Quantum Testbed Stakeholder Workshop

Hosted by the Advanced Scientific Computing Research Program

Pacific Northwest National Laboratory

Quantum Computing Capabilities and Interests

February 14 – 16, 2016

U.S. DEPARTMENT OF ENERGY | Office of Science

Pacific Northwest NATIONAL LABORATORY

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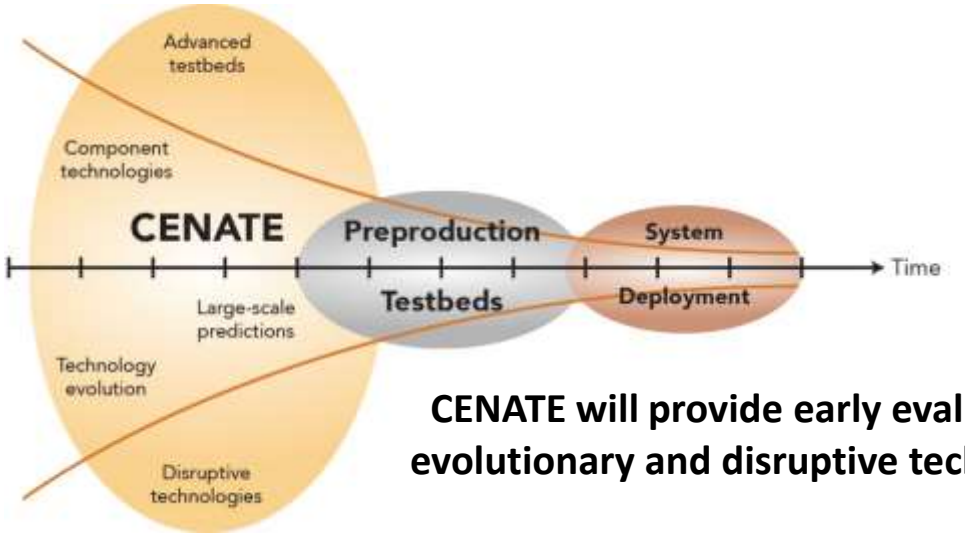
PNNL capabilities & interests summary slide

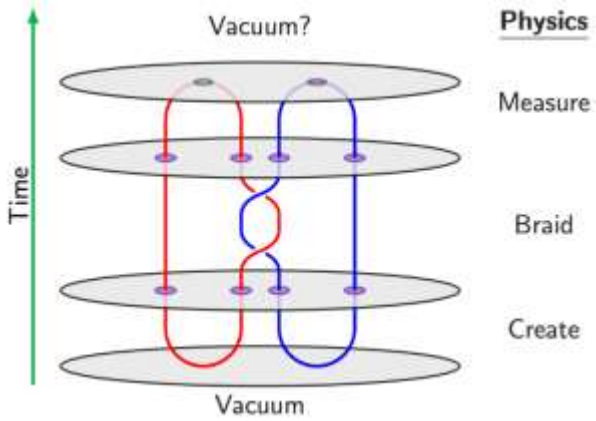
- Primary expertise & interest areas
  - Computing testbeds (e.g., CENATE)
  - Computing technology performance modeling & simulation
  - Topological quantum computing algorithms (co-design)
  - Computational chemistry (co-design)
- Most differentiating factor(s)
  - Topological quantum computing expertise
  - Testbeds for performance modeling & simulation
- Main contribution/role
  - Topological quantum computing algorithm design
  - Center for testbed evaluation, performance modeling & simulation

Quantum computer science capabilities

- Mathematics
  - Topological quantum computing algorithms
  - Combinatorics approaches to error-correcting codes
  - Lattice modeling of topological (quantum) phases
- Computer science
  - Testbed expertise
  - Performance modeling & simulation
  - Runtime library development
- Quantum materials simulation and modeling

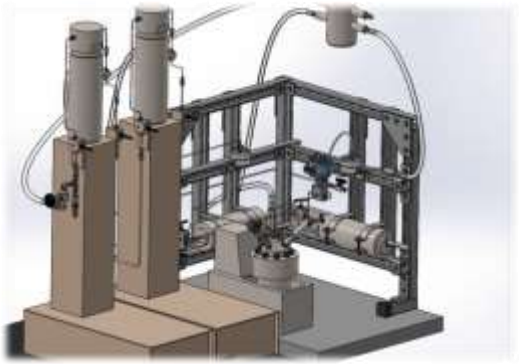


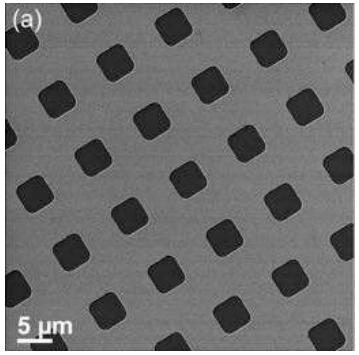
CENATE will provide early evaluation of evolutionary and disruptive technologies.



Fabrication & characterization capabilities

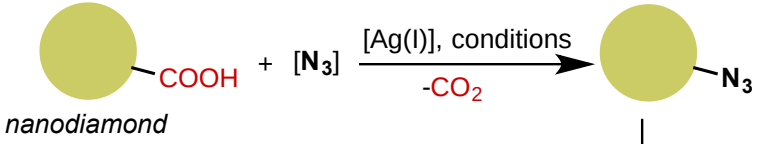
Advanced processing of sensitive features on qubit architectures



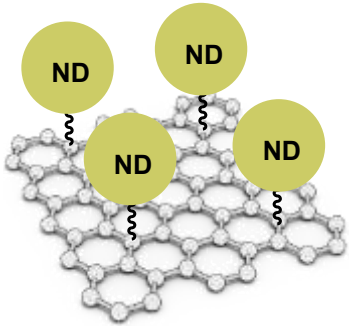


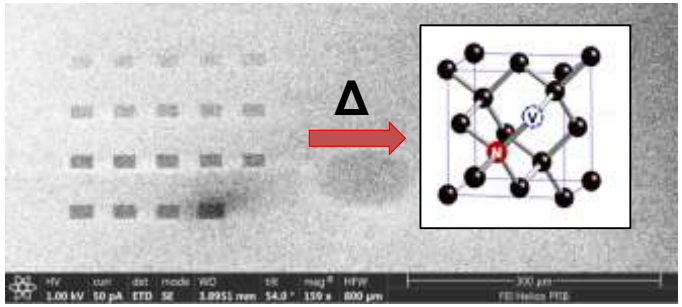
Engineered solvent-assisted supercritical CO_2-based wafer processing

Insight into the chemistry and characterization of nanoscale diamond applicable to development of qubits



Tailoring nanodiamond surfaces to produce heterostructure devices by self-assembly

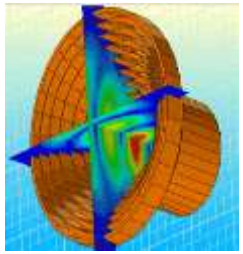


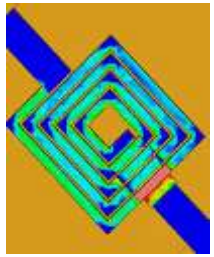


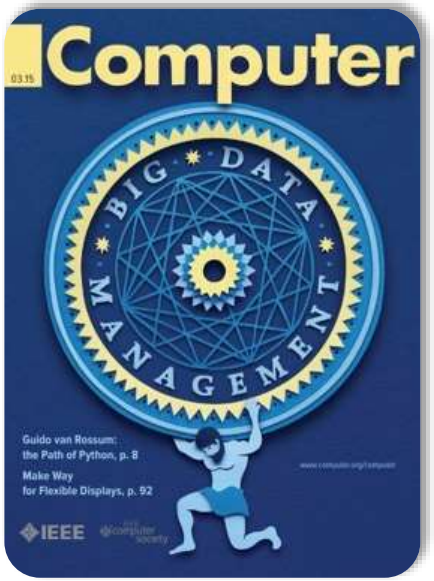
Helium focused ion beam patterning to produce nitrogen-vacancy defect centers in diamond films

Capabilities in engineering & supporting technology

- RF (microwave) engineering for security applications
- Significant data warehousing and analysis capabilities
- Emerging cryogenic capability for physics detection applications

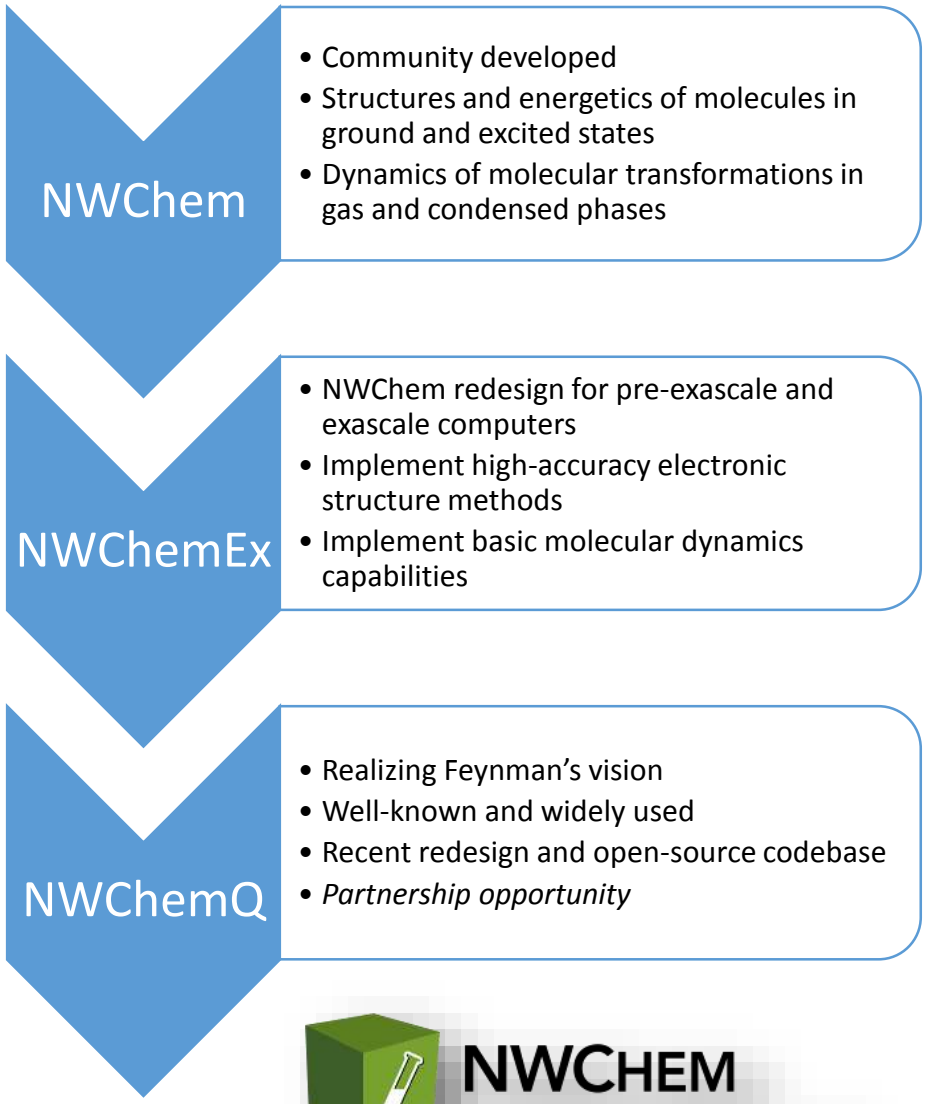






Applications to domain science

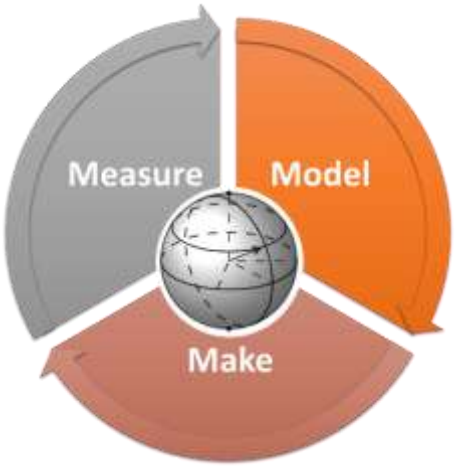
- Computational chemistry
  - Quantum co-processing
  - NWChem: Flagship computational chemistry code
  - NWChemEx: computational chemistry at exascale
  - NWChemQ: realizing Feynman's vision?
- Condensed matter and particle physics
  - Quantum simulation of topological phases
- Applied mathematics
  - Quantum acceleration of combinatorics algorithms

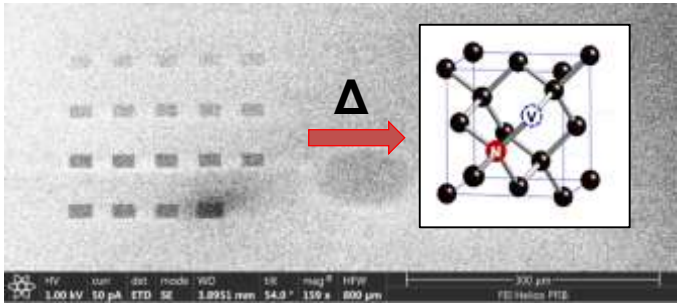


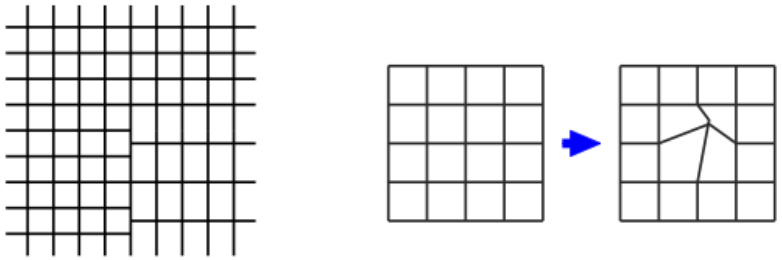
NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

LDRD investments in quantum computing technology

- Motivation
  - Scalable synthesis for atomically precise structures
  - Control of material defects, disorder, and noise
  - Understanding and reducing changes in structure and function over process cycles
- Expertise
  - Quantum materials FIB and characterization
  - Quantum device cleaning
  - New candidate topological phases of matter
  - New topological quantum computing capabilities

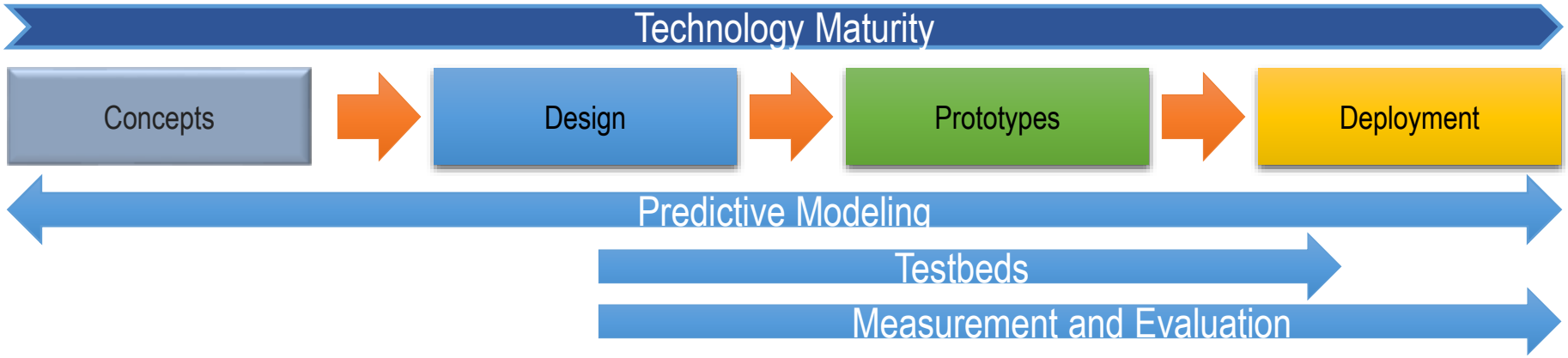






Facility management experience

Center of Advanced Technology Evaluation (CENATE)



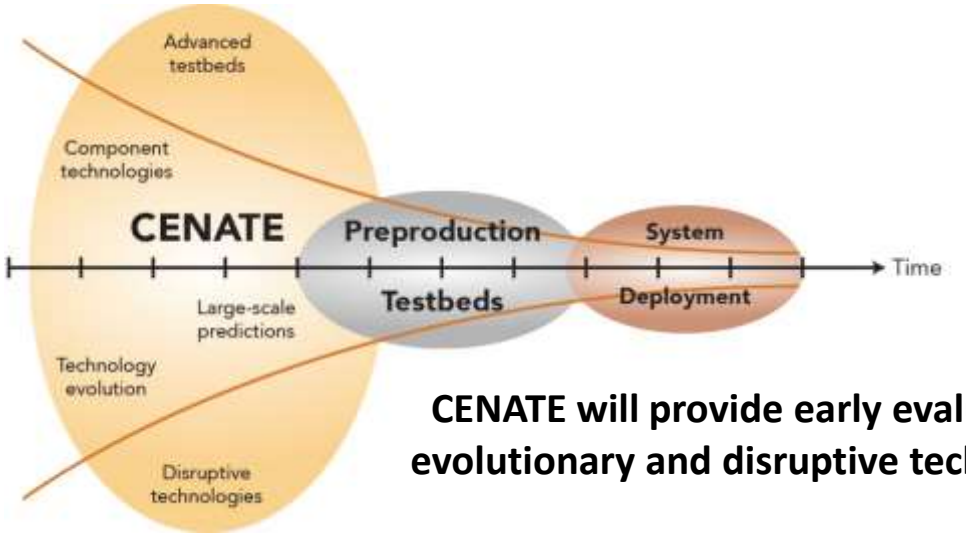
Sub-systems	Processing	Memory	Network	Storage and I/O
Emerging Paradigms	Approximate	Quantum	Neuromorphic	Superconductive
Workloads	Numeric	Machine Learning	Data Analytics	Graph Analytics

External partnerships

- Partnerships
  - Topological phases – Microsoft Station Q, LSU, Texas A&M, UCSB
  - Device modelling – SNL and LLNL
  - Defect measurement and analysis – UMD
- Significant experience working with industry, including IP protection and technology transition
- New partnerships desired
  - Computational chemistry quantum co-processing
  - Hardware testbed for surface code schemes
  - Device modelling for testbed hardware analysis
  - Combinatorial problems in quantum computing

Extra Slide
CENATE: Potential to Leverage

- Testbeds targeted at several areas
  - System Technologies with future high impact to HPC
  - Novel Processing Paradigms beyond traditional computing
  - Emerging Technologies beyond Moore's Law
- Evaluation of workloads of interest
  - Scientific Computing
  - Irregular Applications
  - DOE-focused
- Integrated measurement and ModSim



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