Functionalization of nitrogen vacancy-containing nanodiamonds with a metal-organic framework for quantum sensing applications

Scott E. Crawford, PhD
Research Physical Scientist
Research & Innovation Center
NATIONAL ENERGY TECHNOLOGY LABORATORY

Presented to the 2024 Central Regional Meeting of the American Chemical Society

November 7th, 2024

Disclaimer

NATIONAL ENERGY TECHNOLOGY LABORATORY

Authors and Contact Information

Scott E. Crawford[1], Gary Lander[1,2], Hari Paudel[1,2], Roman A. Shugayev,[1] Yuhua Duan[1], John P. Baltrus[1], Nathan A. Diemler[1,2], James E. Ellis[1,2], Ki-Joong Kim[1], Patricia C. Cvetic [1,2]

[1]National Energy Technology Laboratory, 626 Cochran Mill Road, Pittsburgh, PA 15236, USA

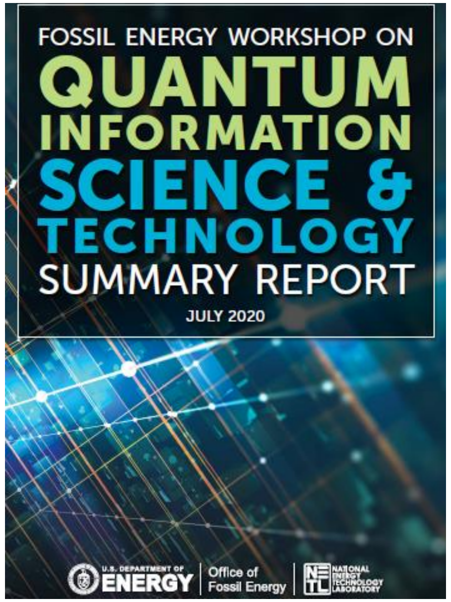
[2]NETL Support Contractor, 626 Cochran Mill Road, Pittsburgh, PA 15236, USA

NETL QUEST (Quantum for Energy Systems and Technologies)

NATIONAL ENERGY TECHNOLOGY LABORATORY

- The National Quantum Initiative Act (NQIA) was signed into law in Dec. 2018. In April 2019, NETL developed a strategy to work on Quantum Information Science (QIS) for energy application.

- In Nov. 18–20, 2019, NETL held the "*Fossil Energy Workshop on Quantum Information Science & Technology*". Co-chaired by Dr. Madhava Syamlal and Prof. Jeremy Levy (PQI).



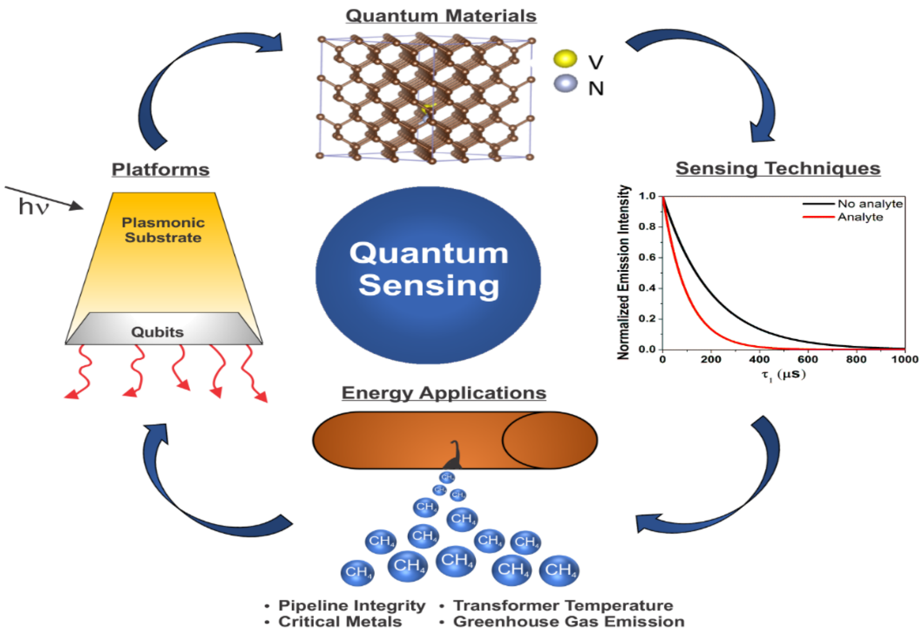
QUEST

- Objectives of QUEST:
  1) Promote QIS activities and capabilities at NETL
  2) Promote collaborations with other QIS entities
  3) Attend QIS meetings
  4) Train NETL QIS workforce
  5) Hold semi-annual update meeting

QUEST external website:

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

QIS In the Energy Sector



Quantum Sensors

-Pipeline integrity

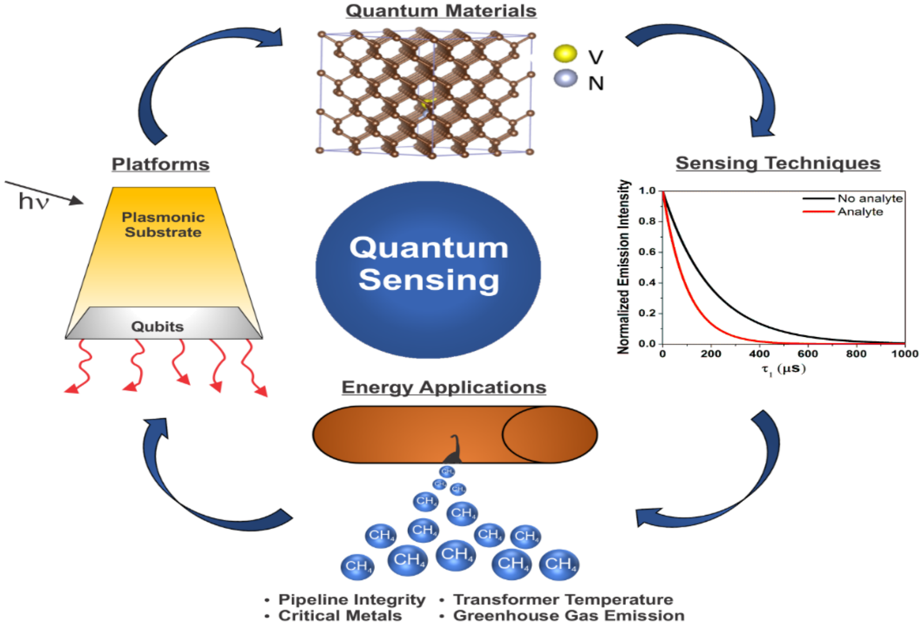
-Gas Leaks/Emissions

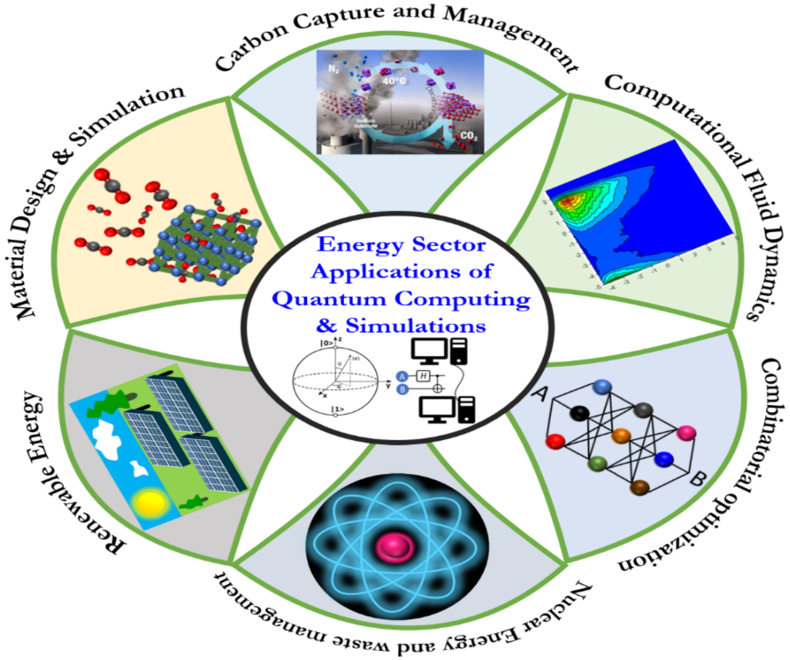
-Abandoned Infrastructure

-Oil & Gas Discovery

Adv. Quantum Technol. 2021, **4**(8), 210049.

QIS In the Energy Sector





Quantum Sensors

-Pipeline integrity

-Gas Leaks/Emissions

-Abandoned Infrastructure

-Oil & Gas Discovery

Adv. Quantum Technol. 2021, **4**(8), 210049.

Quantum Computers & Simulations

-Material design (catalysts, sorbents, etc.)

-Reaction modelling (e.g. carbon capture)

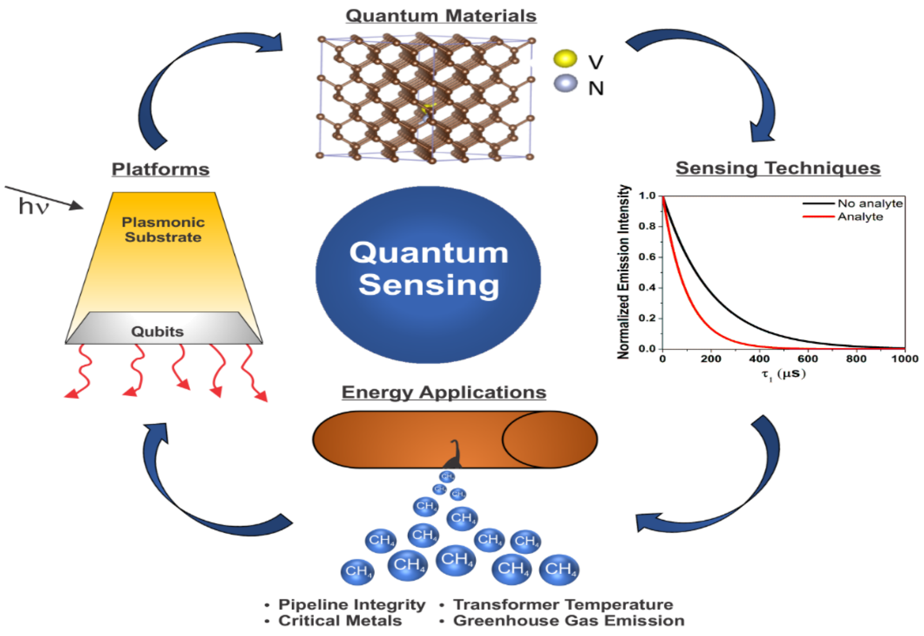
-Grid optimization

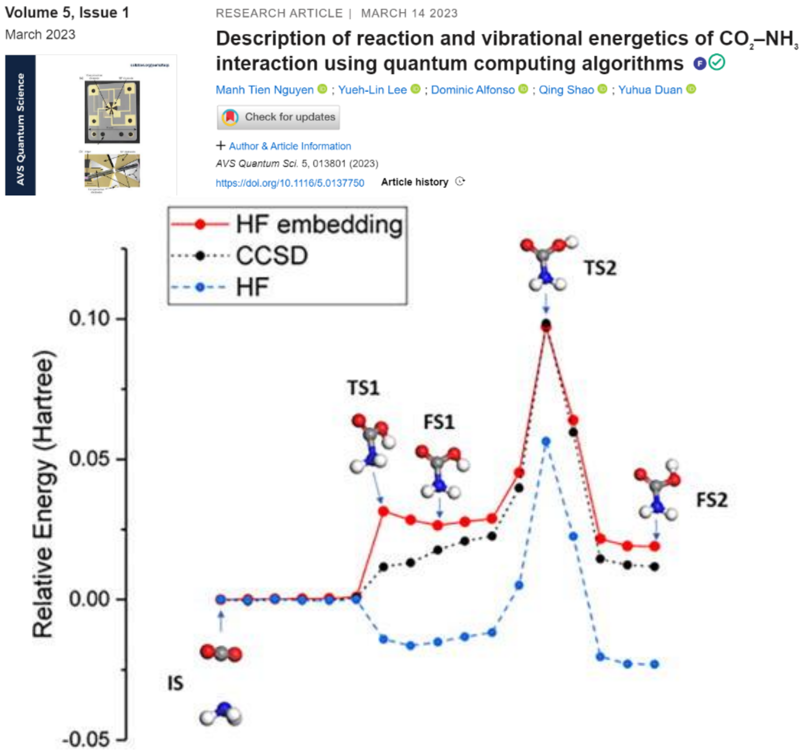
-Simulating Fluid Dynamics

ACS Eng. Au, 2022, **2**(3), 151-196

QIS In the Energy Sector

NATIONAL ENERGY TECHNOLOGY LABORATORY





Quantum Sensors

-Pipeline integrity

-Gas Leaks/Emissions

-Abandoned Infrastructure

--Oil & Gas Discovery

Adv. Quantum Technol. 2021, **4**(8), 210049.

Quantum Computers & Simulations

-Material design (catalysts, sorbents, etc.)

-Reaction modelling (e.g. carbon capture)

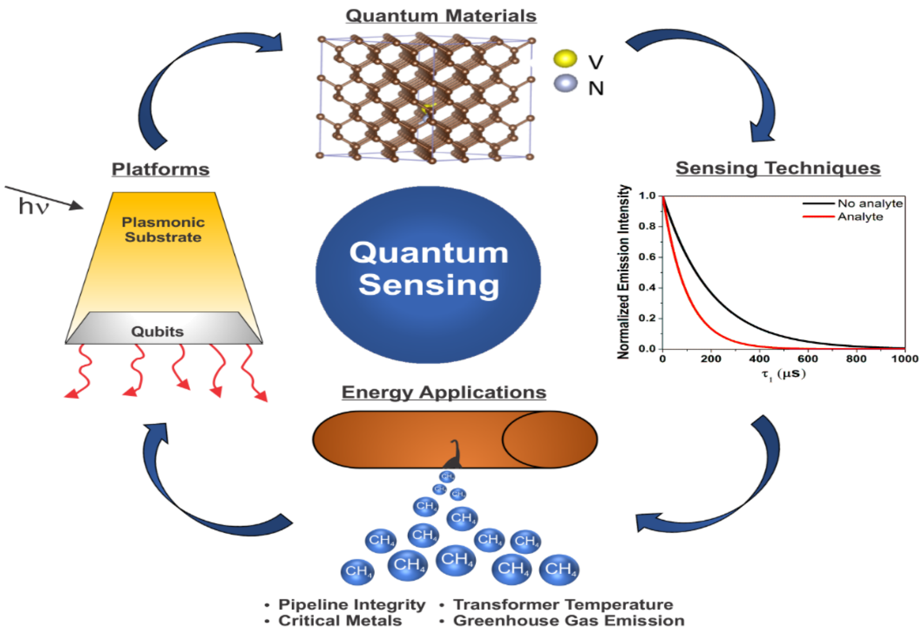
-Grid optimization

-Simulating Fluid Dynamics

AVS Quantum Sci. 2023, **5**(1), 013801

QIS In the Energy Sector

NATIONAL ENERGY TECHNOLOGY LABORATORY



Quantum Sensors

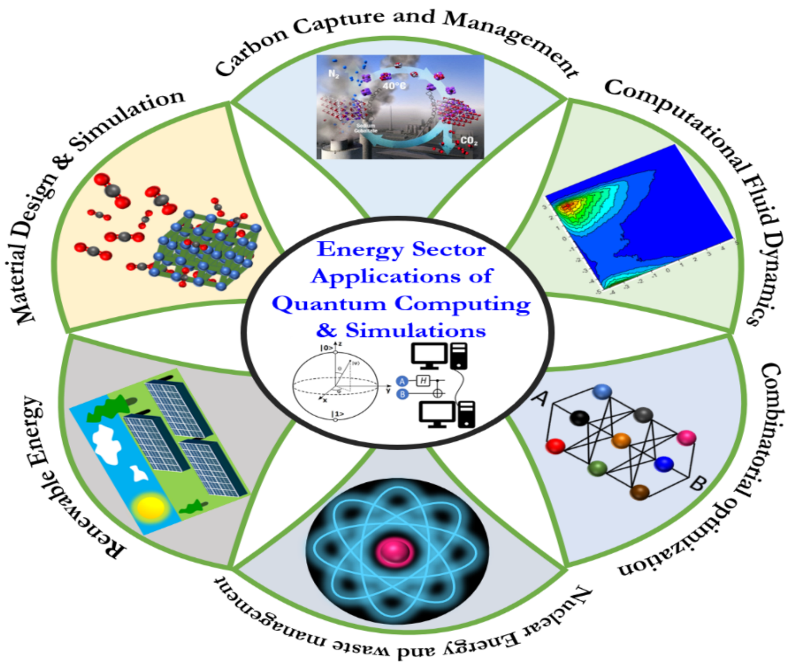
-Pipeline integrity

-Gas Leaks/Emissions

-Abandoned Infrastructure

-Oil & Gas Discovery

Adv. Quantum Technol. 2021, **4**(8), 210049.



Quantum Computers & Simulations

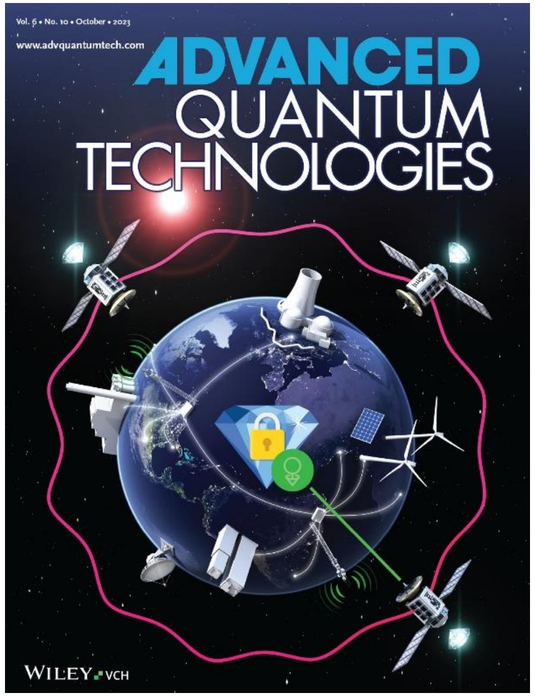
-Material design (catalysts, sorbents, etc.)

-Reaction modelling (e.g. carbon capture)

-Grid optimization

-Simulating Fluid Dynamics

ACS Eng. Au, 2022, **2**(3), 151-196



Quantum Networking/Communication

-Secure data collection + dissemination for:

a) Microgrids

b) Smart grids/meters

c) Vehicle charging stations…

Adv. Quantum Technol. 2023, **6**(10), 2300096

QIS: The Future is Now

Quantum Sensors

~50+ companies

-Both start-ups and multinational corporations

~$610 million market valuation (2023)

-$1.26 billion value projected by 2029

-Gravimeters, atomic clocks, magnetometers, quantum diamond microscopes, etc.

Source: Mordor Intelligence

Quantum Computers

-$1.1 billion market valuation (2022)

-19.6% expected CAGR

-Deployment in banking, chemicals, energy, government, and other sectors

-Significant private and public investments

Source: Grand View Research

Quantum Networking/Communication

-$570 million market valuation in 2022

-29.3% (!!!) CAGR projected until 2032

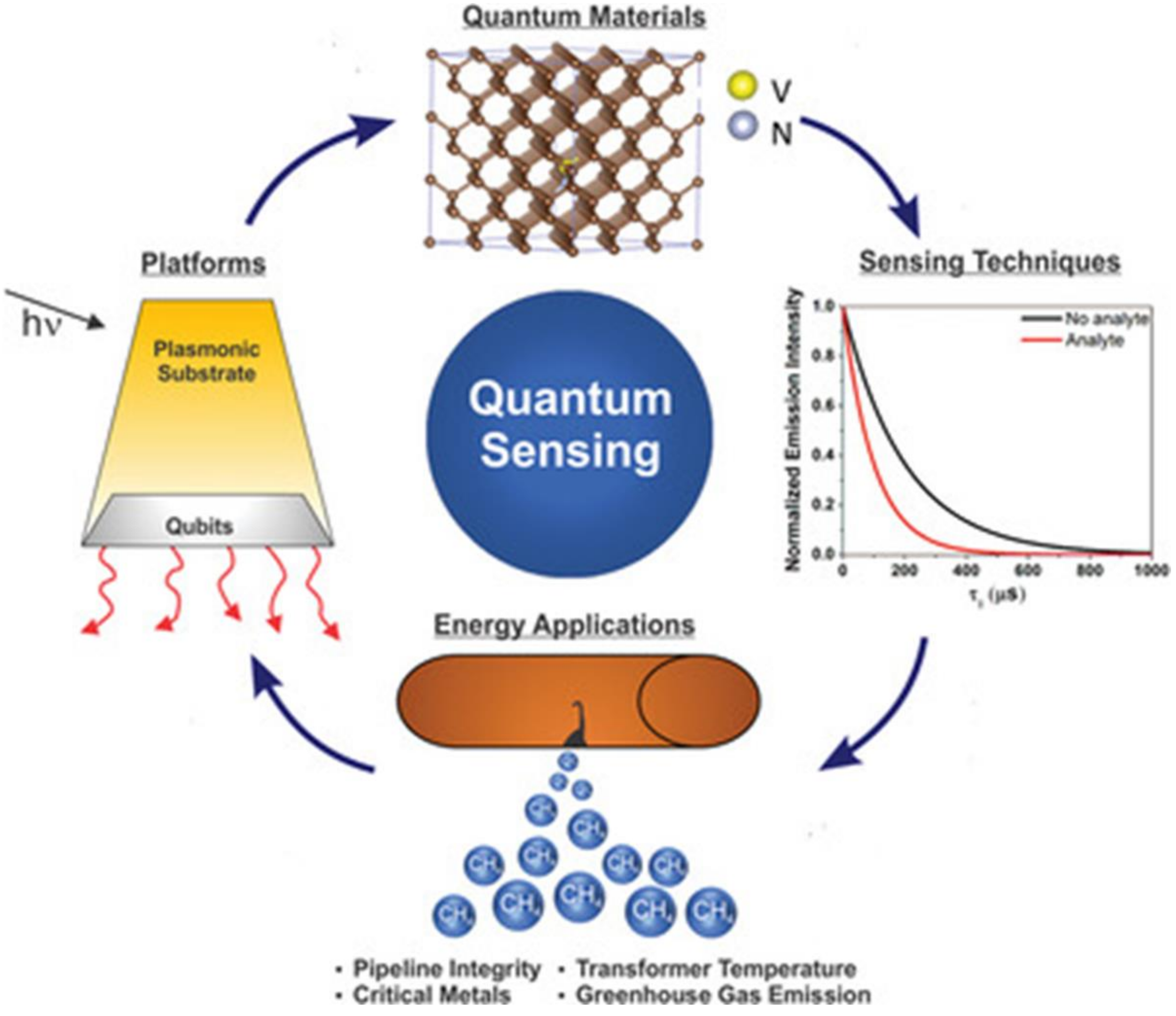
-2032 market value projected to be $8.3 billion

-Driven by cybersecurity threats

Source: Market Research Future

Identifying Application Areas of QIS

- Overview of quantum sensing materials and techniques
- Identifies application areas relevant to the energy industry where high-performance sensors are needed:
  - Pipeline integrity/gas leaks
  - Oil and gas discovery (navigation, subsurface)
  - Electric field sensors
  - Temperature in mines, pipelines, transformers…
- Outlook on future challenges/innovation areas for deployment
  - Packaging/ruggedization
  - Isolating variables of interest/mitigating cross-sensitivity
  - Material innovation
  - Integration with sensing platforms (e.g., fiber optics)



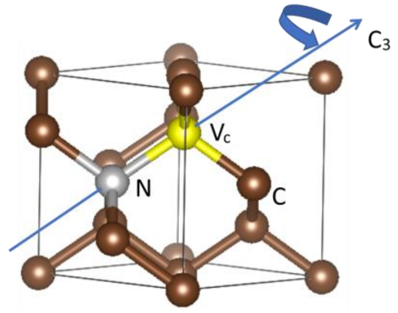
Adv. Quantum Technol. 2021, **4**(8), 210049.

Quantum Materials for Sensing: Diamond Centers

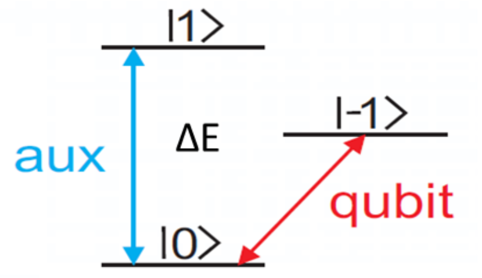
Promising quantum material: Capable for use in elevated temperature and pressure conditions

Vacancy centers in nanodiamonds (ND):

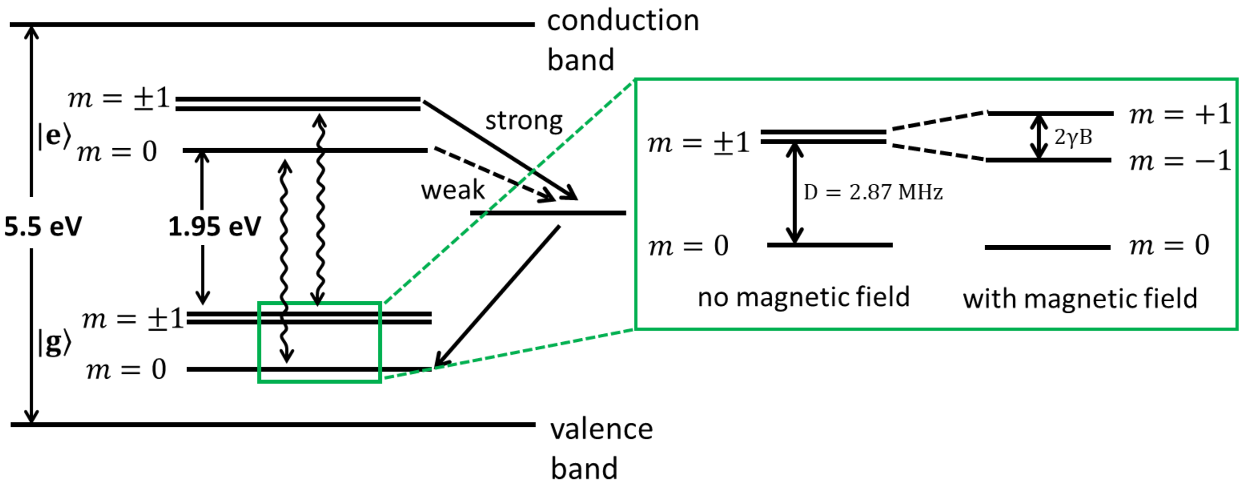
- Atomic impurity (N, Si, Sn, etc.) and carbon vacancy in a diamond lattice: spin qubits
- Information stored in spin states are optically readable
  - Optically-detected magnetic resonance (magnetometry, thermometry, electrometry)
  - Spin relaxometry (ion and pH sensing)
  - Zero-phonon lime emission (thermometry)
  - Room temperature operation



Vacancy in nano-diamond

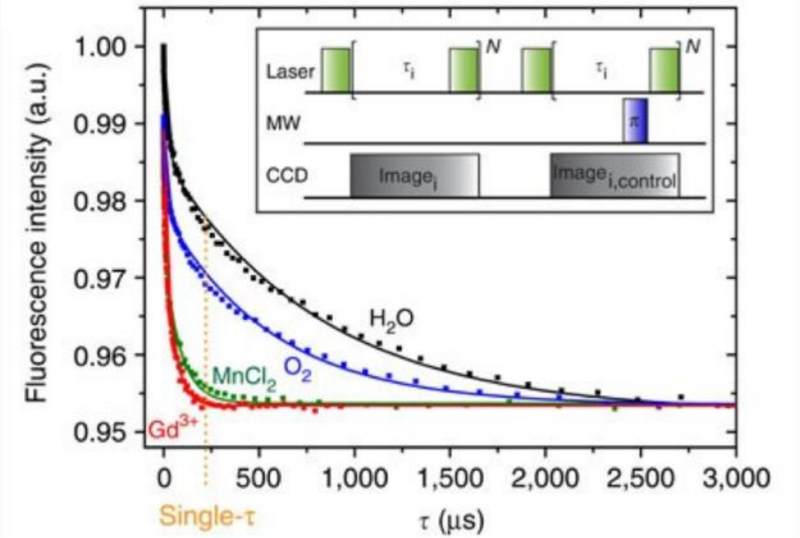


Solid state quantum system



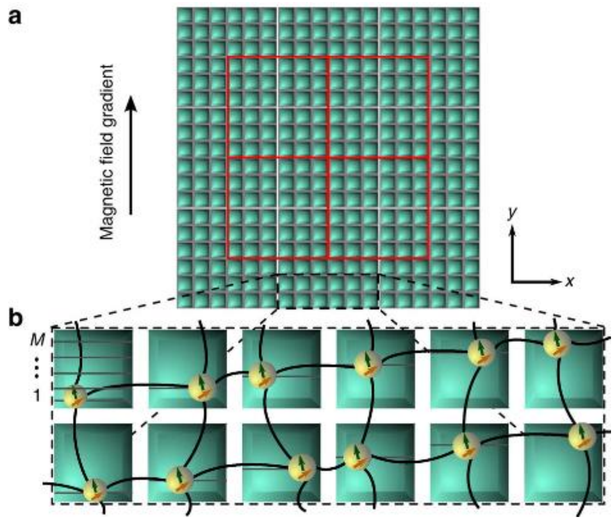
Electronic bands of nitrogen vacancy (NV) center in nano-diamond

Applications of Fluorescent Nanodiamonds



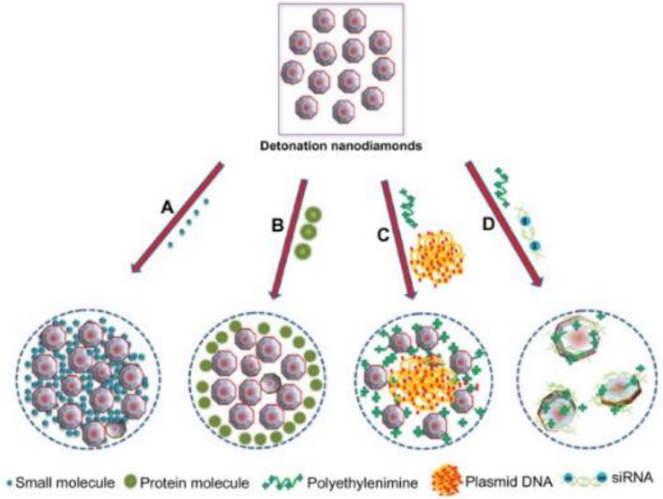
Quantum Sensing

DOI: 10.1038/ncomms2588



Quantum Information Processing

DOI: 10.1038/ncomms1788

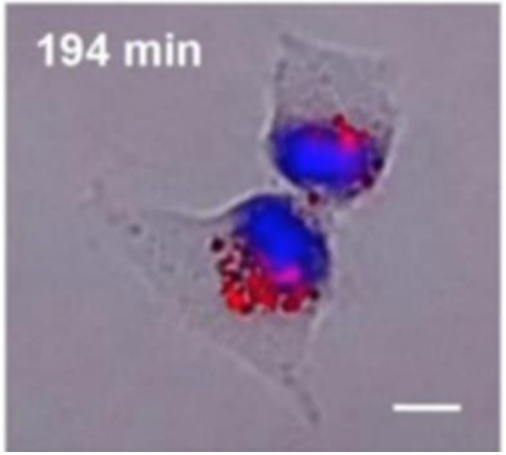


Drug Delivery

DOI:10.2147/IJN.S37348

Catalysis

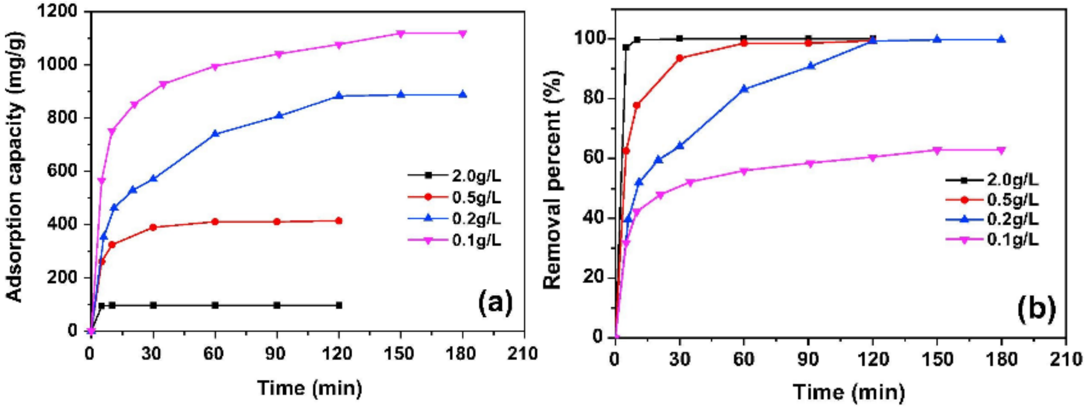
DOI: 10.1002/ange.201002869



Biological Imaging

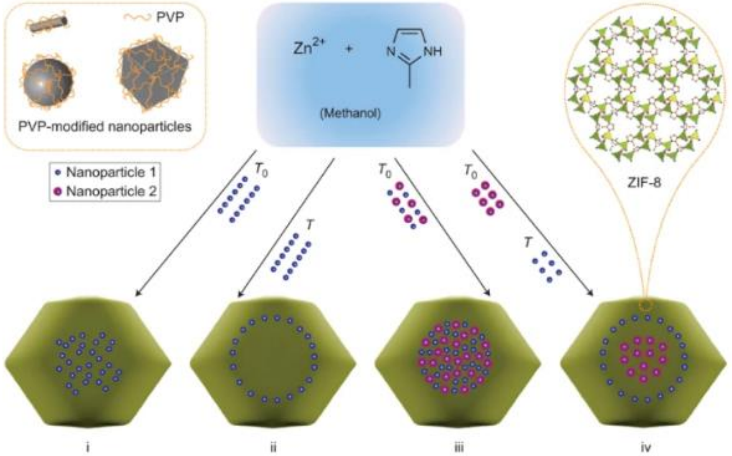
DOI: 10.1021/acs.accounts.5b00484

How Can MOFs* Help?



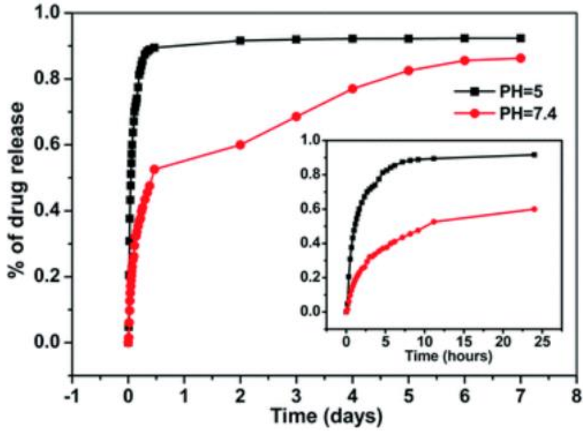
Selective Ion/Gas Uptake

DOI: 10.1016/j.seppur.2017.11.068



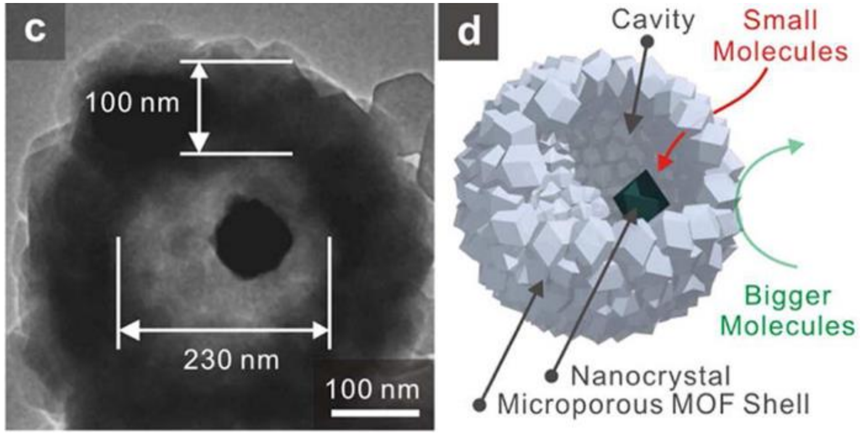
Spatial Control

DOI: 10.1038/nchem.1272



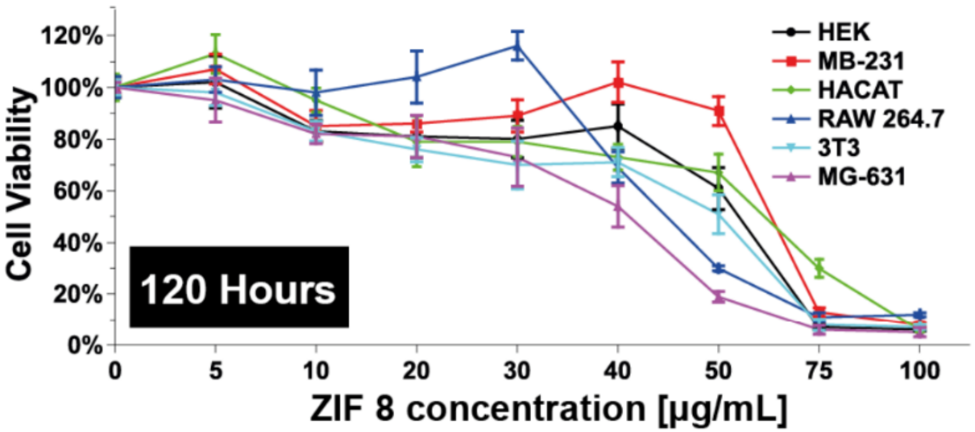
Drug-Delivery Scaffold

DOI: 10.1039/C2DT30357D



Selective Catalysis

DOI: 10.1021/ja306869j

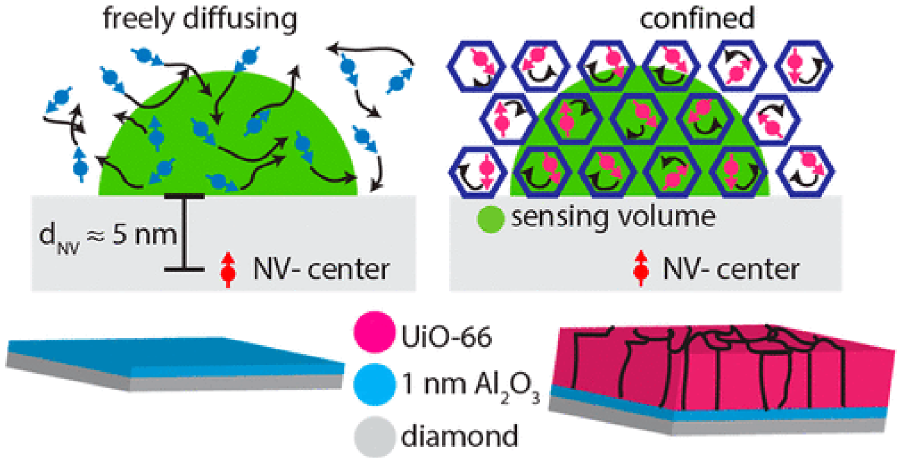


Biocompatibility

DOI: 10.1016/j.apmt.2017.12.014

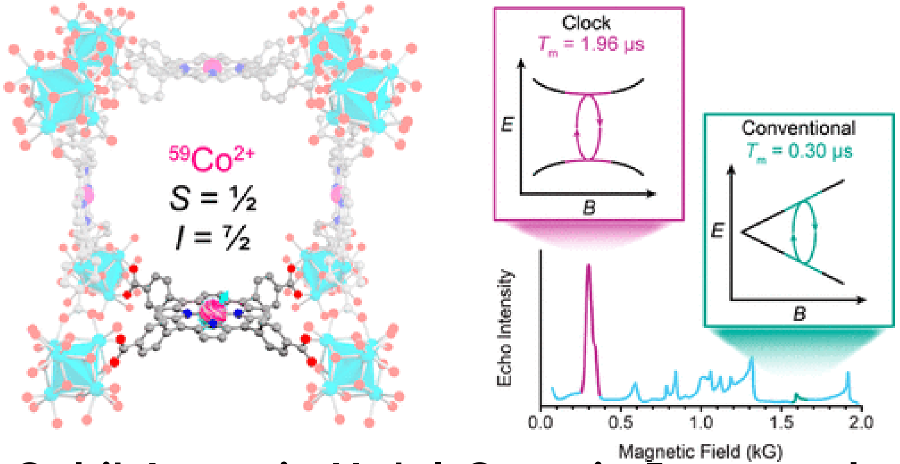
*MOFs = Metal-Organic Framework

Integration of Qubits into Porous Materials



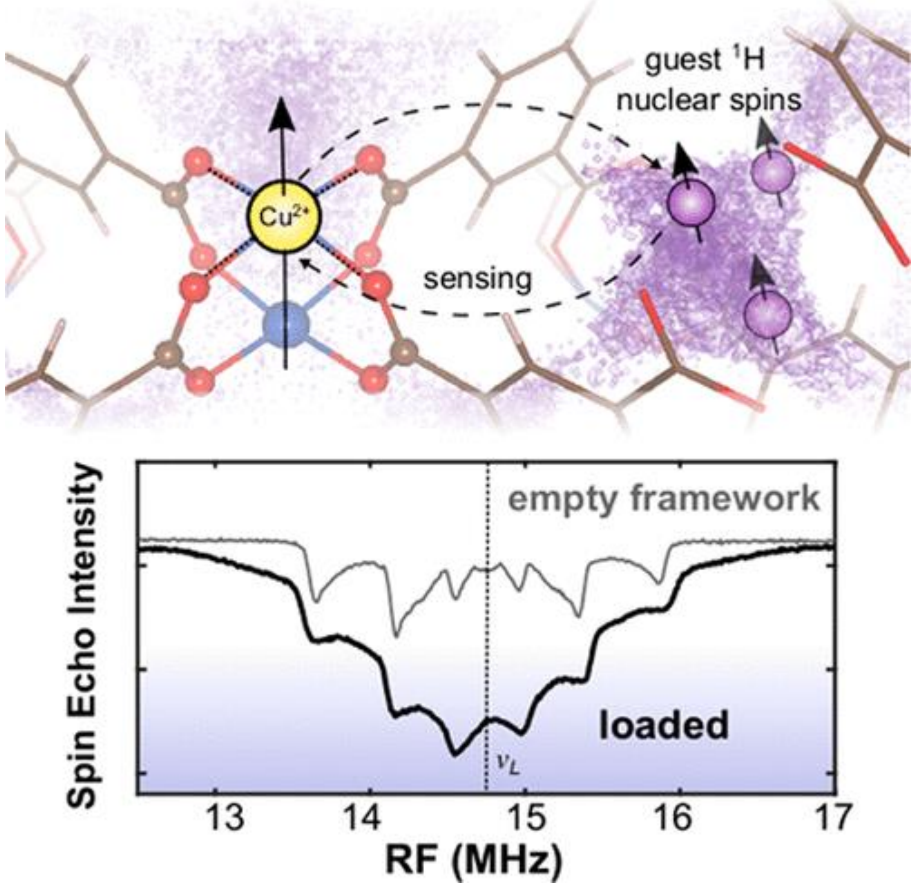
Quantum-Enhanced Nuclear Magnetic Resonance

Nano Lett. 2022, 22, 24, 9876–9882



Qubit Arrays in Metal-Organic Frameworks

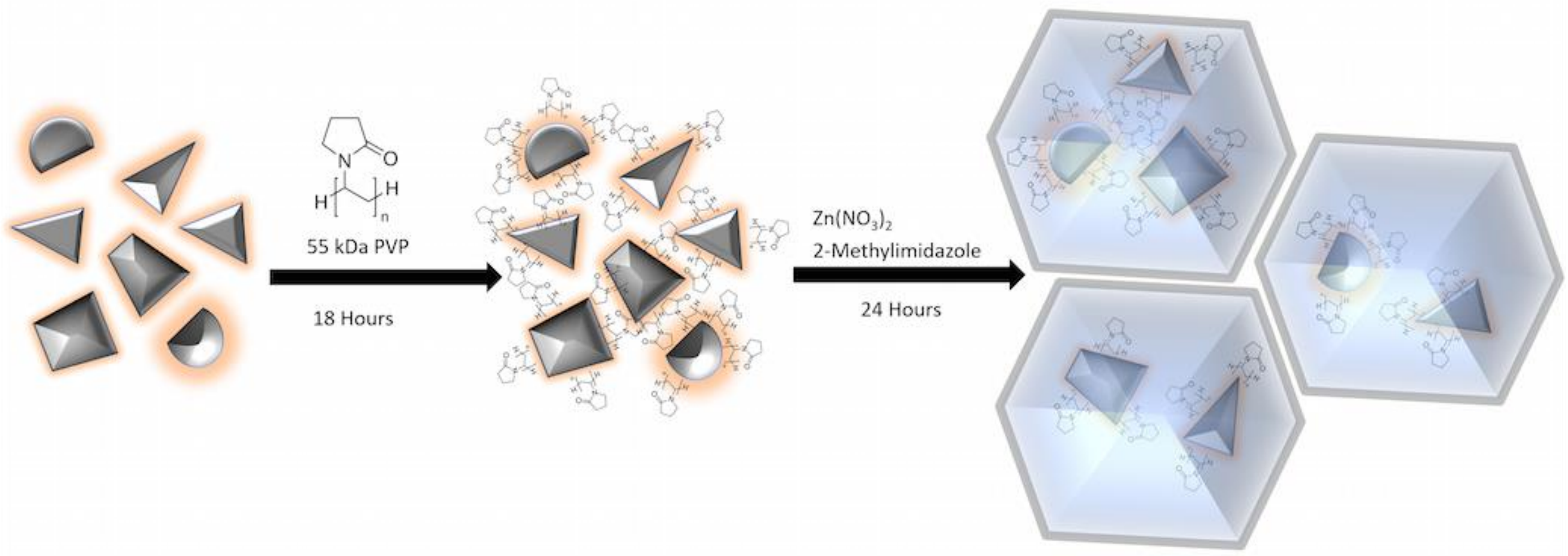
J. Am. Chem. Soc. 2017, 139, 20, 7089–7094

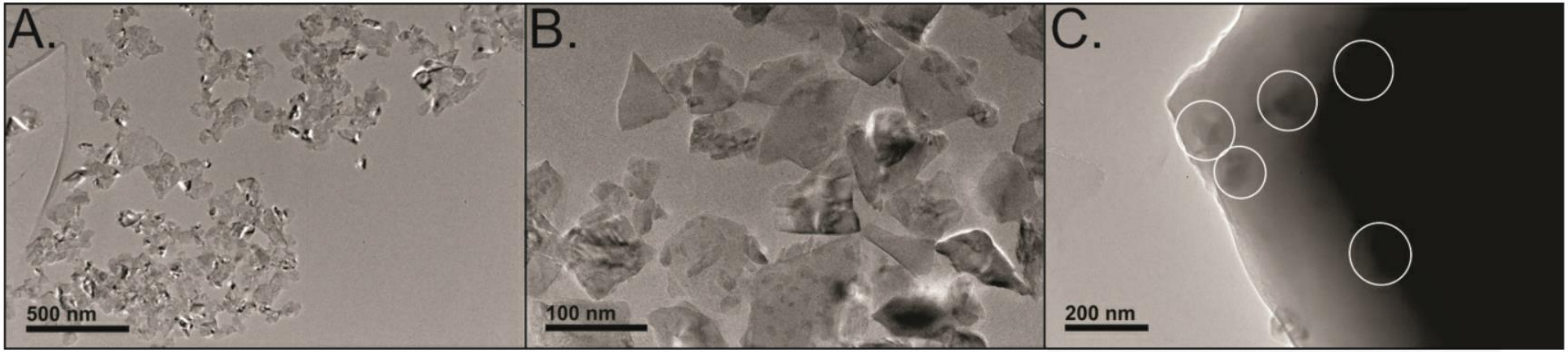


Quantum Sensing of Non-Interacting Gasses

J. Phys. Chem. Lett. 2022, 13, 29, 6737–6742

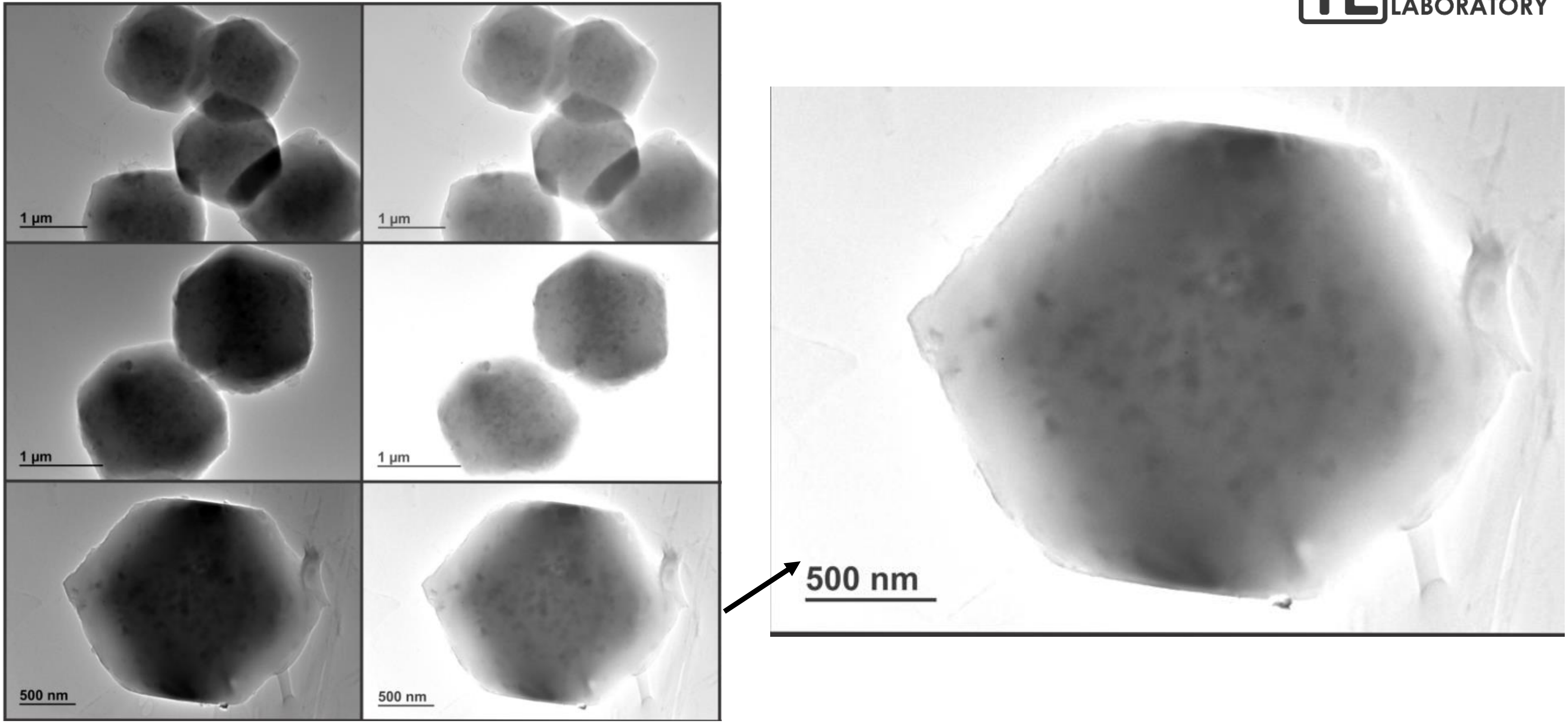
Simple Fabrication Process for NDs@ZIF-8



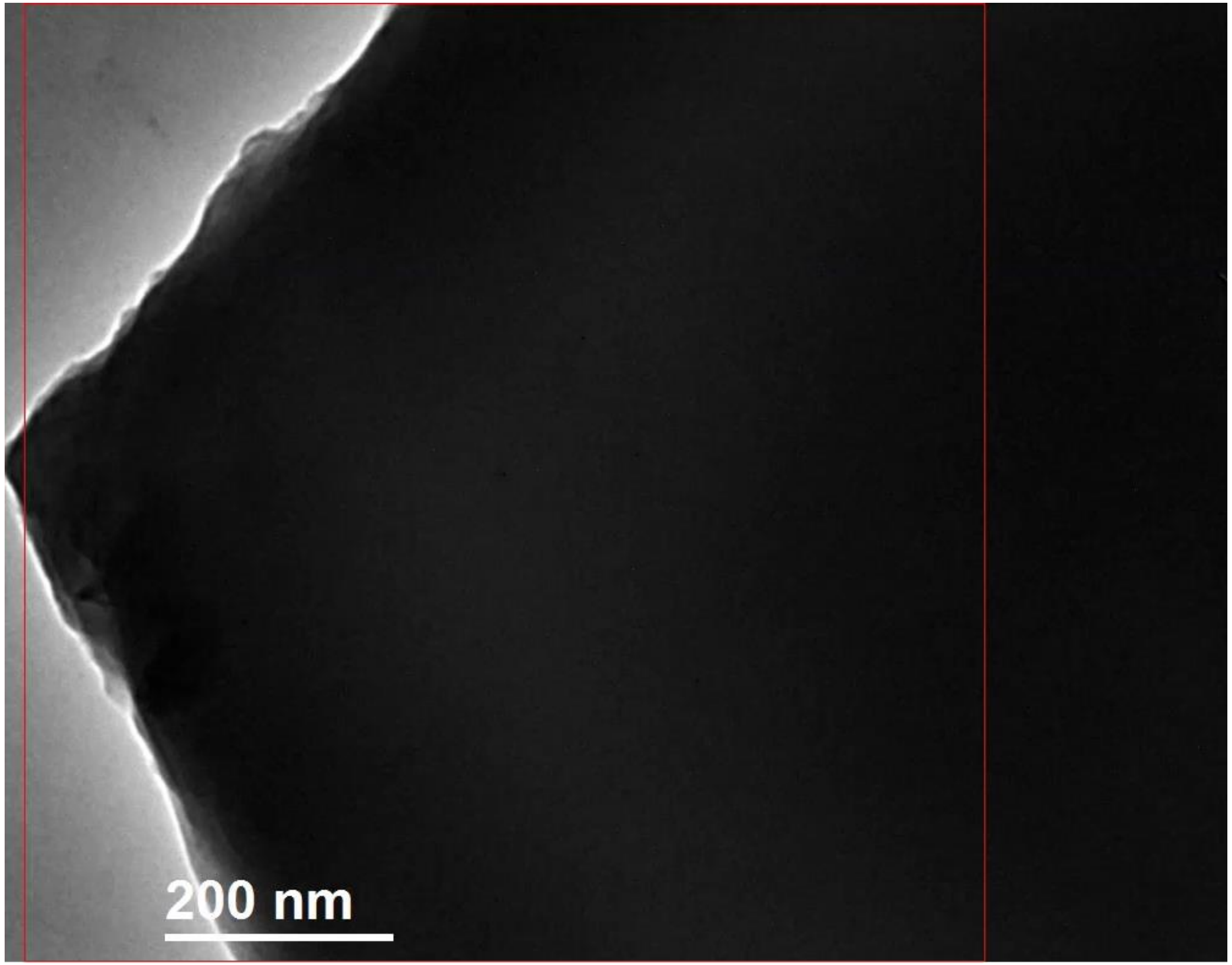


Transmission Electron Microscope Characterization

NATIONAL ENERGY TECHNOLOGY LABORATORY



Dispersion of Nanodiamonds in MOF



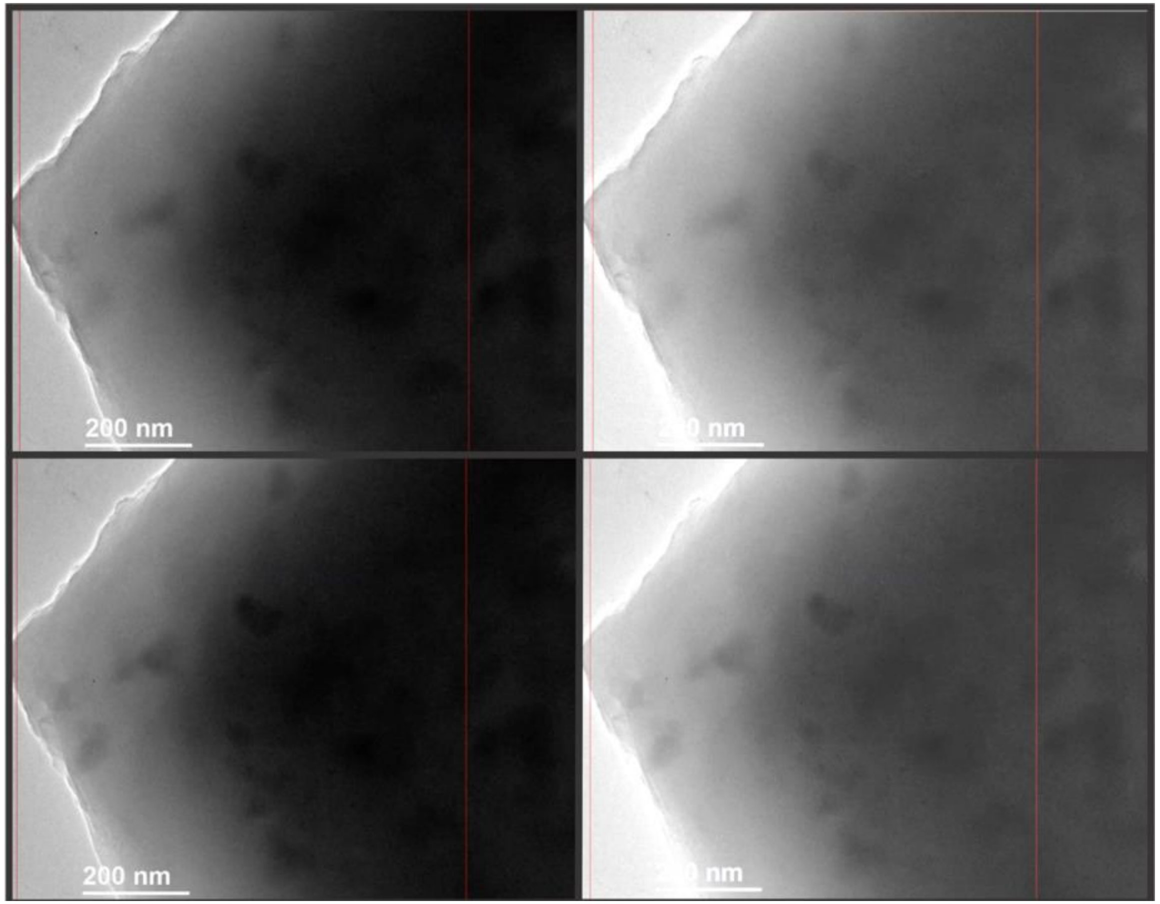
Images at Different Focuses

NATIONAL ENERGY TECHNOLOGY LABORATORY

Raw Image	Enhanced Contrast

1.

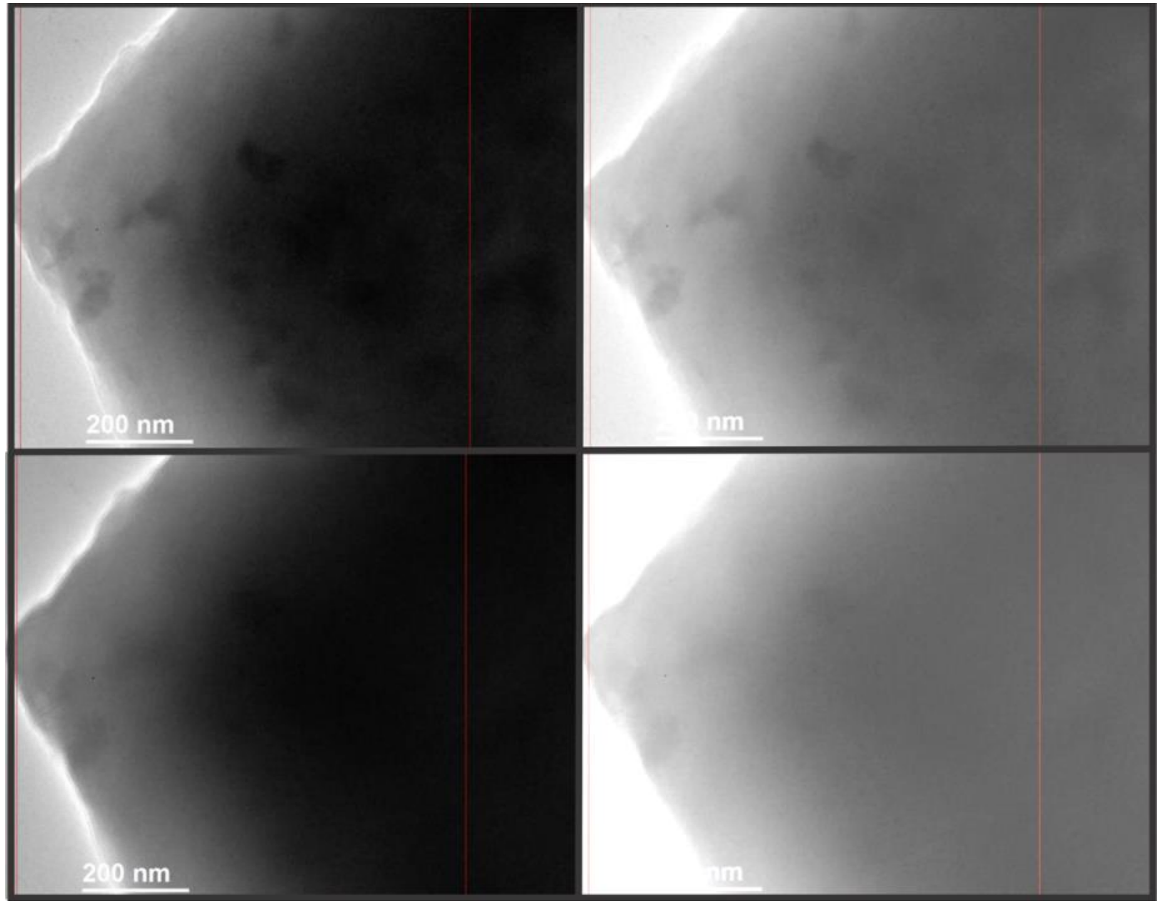
2.



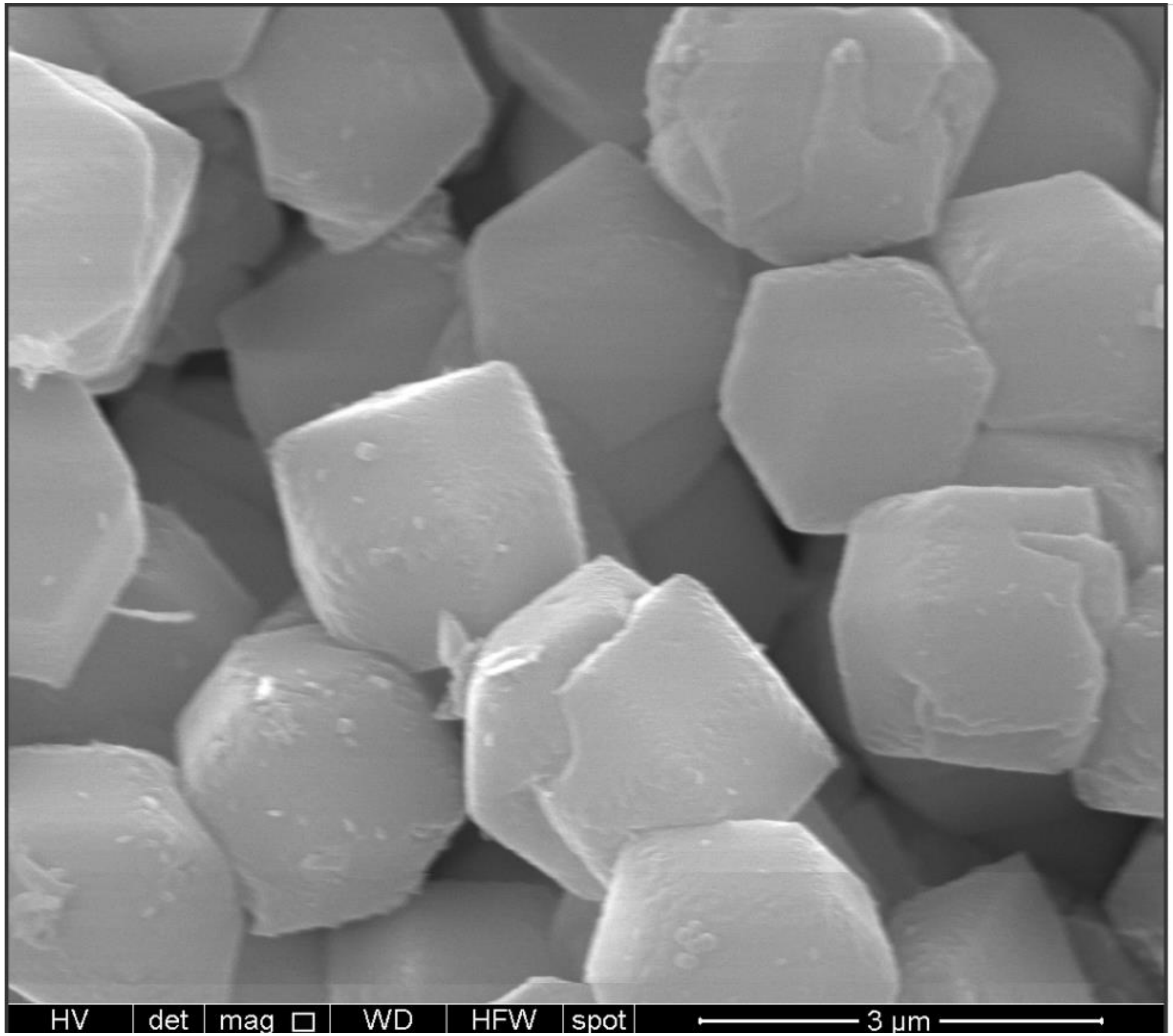
Raw Image	Enhanced Contrast

3.

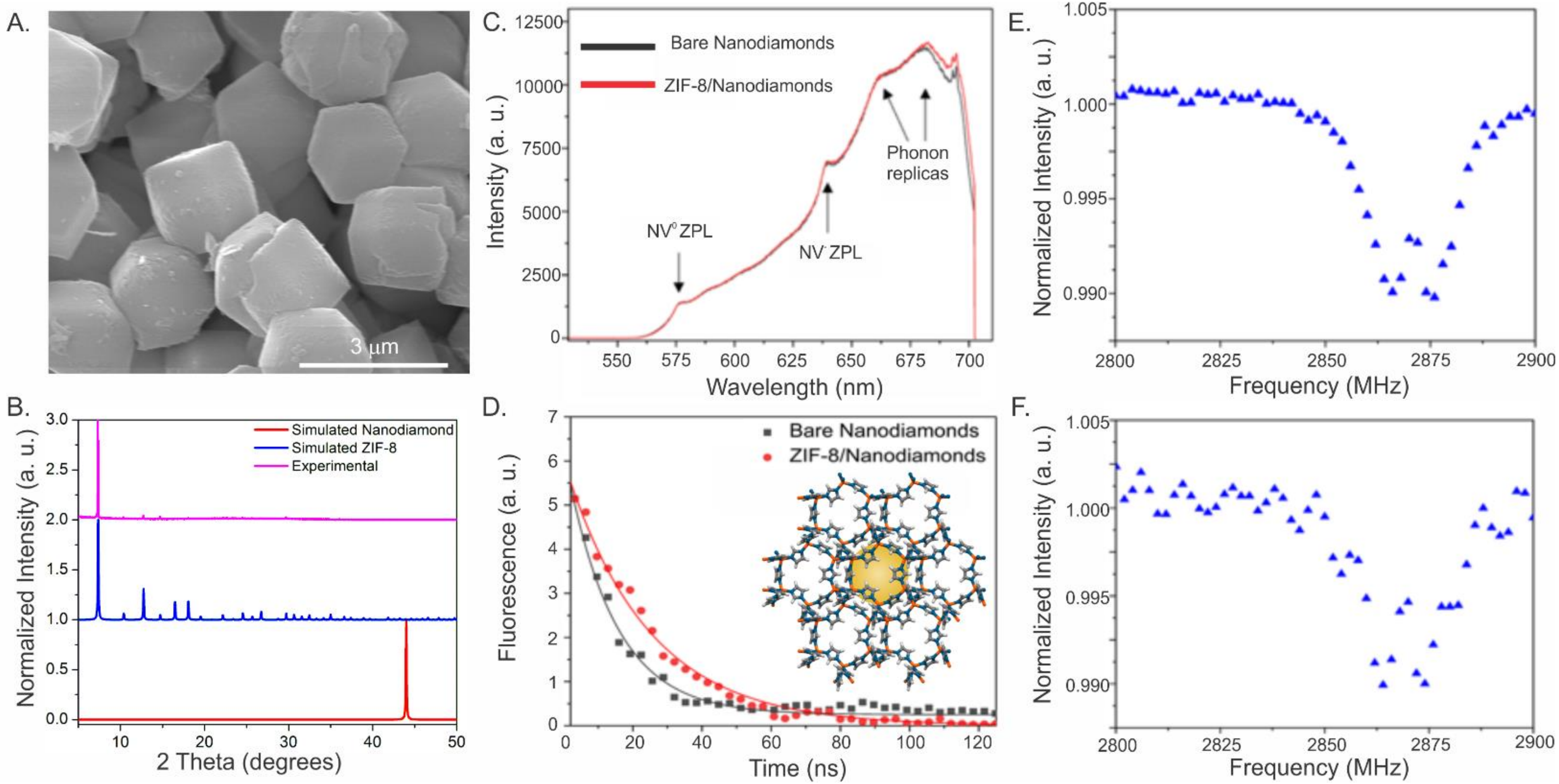
4.



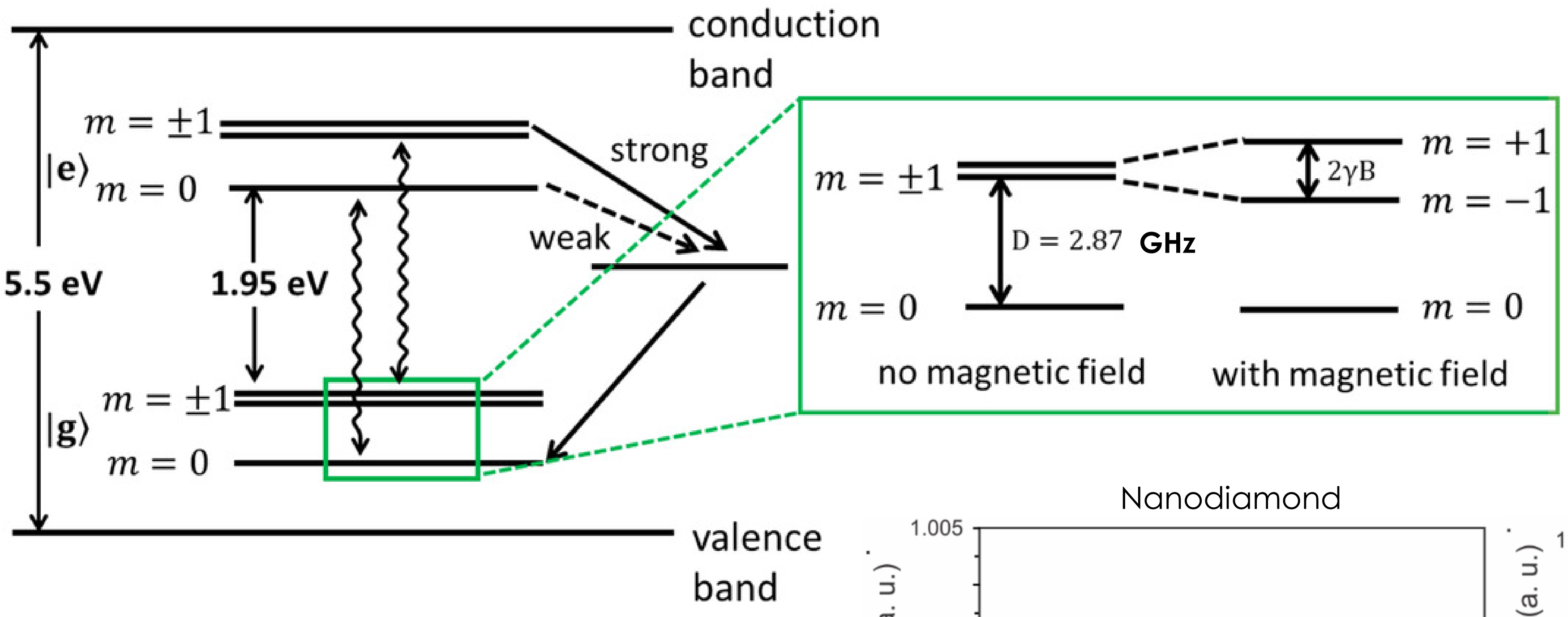
SEM Indicates few Nanodiamonds on MOF Surface

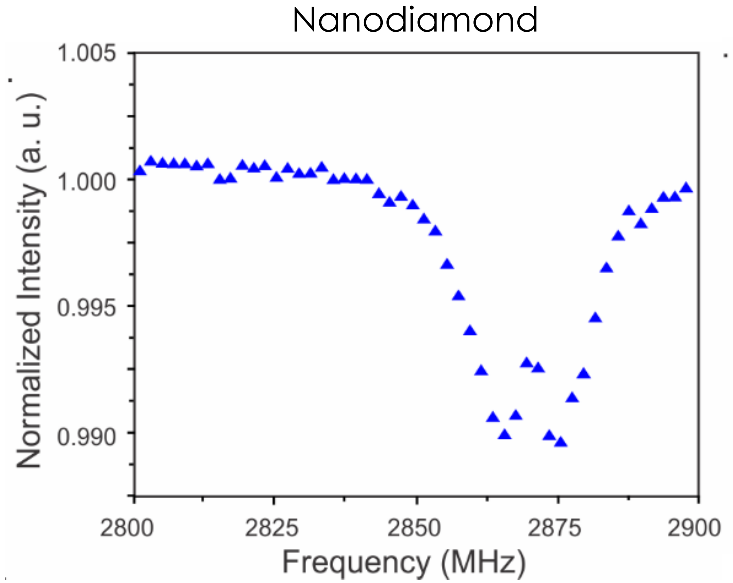


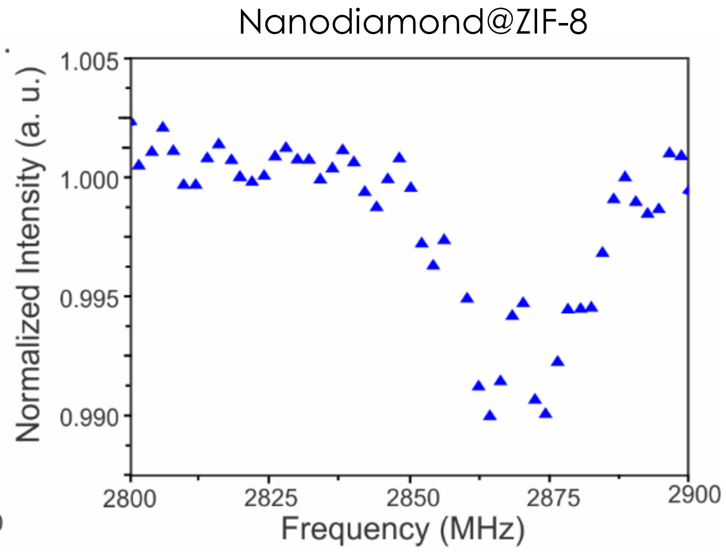
Optical Properties are Unchanged in MOF



Quantum Sensing Experiments: ODMR*

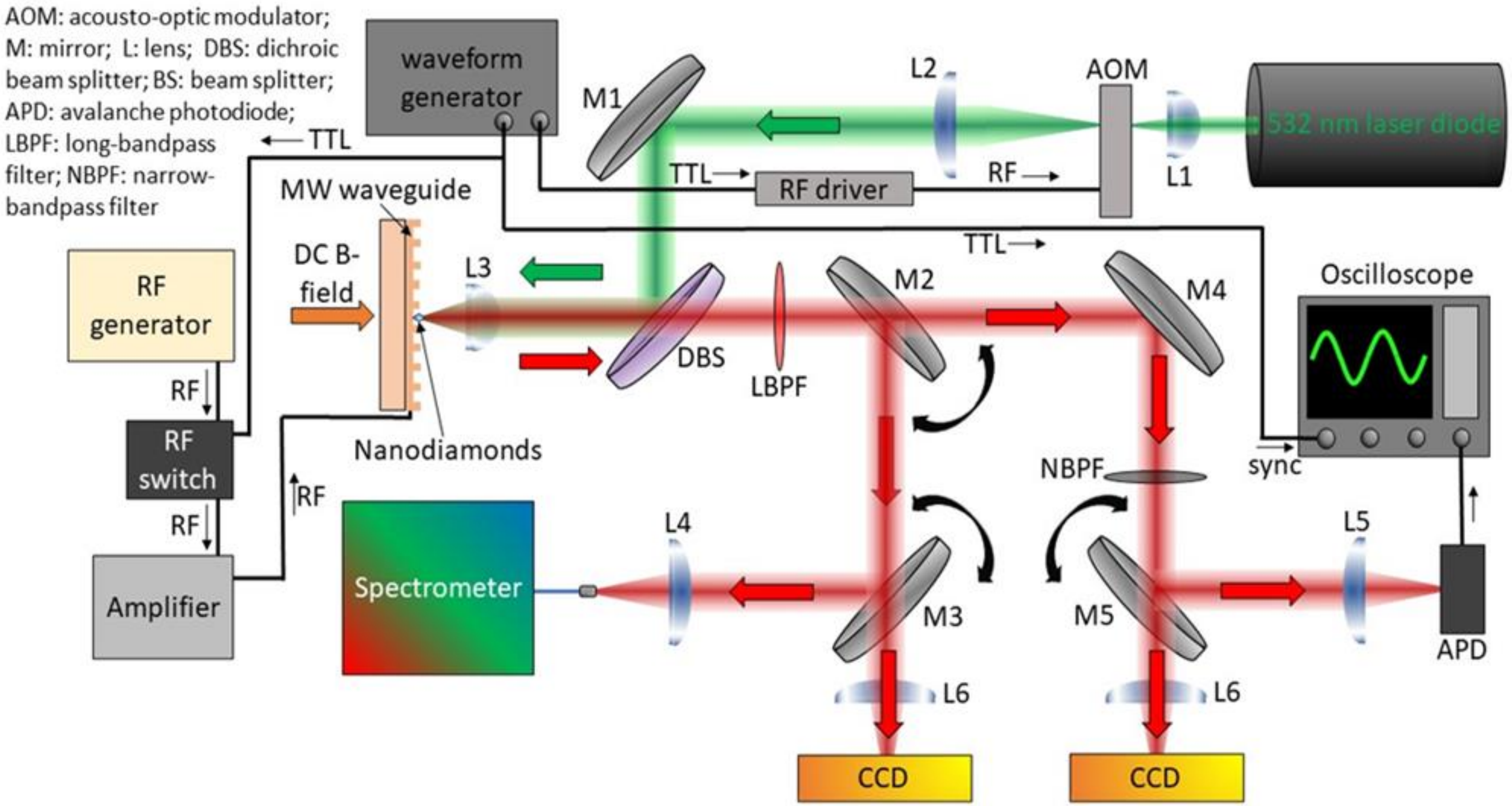






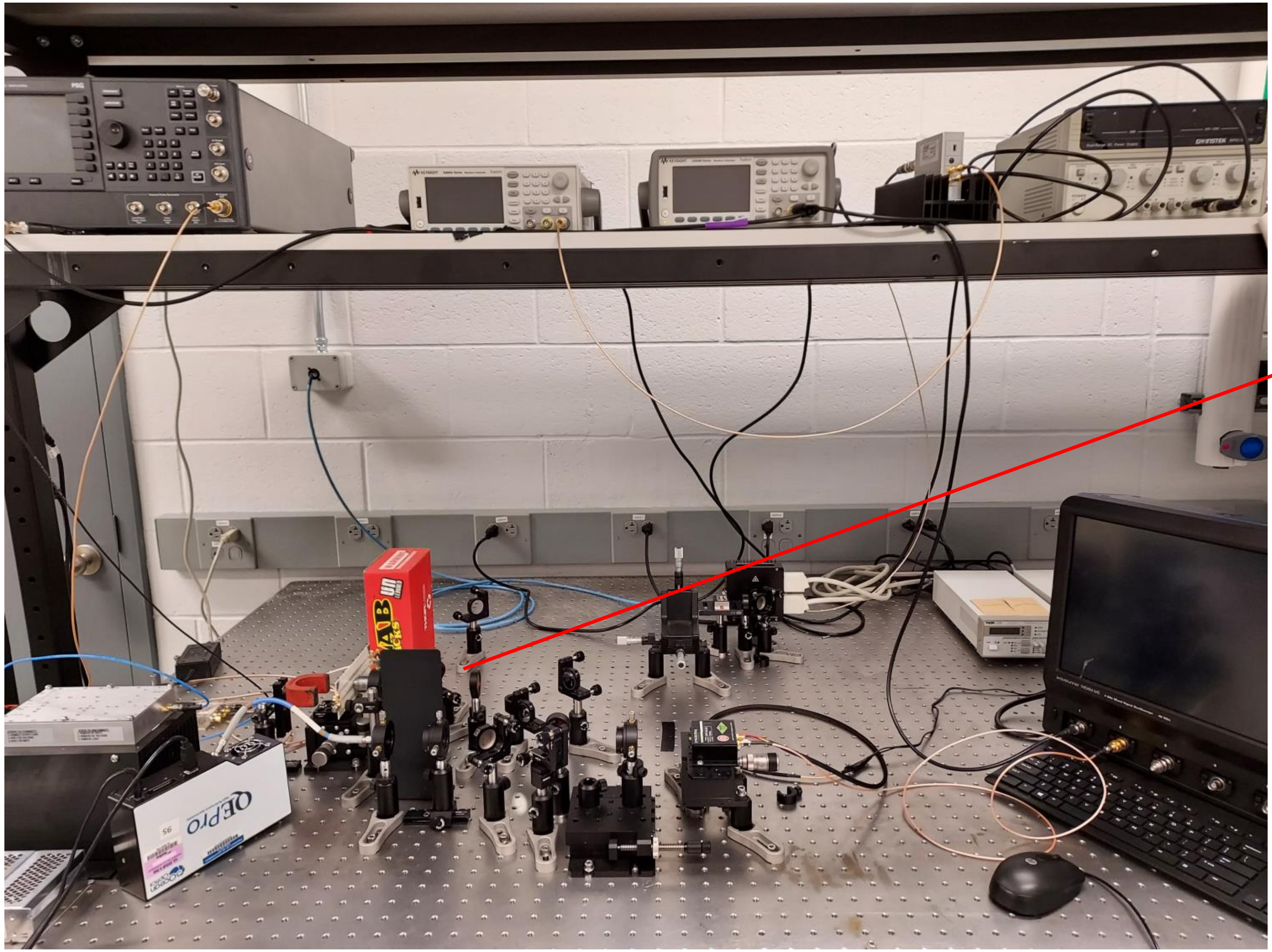
*ODMR: Optically Detected Magnetic Resonance

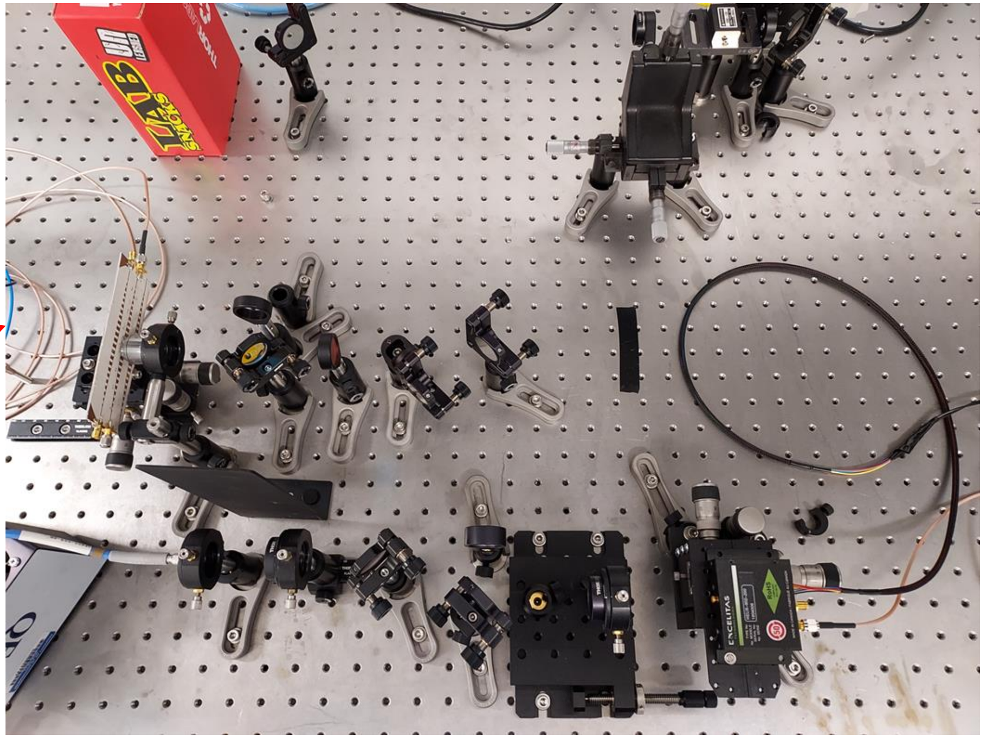
Setup for ODMR/Spin Relaxometery



Gary Lander, et. al., DOI: 10.1117/12.3014019

Setup for ODMR/Spin Relaxometery

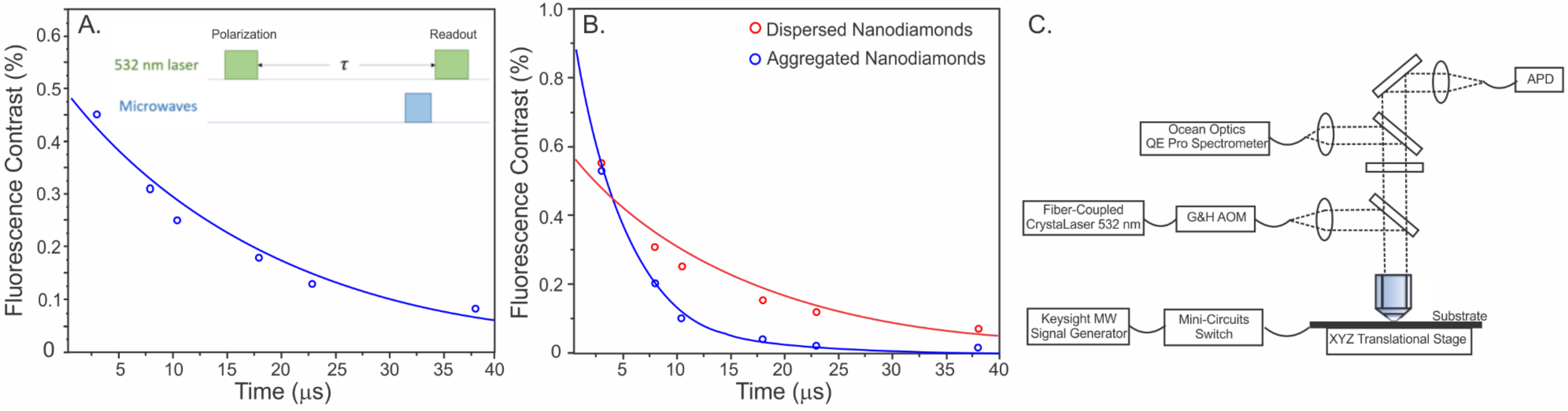




Gary Lander, et. al., DOI: 10.1117/12.3014019

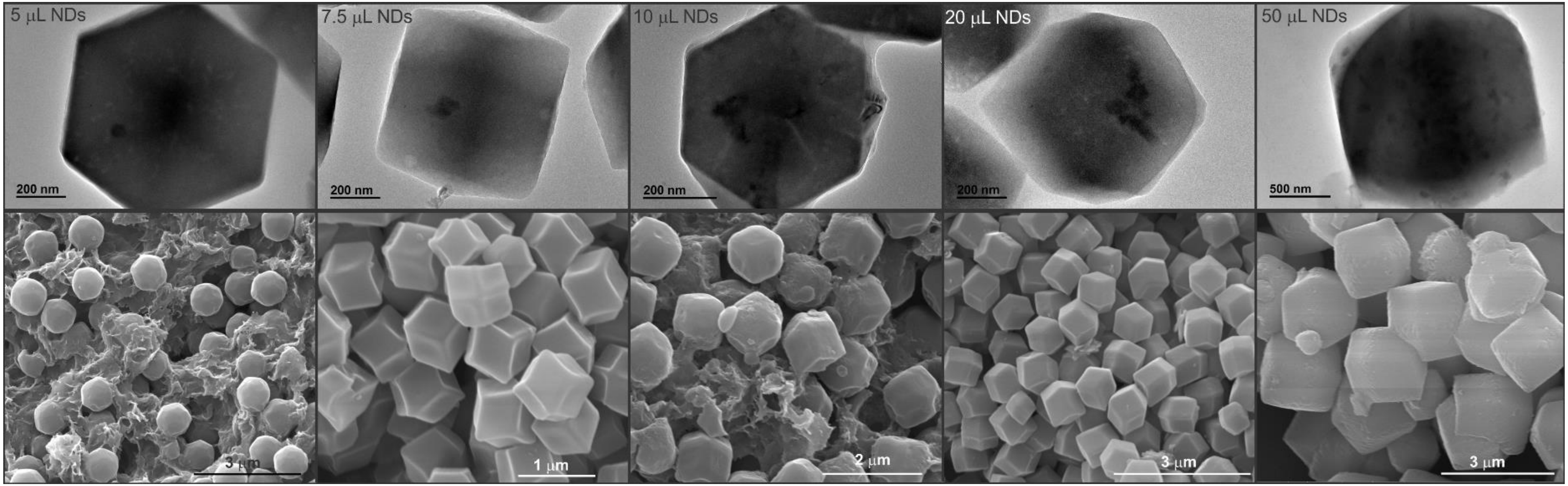
ZIF-8 Enhances Spin Relaxometry Performance

NATIONAL ENERGY TECHNOLOGY LABORATORY



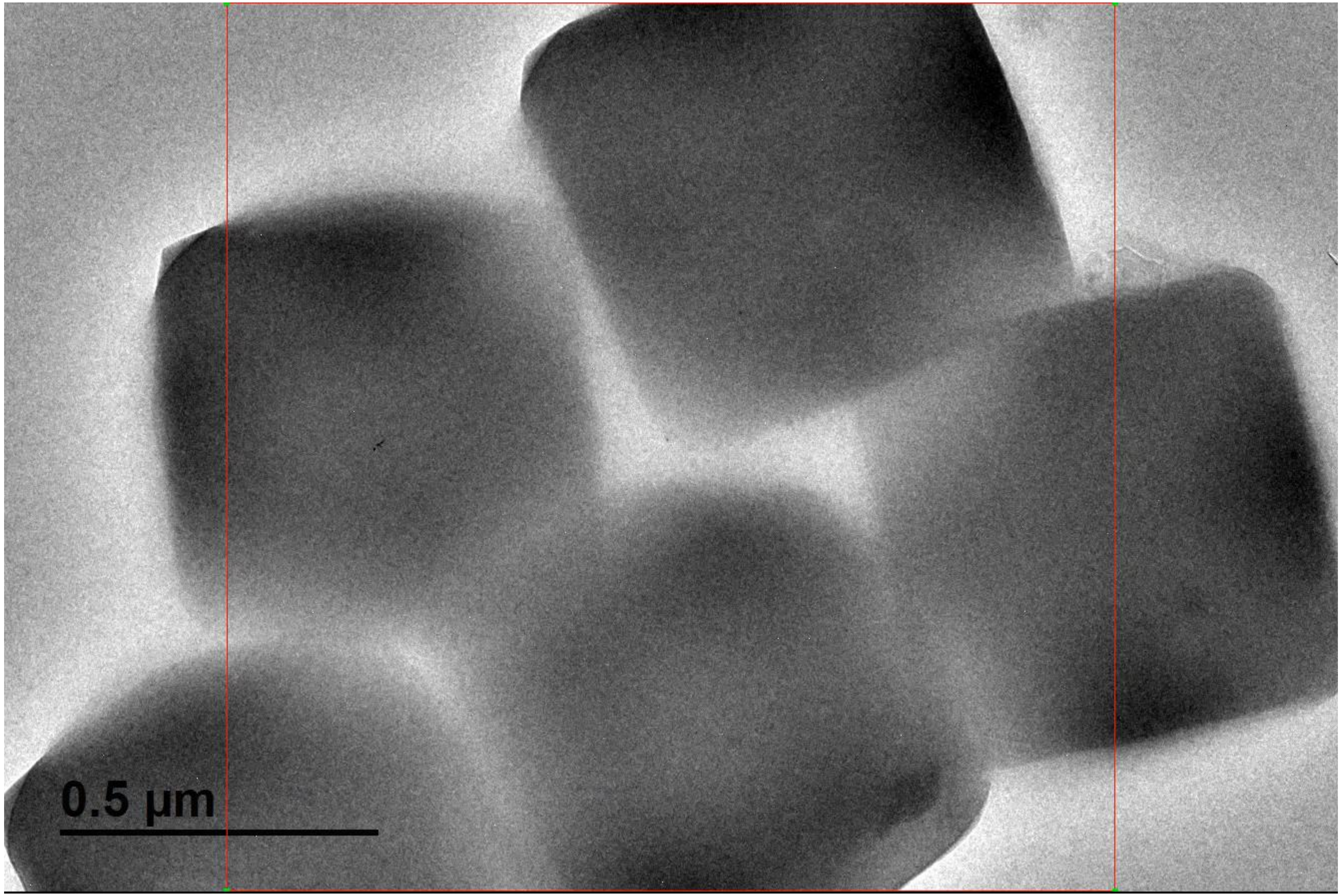
Longitudinal spin relaxation time T_1 is 5 μs for aggregated, bare nanodiamond, 15 μs for dispersed, bare nanodiamond, and enhanced to 20 μs for the MOF-coated diamond

Control over Nanodiamond Loading



Increasing the concentration of nanodiamonds used in the synthesis correlates with the number of nanodiamonds per MOF

Imaging Single Nanodiamonds in ZIF-8



Conclusions and Next Steps

NATIONAL ENERGY TECHNOLOGY LABORATORY

- Established facile synthetic approach for ZIF-8 functionalization of nanodiamonds
- Optical properties of the nanodiamonds are conserved, indicating that the composites have utility in sensing and bioimaging applications
- The system is characterized by XRD, Raman, FT-IR, TEM, SEM, and XPS
- Sensing targets include high spin ions, electric and magnetic fields, etc.
- Other porous material/nanodiamond composites are also being explored

NETL Resources

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

@NETL_DOE

@NETL_DOE

@NationalEnergyTechnologyLaboratory

Contact:
Scott.Crawford@netl.doe.gov