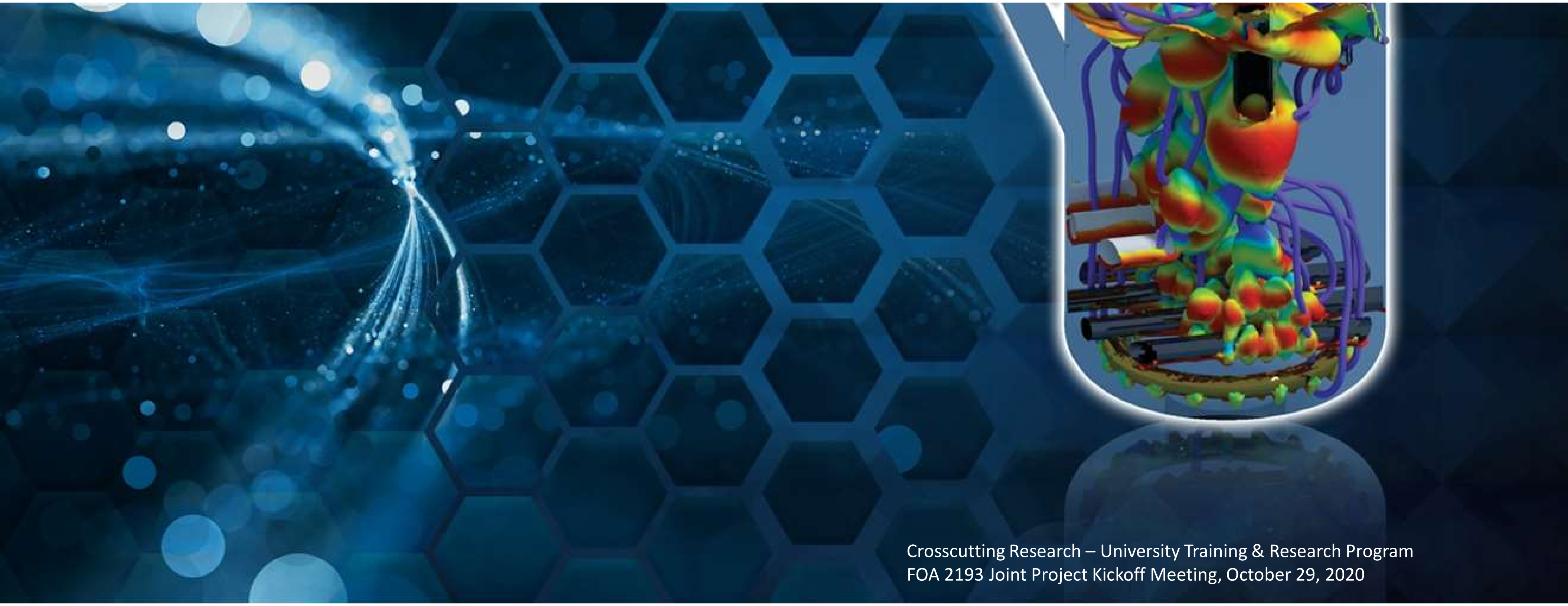


NETL Quantum Activities Overview

Madhava Syamlal (Syam)
Senior Fellow, Computational Engineering
National Energy Technology Laboratory

National Quantum Initiative Act

- The National Quantum Initiative Act was signed into law on 21 December 2018
- The act has launched 10 years of sustained effort at three lead agencies: NIST, NSF and DOE.
- The act directs DOE to carry out a basic research program on quantum information science; leverage knowledge from existing QIS research; provide QIS training for additional undergraduate and graduate students; and coordinate research efforts with currently funded programs.

FY21 Budget Request for QIS Research

- Greatly bolsters funding by nearly 50%, putting QIS R&D on the path to double to over $860 M by 2022.
- **NSF** funding would double to $230 M
- **DOE-SC** funding would increase from $195 M to $237 M
  - $25 M to support early state research for a quantum internet
  - Five multidisciplinary QIS research centers, collectively receiving up to $625 M over five years.
- **NIST** funding would be $40 M to focus quantum networking and support Quantum Economic Development Consortium
- **NASA**'s initial funding will allow it to explore the potential for a space-based quantum entanglement experiment.

QIS will improve our industrial base, creating new jobs and entirely new industries in the process, while helping keep America safe.

-- FY21 Budget Request

consequences of mastering quantum computing … are no less significant than those faced by the scientists who lit up the New Mexico sky with the detonation at the Trinity test site 72 years ago.

-- Rep. Will Hurd (R-Tex.)

QIS Centers: create and steward the ecosystem needed to foster and facilitate advancement of QIS

NATIONAL ENERGY TECHNOLOGY LABORATORY

DOE is awarding $625 million over five years to establish five QIS Centers. This award was met with $340 million in contributions from the private sector and academia.

Q-NEXT · Next Generation Quantum Science and Engineering

Director: David Awschalom

Lead Institution: ANL

C2QA · Co-design Center for Quantum Advantage

Director: Steve Girvin

Lead Institution: BNL

SQMS · Superconducting Quantum Materials and Systems Center

Director: Anna Grassellino

Lead Institution: FNAL

QSA · Quantum Systems Accelerator

Director: Irfan Siddiqi

Lead Institution: LBNL

QSC · The Quantum Science Center

Director: David Dean

Lead Institution: ORNL

Enterprise quantum computing appears poised for rapid growth

- Among Gartner Top 10 Strategic Technology Trends for 2019[1]
- By 2023, 20% of organizations will be budgeting for quantum computing projects[2]
- Annual budget for enterprise quantum computing reported to rise from $39.2 million in 2017 to $2.2 billion by 2025[3].

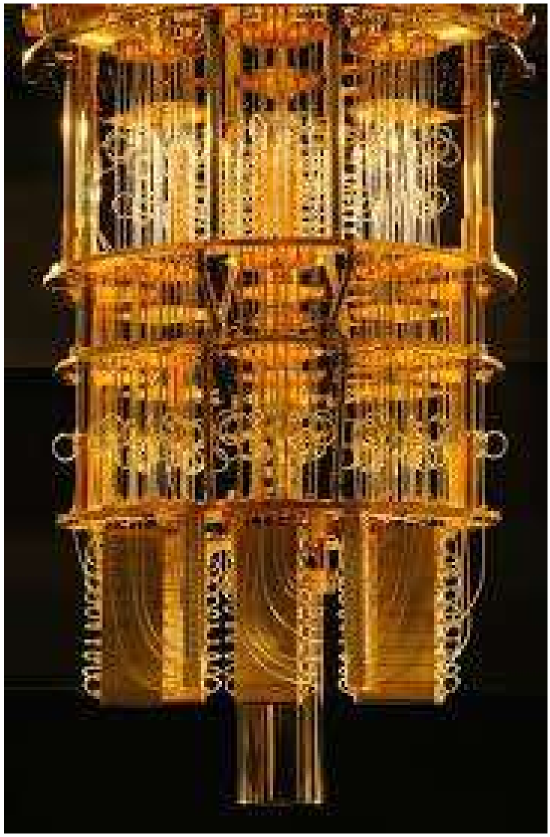
1. https://www.gartner.com/smarterwithgartner/gartner-top-10-strategic-technology-trends-for-2019/
2. https://www.gartner.com/smarterwithgartner/the-cios-guide-to-quantum-computing/
3. https://www.tractica.com/newsroom/press-releases/enterprise-quantum-computing-market-to-reach-2-2-billion-by-2025/

Four areas of QIS – 1-3

1. **Sensing**
   - Exploits the strong sensitivity of quantum systems to external disturbances
   - e.g., GPS–free navigation, atomic clocks, magnetometers, functional imaging of individual molecules
2. **Networking**
   - Transmit information with the help of *entangled* particles, whose states are inextricably linked even when the particles are separated by a large distance
   - e.g., BNL and Stony Brook U. transmitted *qubits* 87 miles over commercially available telecommunications fiber; DOE plans to connect all 17 national labs through *quantum internet*
3. **Simulation or Emulation**
   - Use a controllable quantum system to study another inaccessible or impossible-to-model quantum system
   - e.g., H. Häffner group (UC Berkeley) uses two calcium-ion qubits to simulate a quantum process underlying photosynthesis

Four areas of QIS – 4: Computation

- **Quantum bits or qubits**
  - Superposition: the bit has amplitude α for being 0 (β for being 1) and will become 0 (or 1) with probability $|\alpha|^2$(or $|\beta|^2$) when measured
  - Interference: the amplitudes can interfere and even cancel out
  - Entanglement: states of a group of qubits are linked even at a distance
- **Hardware manifestations**
  - Quantum annealer: D-Wave
  - Noisy intermediate-scale quantum (NISQ) computers: IBM, Google, Rigetti, IonQ, ...
  - Universal, fault-tolerant quantum computer: 1 or 2 *decades away*
- **Algorithms**
  - Hybrid: Quantum approximate optimization algorithm (QAOA), variational quantum eigen (VQE) solver for finding ground state energy
  - Provable speed up: Bernstein–Vazirani (1993), Shor (1994), Grover (1996), Harrow-Hassidim-Lloyd (2009)



Timeline of QIS capability development at NETL

4/19 NETL QIS strategic plan developed

5/19 ASFE briefed about the strategic plan

6/19 NETL/FE team visited IBM-Q

8/19 NETL/FE team visited Pittsburgh Quantum Institute (PQI)

9/19 Started a seed project in quantum sensing

11/19 Fossil Energy Workshop on Quantum Information Science & Technology held at NETL, bringing together experts from fossil energy and QIS

https://www.netl.doe.gov/onsite-research/quest

1/20 Quantum for Energy Science and Technology (QUEST) Technical Working Group established at NETL

1/20 Two preapplications submitted

3/20 NETL/FE team visited NIST

5/20 QUEST external website went live

6/20 Two extramural projects selected under University Training Program

6/20 Training workshop in quantum computing by QCWare

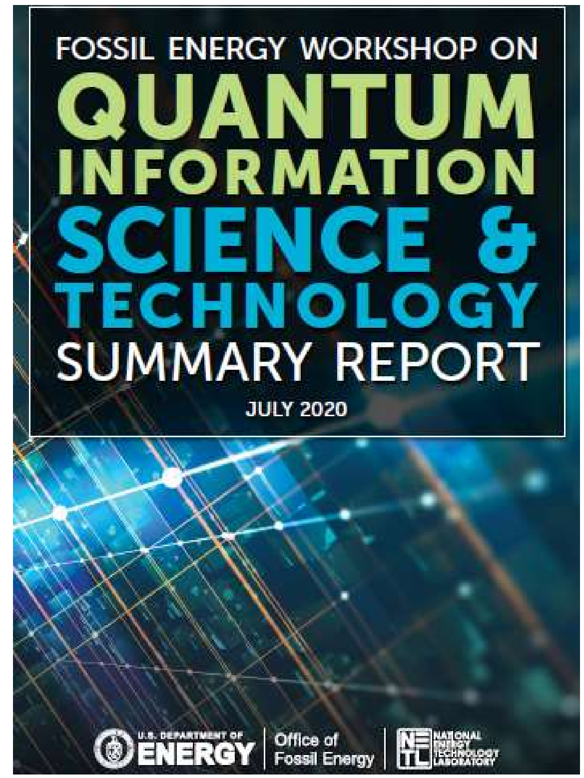
7/20 Review article on the applications of QIS in energy written

7/20 Workshop report published

9/20 Quantum computing study group started

QIS Workshop, November 2019

- Organized the “Fossil Energy Workshop on Quantum Information Science & Technology” in November 2019.
- The workshop brought together 54 participants with expertise in a variety of relevant areas in fossil energy (33) and QIS (21). They came from DOE (2), industry (12), universities (17), and national labs (23).
- The workshop report containing specific recommendations for NETL and FE was published in July 2020.



Bush, S.; Duan, Y; Gilbert, B.; Hussey, A.; Levy, J.; Miller, D.; Pooser, R.; Syamlal, M. Fossil Energy Workshop on Quantum Information Science & Technology Summary Report; U.S. Department of Energy, National Energy Technology Laboratory: Pittsburgh, PA, 2020; DOI: 10.2172/1639026.

Review article on the applications of QIS in energy under review

QUEST

NATIONAL ENERGY TECHNOLOGY LABORATORY

Main topics

- ❑ Quantum sensing: Focused to fossil energy applications
- ❑ Quantum networking: Focused to basic concepts and quantum communication for energy applications
- ❑ Quantum simulations: Focused to basic concepts and simulation of quantum chemistry problems
- ❑ Quantum computing: Focused to basic concepts and quantum computation of combinatorial and material chemistry problems.

Quantum Information Science: Review and Perspective for Energy Applications

Hari P. Paudel,[a,b] Scott E. Crawford,[a] Roman A. Shugayev,[a] Ping Lu,[a, b] Madhava Syamlal,[a] Paul R. Ohodnicki,[a] Randall Gentry,[a] Yuhua Duan Duan[a1]

[a] National Energy Technology Laboratory, United States Department of Energy, 626 Cochrans Mill Road, Pittsburgh, Pennsylvania 15236, USA

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Abstract

On its revolutionary threshold, quantum information science (QIS) is creating potential transformative opportunities to exploit the intricate quantum mechanical phenomena in new ways for obtaining and processing information. QIS has already found its initial applications in communications and computations and has further expanded its uses into a variety of new areas, such as sensing and networking. Concurrently, the growing interest in QIS has created opportunities for its deployment processes pertaining to energy production, distribution, and consumption. Safe and secure utilization of energy depends on the challenges related to material stability and function, secure monitoring of infrastructures, accuracy in detection and measurement, and economic

Quantum Sensing Pilot Projects at NETL

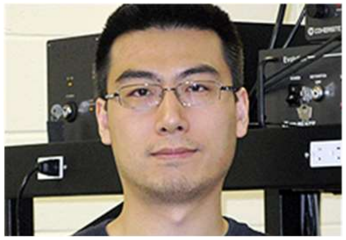
- Integrate quantum sensing materials for chemical sensing in subsurface monitoring (e.g., pH, CO_2), natural gas infrastructure monitoring (e.g., pipelines, CH_4), and rare earth element detection.
- Leverage quantum squeezed and entangled photons for optimizing performance of distributed interrogation methodologies for the optical fiber sensor platform.

NETL Team


Dr. Hari Paudel


Dr. Yuhua Duan


Dr. Scott Crawford

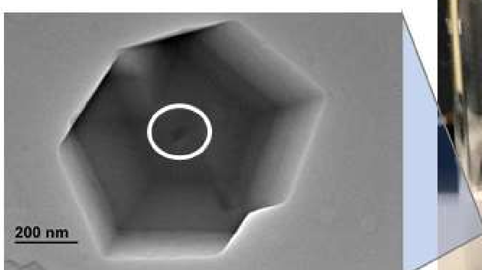

Dr. Ping Lu


Dr. Roman Shugayev

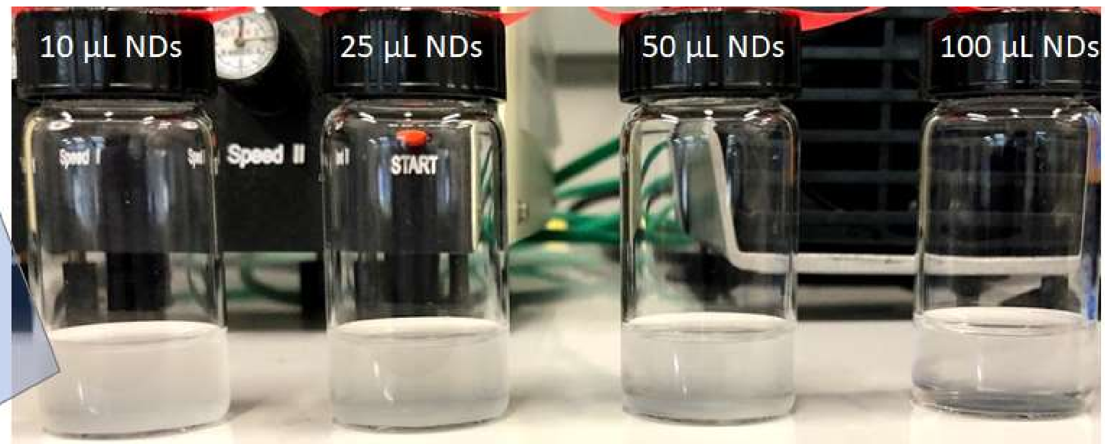

Dr. Yueh-Lin Lee

Nanodiamonds encapsulation in metal-organic framework materials

Nitrogen vacancies in nanodiamonds represent an intriguing quantum material with potential applications in quantum sensing and computing. At NETL, we are designing and investigating composite materials in which nanodiamonds are encapsulated in the metal-organic framework (MOF; ZIF-8), which may be used to create a well-defined chemical environment around the nanodiamond and enhance its performance in these applications. Furthermore, the MOF may also act as scaffold for incorporating and positioning the nanodiamonds for nearest neighbor entanglement applications



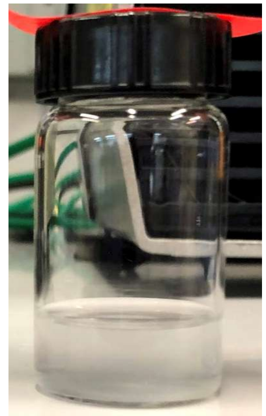
White circle denotes nanodiamond in metal-organic framework (MOF)

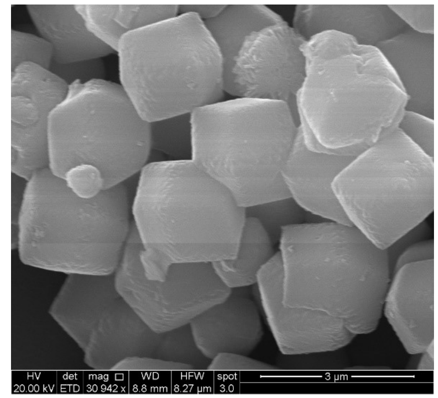


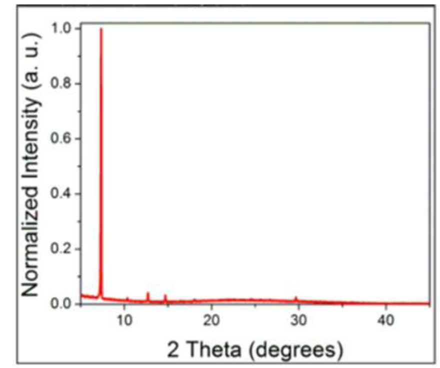
ZIF-8 growth solution with varying concentrations of the polyvinylpyrrolidone (PVP)-functionalized nanodiamonds.

Progress in nanodiamond encapsulation

- NV centers have been successfully encapsulated for sensing applications
- Crystal imaging has been obtained (SEM images)
- Florescence spectrum and carrier population are measured for NV center in nano-diamond

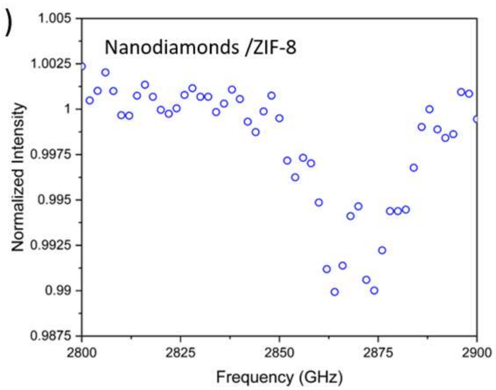




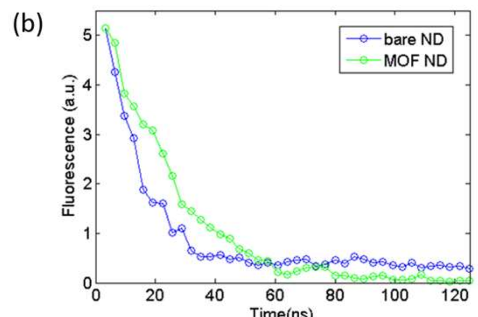


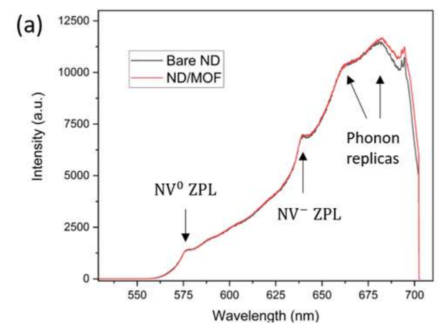
NV center encapsulated in MOF surfaces

Shugayev et. al
(Manuscript under preparation)



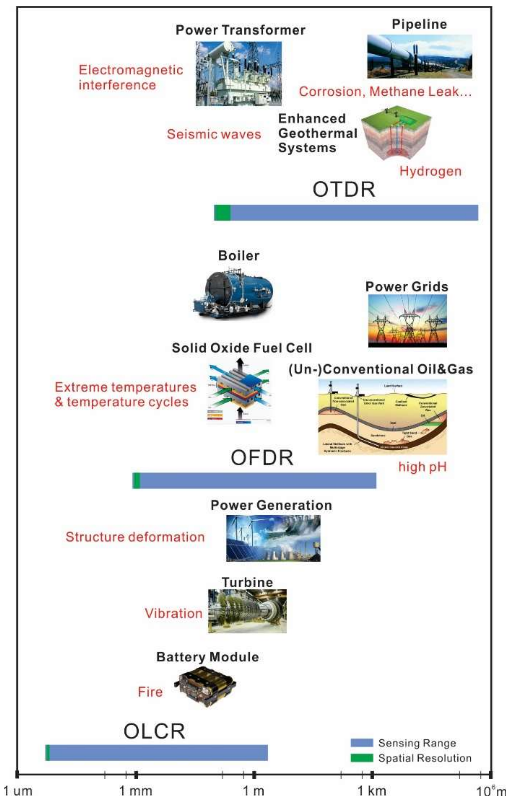
Optically detected magnetic resonance of NV center





Florescence spectrum (a) and loss of carrier population (b) in NV center of nano-diamond

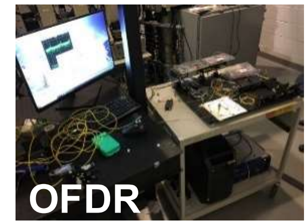
Distributed Optical Fiber Sensing Platforms Developed

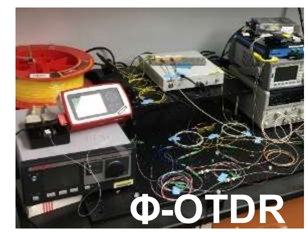


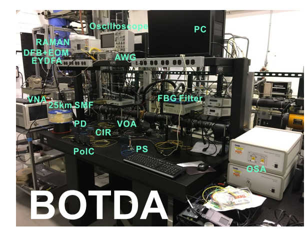
Challenges: Long-distance, trace chemical sensing, cross-sensitivity, field deployment, capital cost

Comparison of sensing performance specifications

Technology	Sensing Range	Spatial Resolution	Measurement Time	Fiber Type	Sensing Performance
Coherent Rayleigh OFDR	m – km	mm – cm	seconds	SMF	Temperature, strain, vibration, chemical sensing
Coherent Rayleigh OTDR	km	m	seconds	SMF	Acoustic wave, vibration
Brillouin OTDR/BOTDA	> 100 km	cm – m	minutes	SMF	Temperature, strain,







Enable Structural Health Monitoring of Energy Infrastructures

Potential Future Directions

1. Develop hybrid quantum-classical optical fiber sensor networks for applications ranging from pipeline monitoring to oil and gas exploration
2. Develop quantum sensors based on nitrogen vacancy (NV) center nanodiamonds incorporated into metal-organic framework materials for sensing rare earth elements and critical materials from coal and coal-based resources.
3. Build quantum simulator to explore the carbonic anhydrase as a biocatalyst for carbon capture with the help of quantum computing.
4. Collaborate with industry and national lab partners to found Energy-Q, a group that will identify and promote pre-competitive research that will benefit all QIS applications to energy R&D.
5. Train NETL work force on quantum sensor & quantum computer through workshops and seminars.

Thank You!

VISIT US AT: **www.NETL.DOE.gov**

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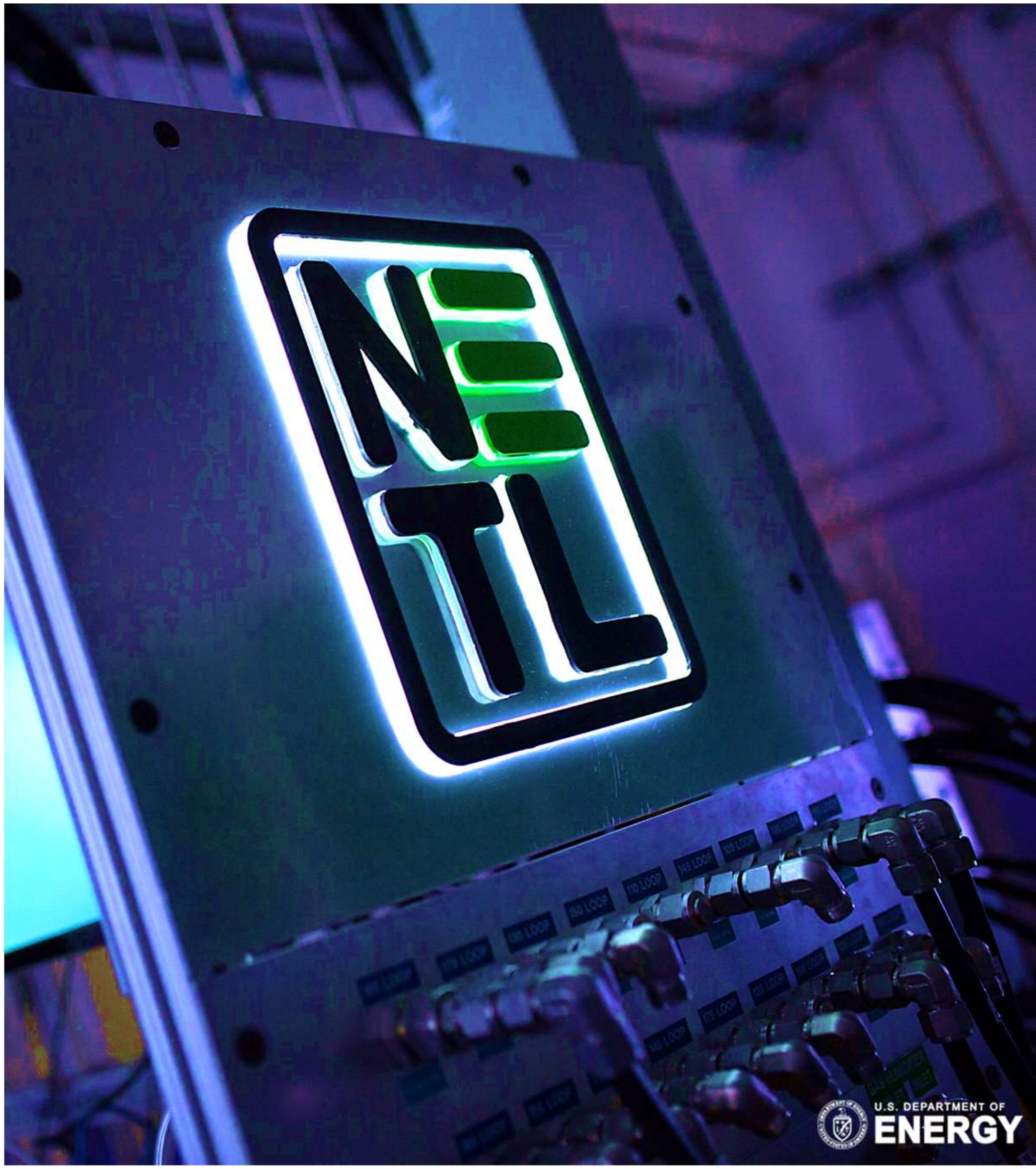

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