hardware : Trapped Ions

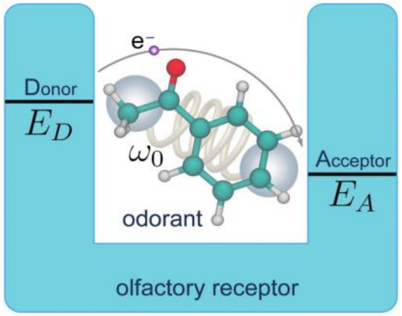
- Energy and Entanglement Dynamics
- Impurities in Crystals
- Dissipation and Thermalization
- Quantum Phase Transitions

Light harvesting



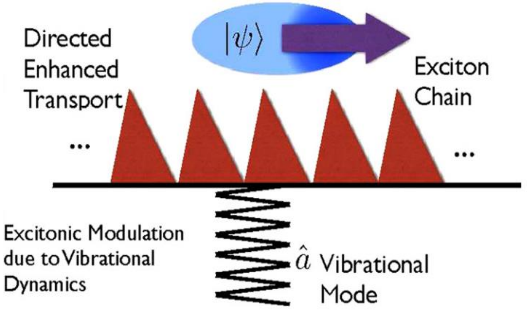
Sarovar et al., Nature Physics **6** 462 (2010)
Irish et al., PRA **90**, 012510 (2014)

Olfaction



Solov'yov et al., PCCP **14** 13861 (2012)

Directed energy transport



Myers et al., NJP **17** 093030 (2015)

Problems scale exponentially in the number of sites, difficult to solve for ~ 5-10 sites.

Quantum Computing Hardware : Ultracold Atoms

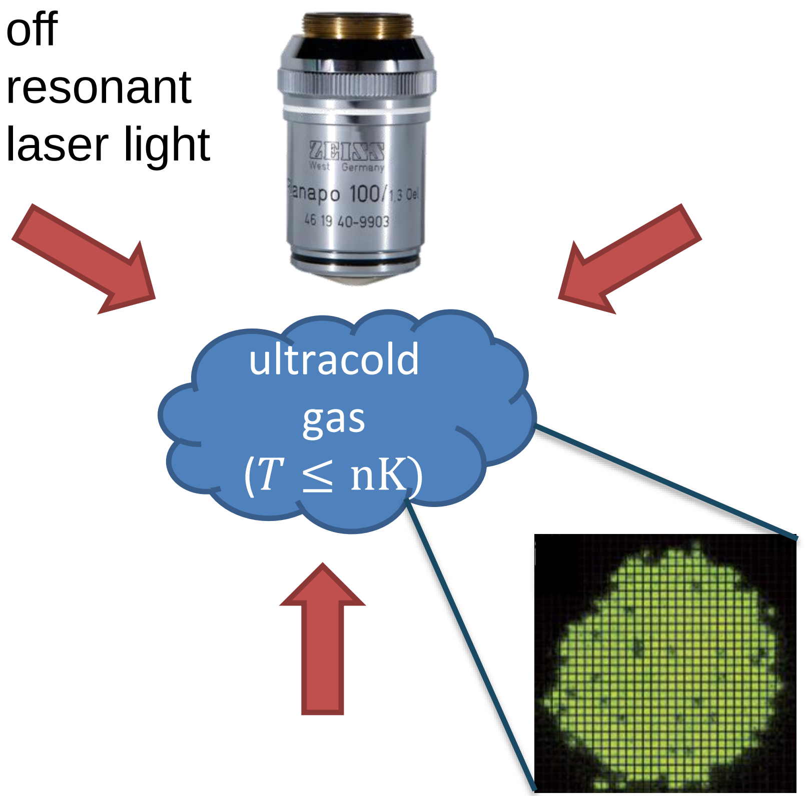


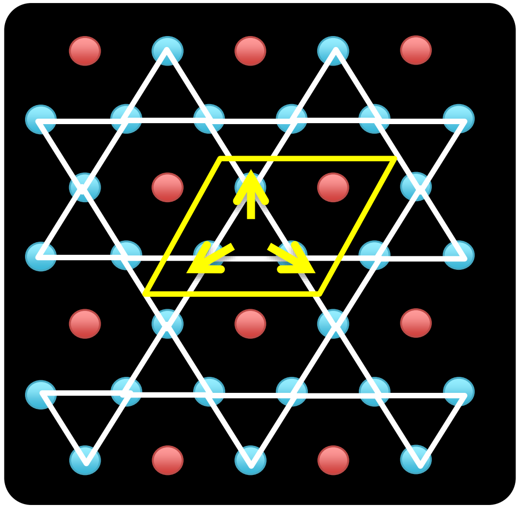
image: Greiner lab

- **Identical atoms (10^2 - 10^6)**
- **Long coherence times, highly entangled cluster states**
- **Single site imaging**
- **State-dependent readout**
- **Multi-species experiments; long/short range interaction**
- **Versatile lattice geometry**

$$\hat{H} = -t \sum_{i,j} \hat{b}_i^\dagger \hat{b}_j + U \sum_i (\hat{n}_i - 1)\hat{n}_i + \mu \sum_i \hat{n}_i$$

Quantum Computing Hardware : Ultracold Atoms

- Low Energy Phases of Frustrated Systems
- Emergent Excitations
- Non-equilibrium Dynamics
  - energy
  - entropy
  - entanglement



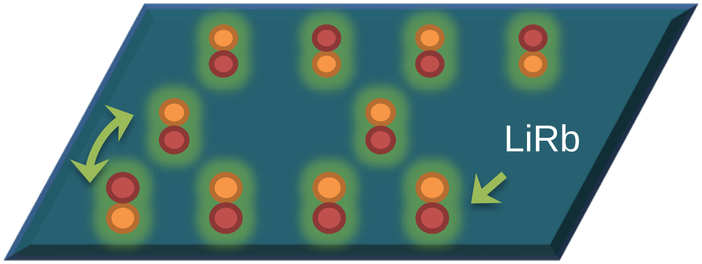
<u>“Very frustrated” quantum magnetism</u>

- What is the antiferromagnetic ground state? A quantum spin liquid of some type? (Z2, Dirac…)

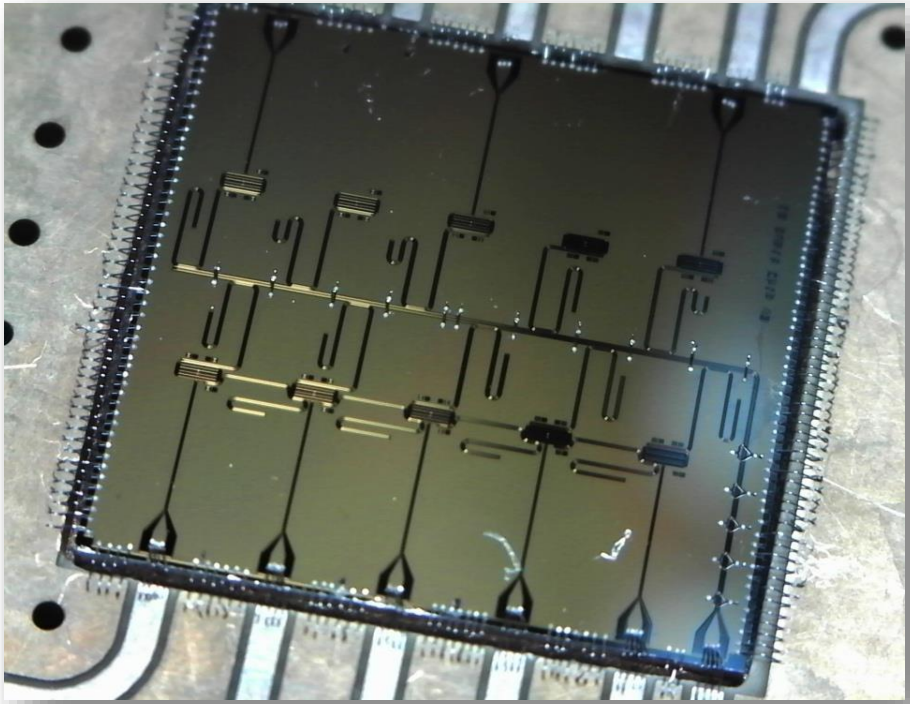
<u>Orbital frustration = flat bands</u>

- Fate of Bose condensation, superconductivity, itinerant ferromagnetism?
- Does flat band strengthen localization into Mott insulator?

- strong direct interactions: nearest neighbor exchange ~ 20 kHz
- reconfigurable: photoassociate into molecules at selected sites
- localized non-destructive measurement: photodissociate at selected site and measure atoms



Quantum Computing Hardware : SC Circuits



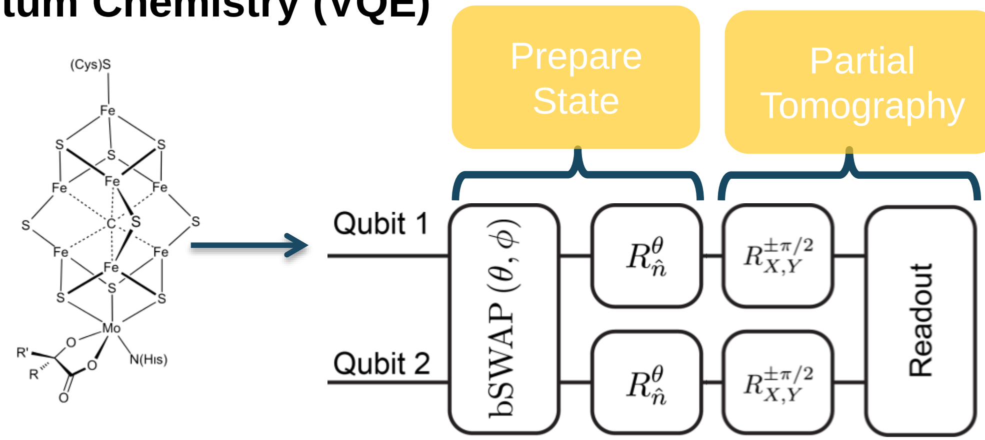
- **Fully engineered quantum system (10-100,…)**
- **In-situ tuning**
- **Fast operating time**
- **Single qubit addressability, readout, and control**
- **QND, pulsed & continuous measurement**
- **Variable connectivity**

$$\hat{H} = \sum_i \epsilon_i \hat{\sigma}_i^z + \chi_i \hat{\sigma}_i^z \hat{a}_i^\dagger \hat{a}_i + J(t)\hat{\sigma}_i^x \hat{\sigma}_{i+1}^x$$

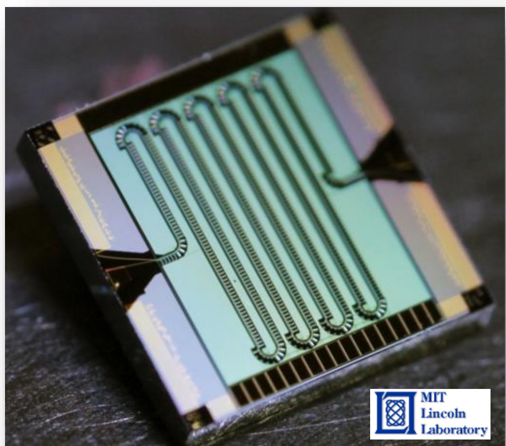
Quantum Computing Hardware : SC Circuits

- Quantum Chemistry: Statics & Dynamics
- Quantum Ising
  Bose-Hubbard
  Fermi-Hubbard
- Topological Materials

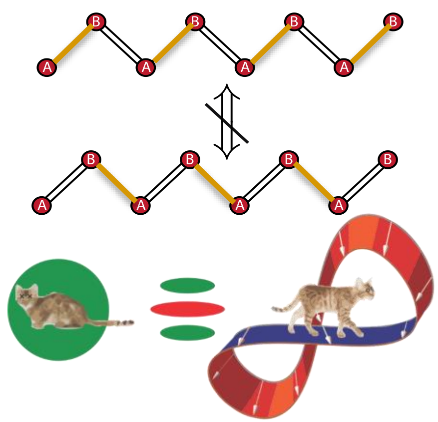
Quantum Chemistry (VQE)

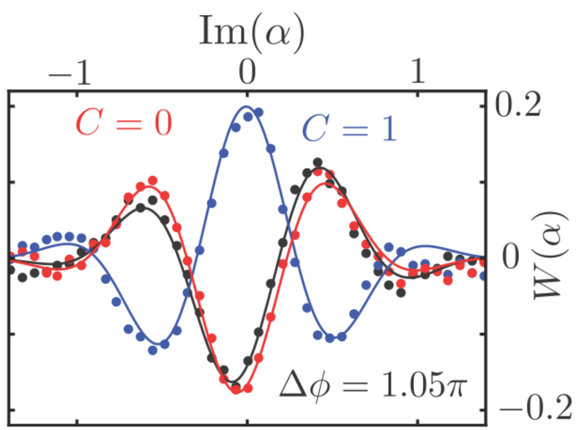


Quantum Limited Detection



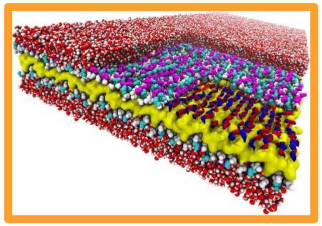
Topology (Q-Walk)



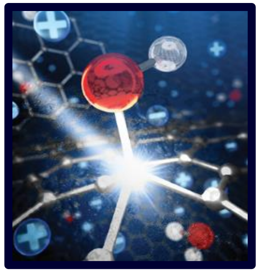


Topological invariant

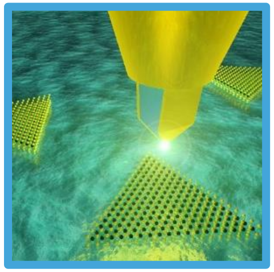
Fabrication and Characterization Capabilities



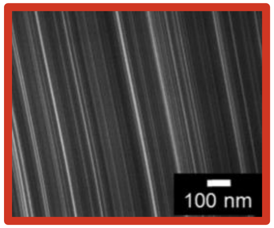
Combinatorial Nanoscience



Functional Nanointerfaces



Multimodal Nanoscale Imaging

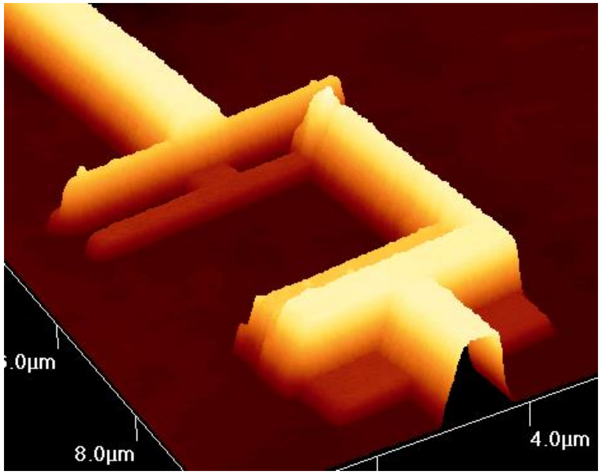


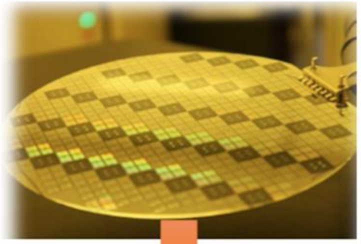
Single-Digit Nanofabrication and Assembly

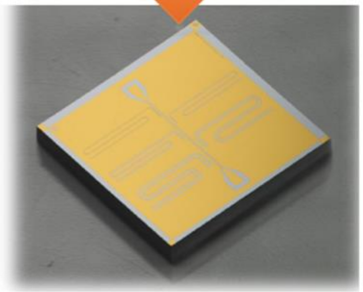
Stefano Cabrini

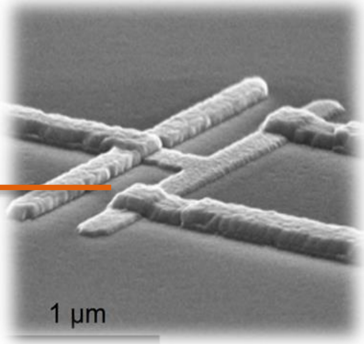
MOLECULAR FOUNDRY

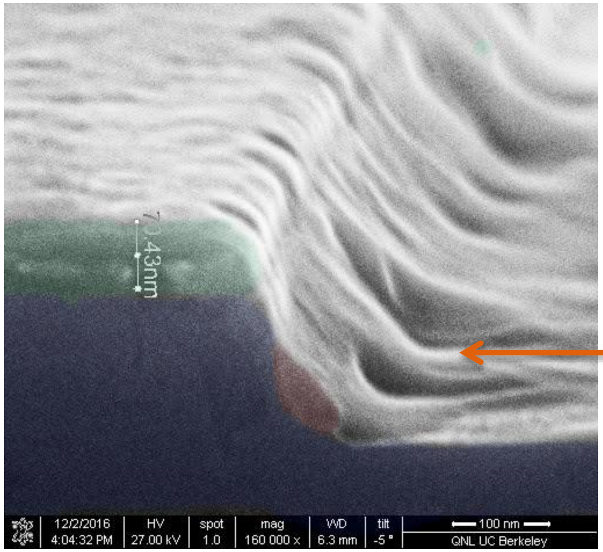
Fabrication and Characterization Capabilities











Quantum Nanoelectronics Laboratory

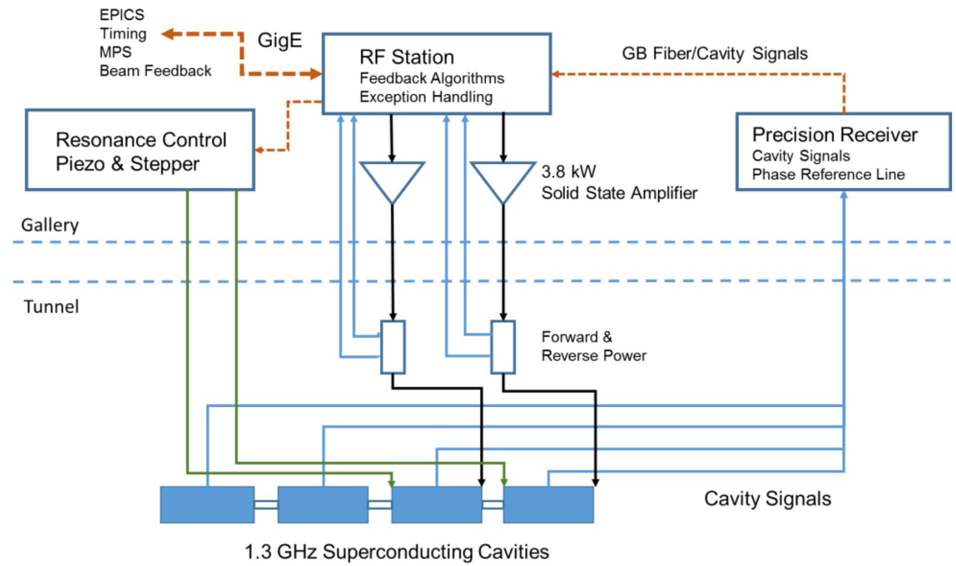
Engineering and Supporting Technology

Wim Leemans (8-10 FTE)
Director, Accelerator Technology and Applied Physics Division

John Byrd
Head, Center for Beam Physics Accelerator Technology and Applied Physics Division

Larry Doolittle
Engineering Division

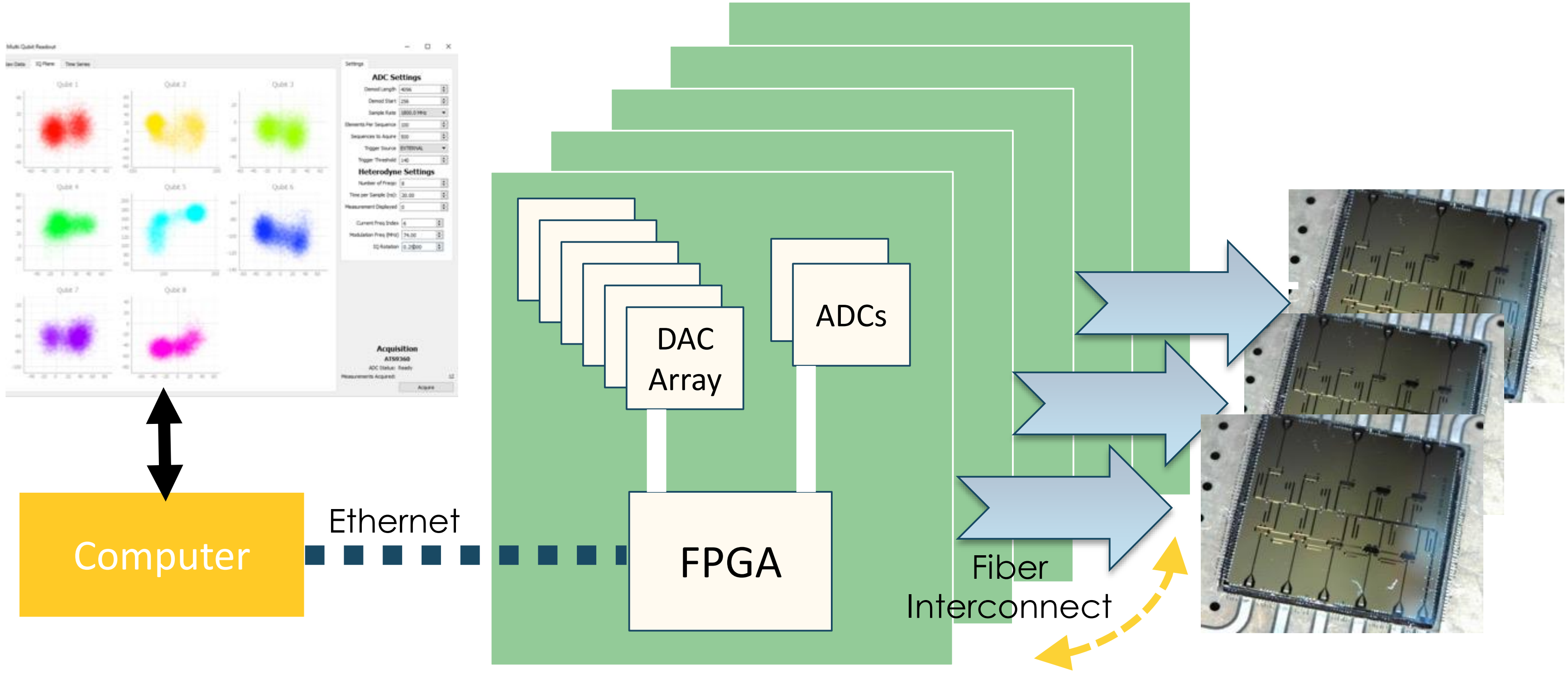
Berkeley Lab is the lead for development of the RF controls, conceptual design, and prototype development. GOAL: RF controller that maintains 10^{-4} amplitude and 0.01 deg phase coherence between hundreds of SC cavities.



LCLS-II RF system schematic layout (SLAC)

Engineering and Supporting Technology

- Single FPGA board controls and measures 6-8 qubits
- Boards connected via fast fiber interconnect
- Local DSP for waveform generation and analysis
- Low latency for feedback across the entire network
- Scalable to arbitrary number of boards



Quantum Computer Science and Computational Science Capabilities

Anastasiia Butko
Computer Architecture

Jonathan Carter
Algorithms

Bert de Jong
Algorithms & Control

Jarrod McClean
Algorithms

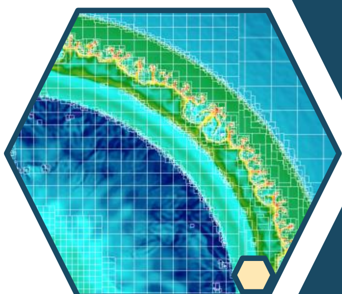
Joel Moore
Cond. Mat., QVV

Umesh Vazirani
QVV

Birgitta Whaley
Chemistry, QVV

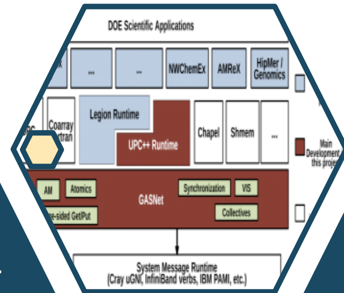
Norman Yao
Cond. Mat., Algorithms

Computer & Computational Science Ecosystem



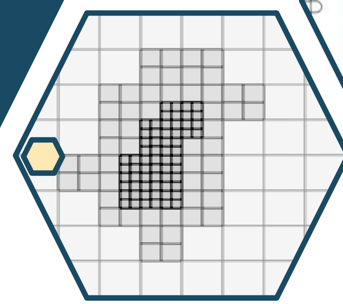
Languages & System Software

Co-Design

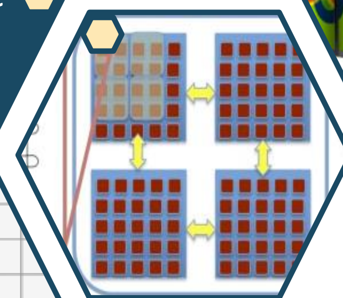


Applied Math

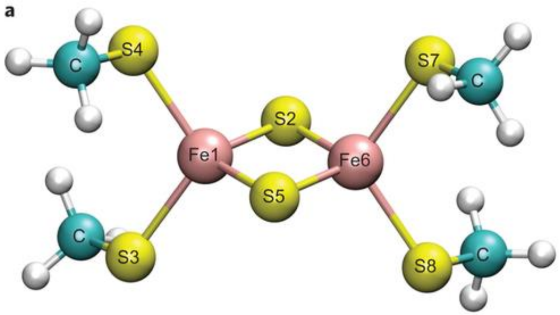
Computer Architecture Group



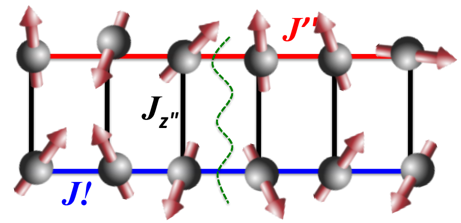
NERSC (Advanced Technology Group)



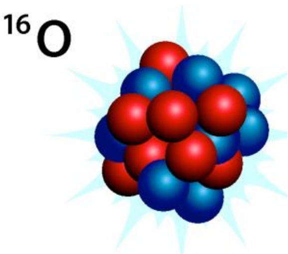
Applications to Domain Science @ Berkeley Lab



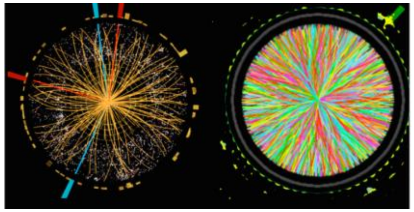
Catalysts - Coupled electron-nuclear motion; beyond single reference methods: de Jong, McClean, Whaley,



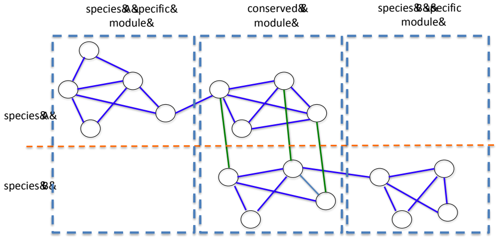
Strongly correlated materials: Moore, Yao, Whaley



Nuclear structure: Haxton



Quantum Associative Memory for HEP particle tracking: Calafiura, Shapoval



Orthology – complex optimization problem in biosciences: Brown, Bouchard

Investments in Quantum Computing Technology

- As part of LDRD initiative in post-Moore computing

Project	PI
Solving Problems in Materials Theory via Quantum Networks	Moore,Joel
Quantum Computing Technology Exploration	Siddiqi, Irfan
Design of Quantum Chemistry Simulations for Superconducting Circuits	McClean,Jarrod
Quantum Chemistry Simulations for Superconducting Circuits	Siddiqi, Irfan
Quantum simulations of magnetism and transport with atomic systems	Stamper-Kurn,Dan
Simulating Excited State Energies and Dynamics with Superconducting Qubits	Siddiqi, Irfan
Nanoscale magnetometry, electrometry, and thermometry of exotic quantum materials using Nitrogen-Vacancy Defects	Yao, Norman

- **Productive multi-disciplinary team consisting of Computing Sciences, Materials Science, Chemical Science, Molecular Foundry and campus**

Facility Management Experience

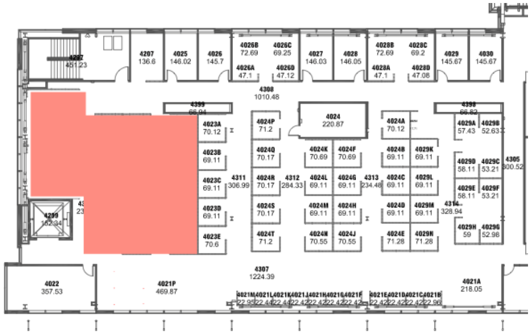
NERSC | ESnet | ALS | Molecular Foundry & NCEM | JGI

- Hosts 2 ASCR, 2 BES, and 1 BER user facilities
- Nearly 10,000 users (remote and onsite)
- JGI, ALS, NERSC, and ESnet staff work exclusively on program activities;

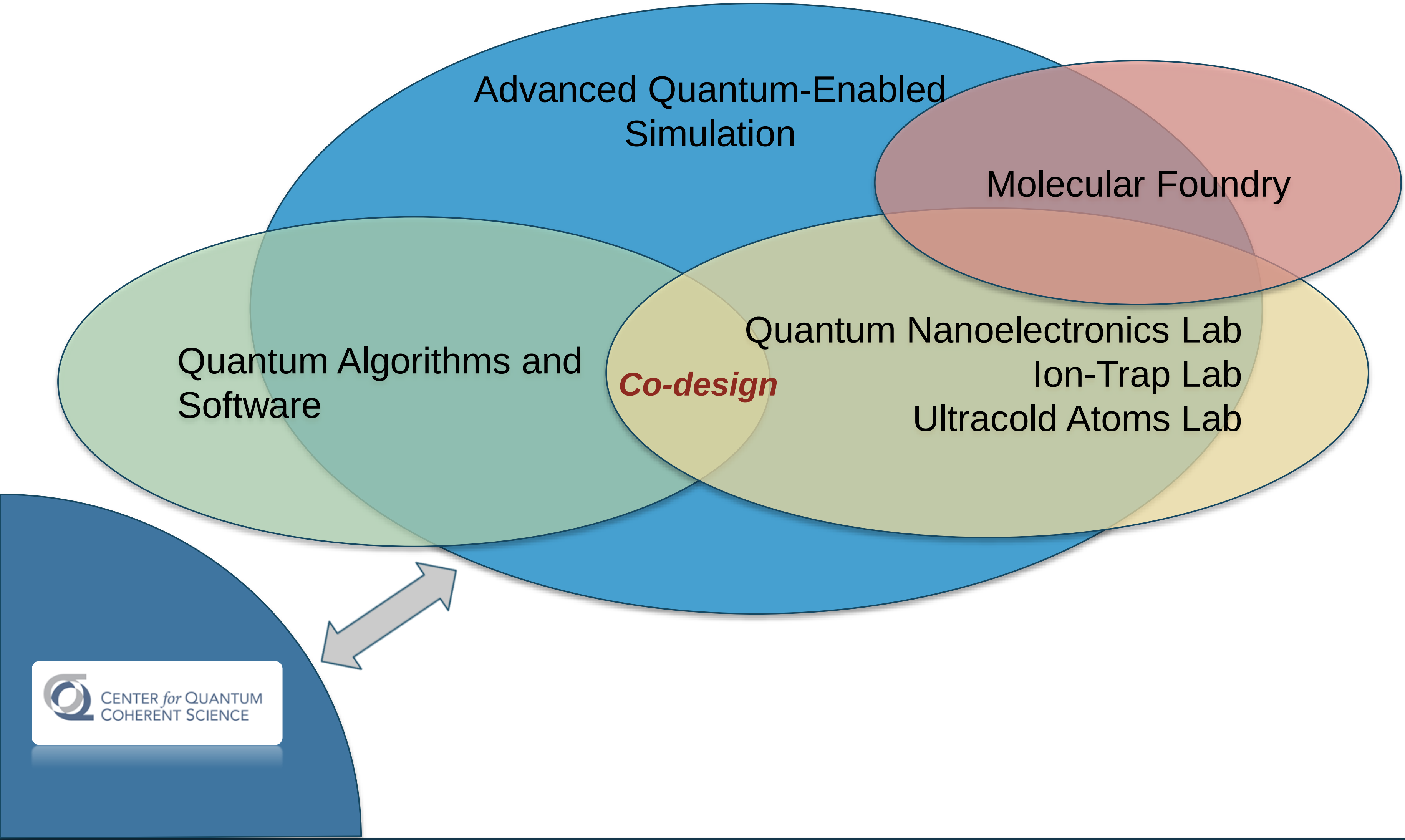
  Molecular Foundry staff work 50% with users
- User group meetings, User information systems, Onboarding office, Guest house

AQuES – Housed with Computing Sciences

- Office & lab space available in Wang Hall
- Internal funding to develop lab space & hardware



AQuES Partnerships



External Partnerships

- Google
  (FermiLib)
- NASA Ames
- LLNL
- Sandia
  (GST)
- UC Riverside, U. Rochester, Chapman U.
  (continuous error correction)
- U. Sherbrooke, McGill U.
  (non-classical light and matter)

Cyclotron Road Science Incubator

- 6 teams generated over $15M in public/private partnership funding from $3M initial EERE AMO funding

Innovation and Partnership Office

- Patents issued: 80 (65 U.S., 15 foreign)
- Patent applications filed to protect LBNL intellectual property: 167
- New technologies disclosed by LBNL researchers: 193
- Royalties: $ 2,995,865
- Companies / investors / entrepreneurs visiting with IPO staff: 111
- New licenses and options for LBNL technology: 11
- Software licenses: 149 (commercial, collaboration, and government use)
- 46 CRADAs
- NDAs Inbound 95 and Mutual (in/out) 157

Thank You