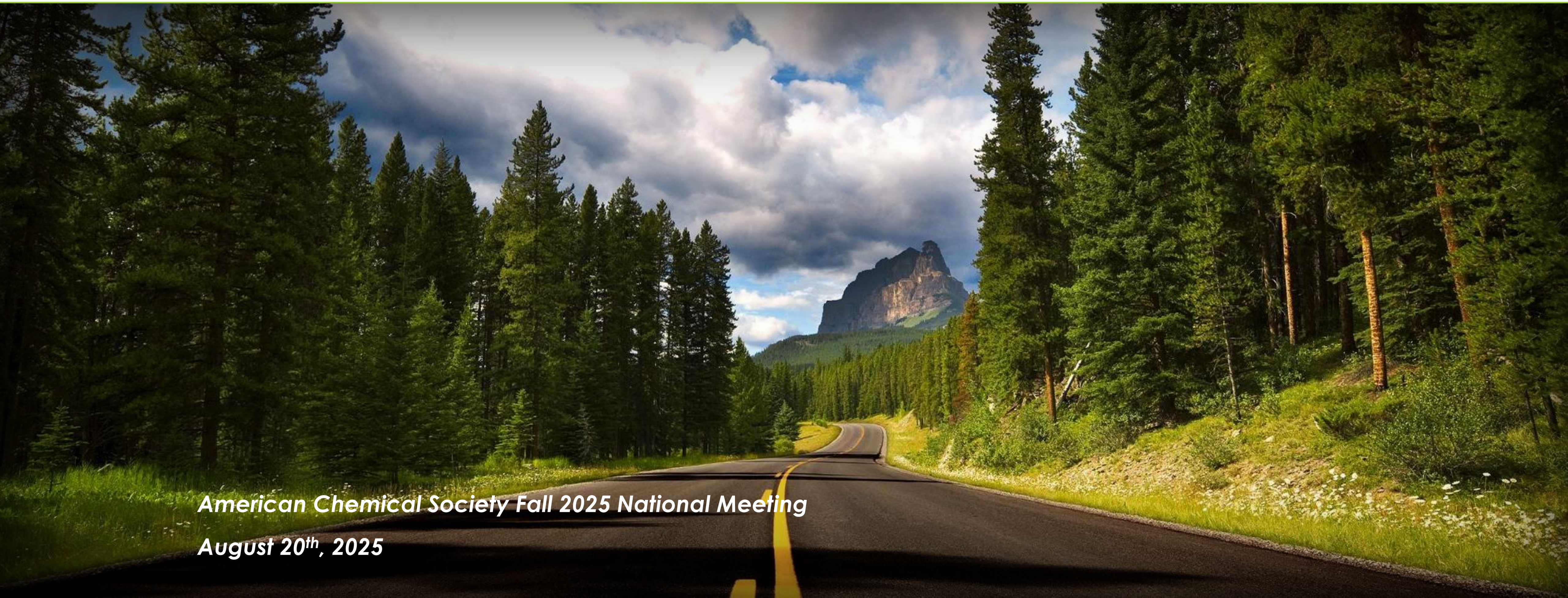
Synthesis of nanodiamonds encapsulated by zeolitic imidazole framework-8 for quantum sensing applications

Scott E. Crawford, PhD
Research Physical Scientist, Research & Innovation Center



American Chemical Society Fall 2025 National Meeting

August 20th, 2025

Disclaimer

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Authors and Contact Information

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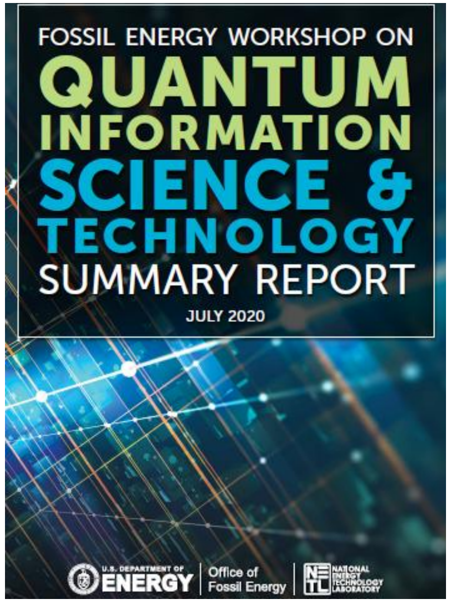
NETL QUEST (Quantum for Energy Systems and Technologies)

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).



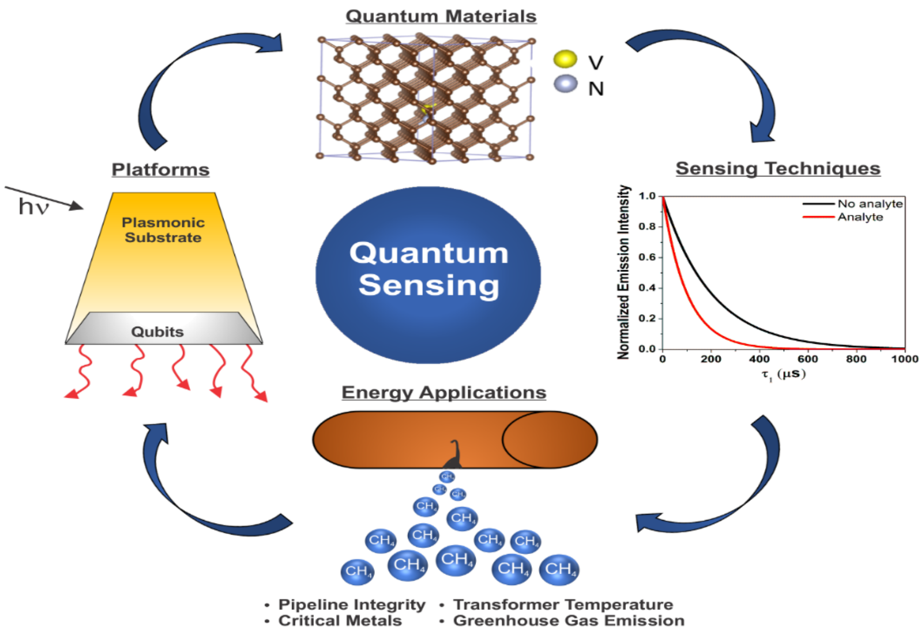
QUEST

- 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

Quantum for the Energy Sector



Quantum Sensors

-Pipeline integrity

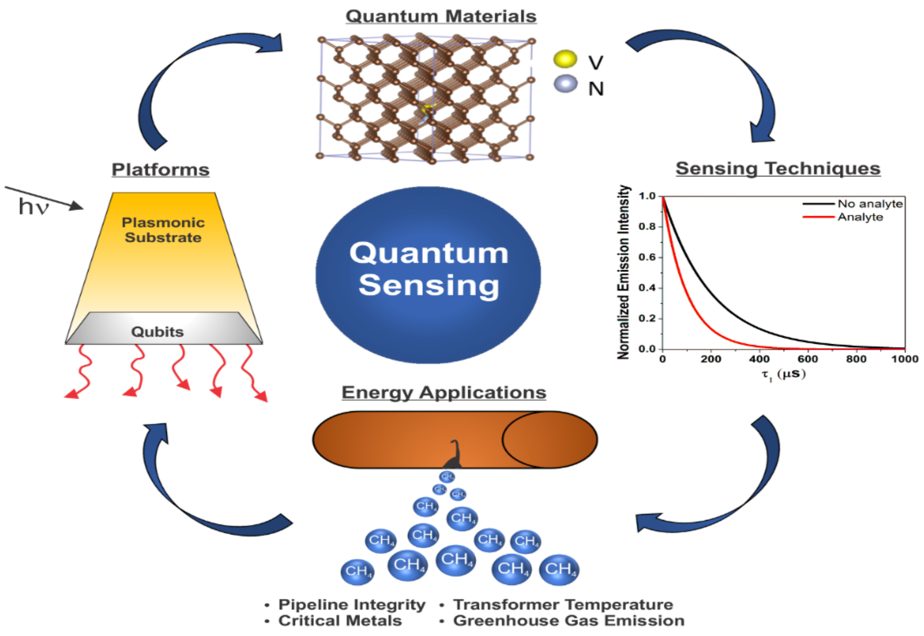
-Gas Leaks/Emissions

-Abandoned Infrastructure

-Oil & Gas Discovery

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

Quantum for the Energy Sector



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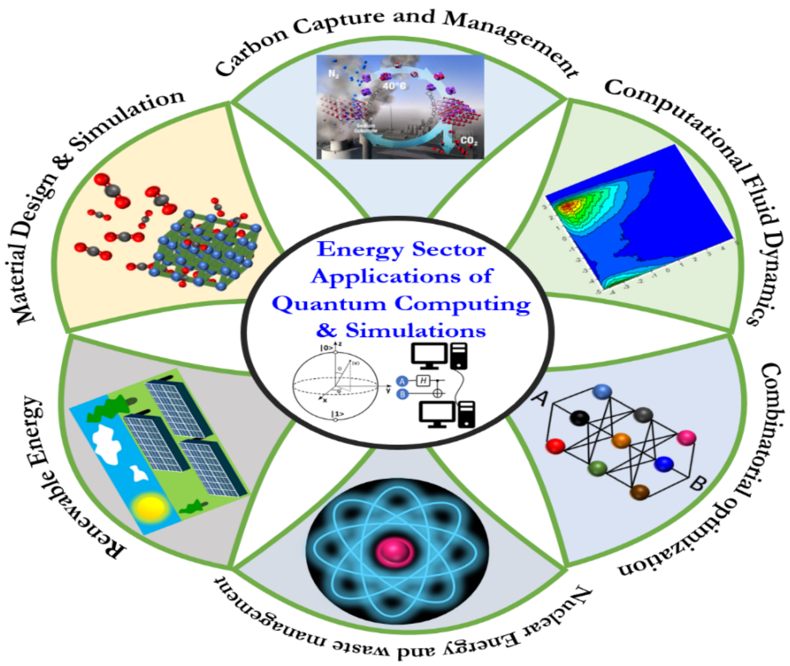


Quantum Computers & Simulations

-Material design (catalysts, sorbents, etc.)

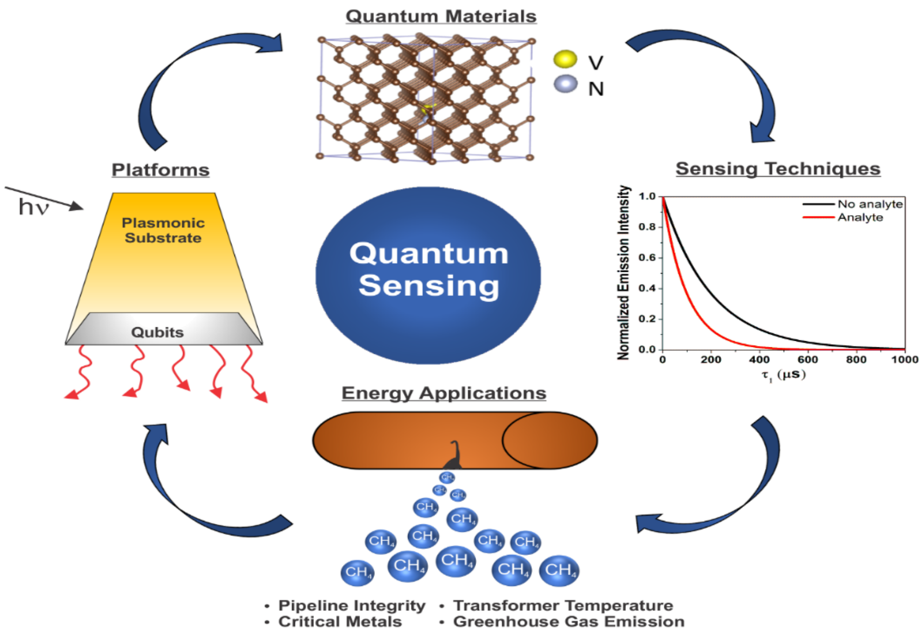
-Reaction modelling (e.g. carbon capture)

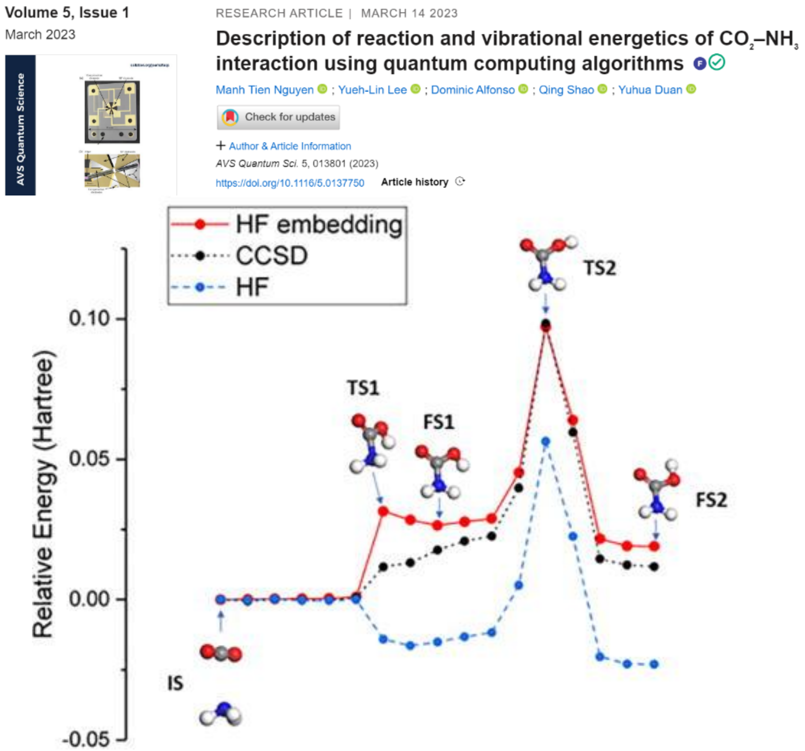
-Grid optimization

-Simulating Fluid Dynamics

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

Quantum for the Energy Sector




Volume 5, Issue 1
March 2023

RESEARCH ARTICLE | MARCH 14 2023

Description of reaction and vibrational energetics of CO_2–NH_3 interaction using quantum computing algorithms

Manh Tien Nguyen ; Yueh-Lin Lee ; Dominic Alfonso ; Qing Shao ; Yuhua Duan

Check for updates

+ Author & Article Information

AVS Quantum Sci. 5, 013801 (2023)

https://doi.org/10.1116/5.0137750 Article history

Quantum Sensors

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

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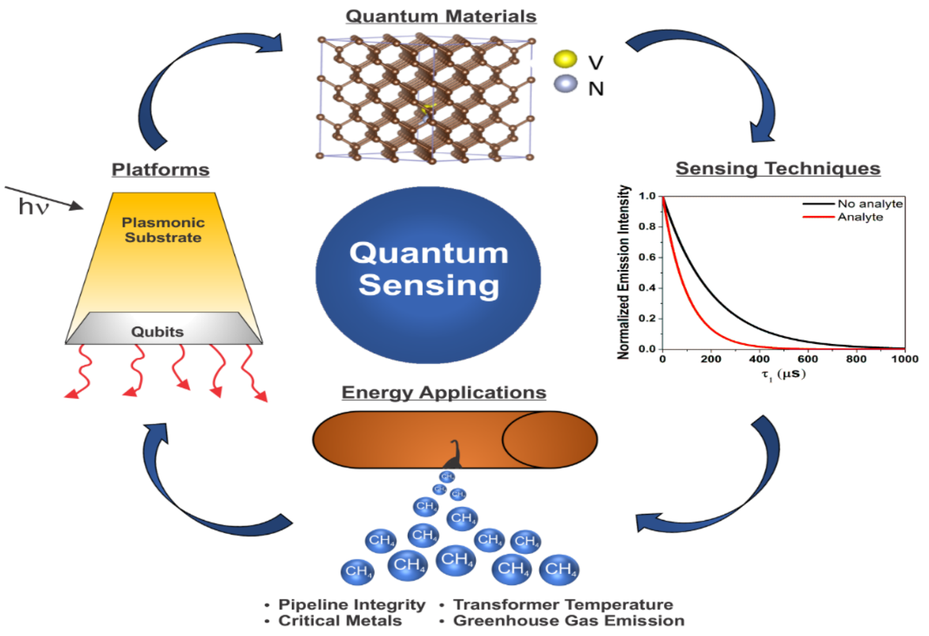
AVS Quantum Sci. 2023, **5**(1), 013801

Quantum for the Energy Sector



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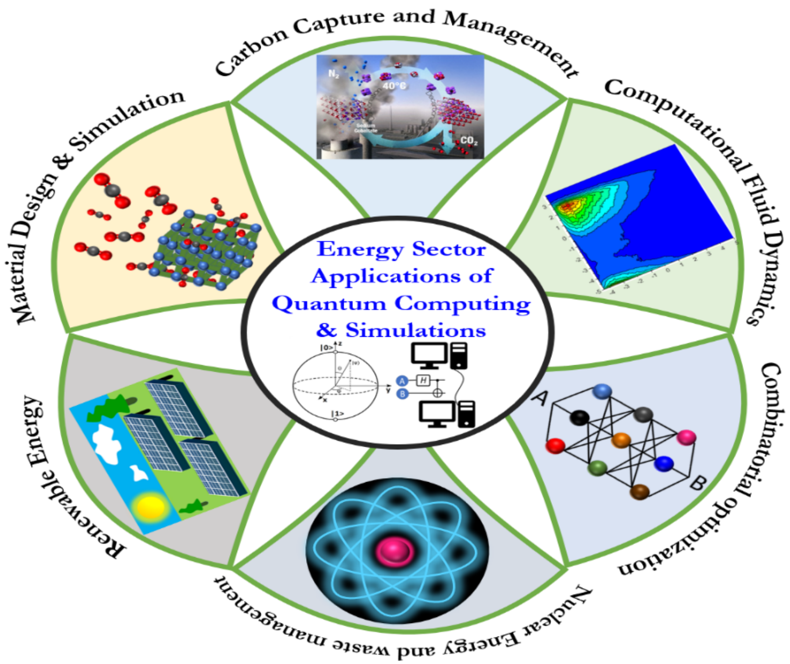
Adv. Quantum Technol. 2021, **4**(8), 210049.



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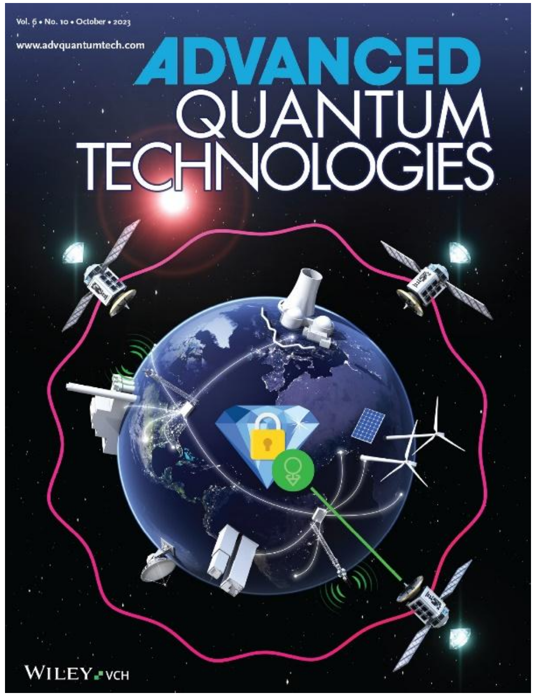
ACS Eng. Au, 2022, **2**(3), 151-196



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

From Science Fiction to Commercialization

NATIONAL ENERGY TECHNOLOGY LABORATORY

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

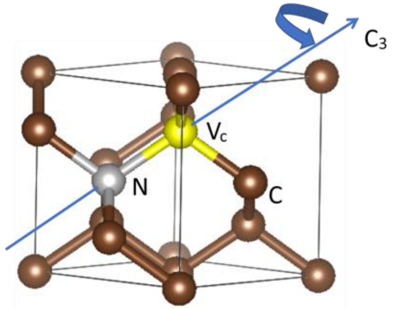
Source: Market Research Future

Quantum Materials for Sensing: Diamond Centers

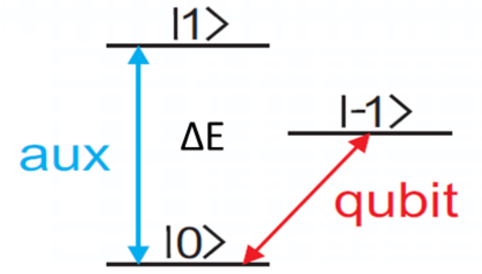
Promising quantum material: Capable for use in elevated temperature and pressure conditions

Vacancy centers in nanodiamonds (ND):

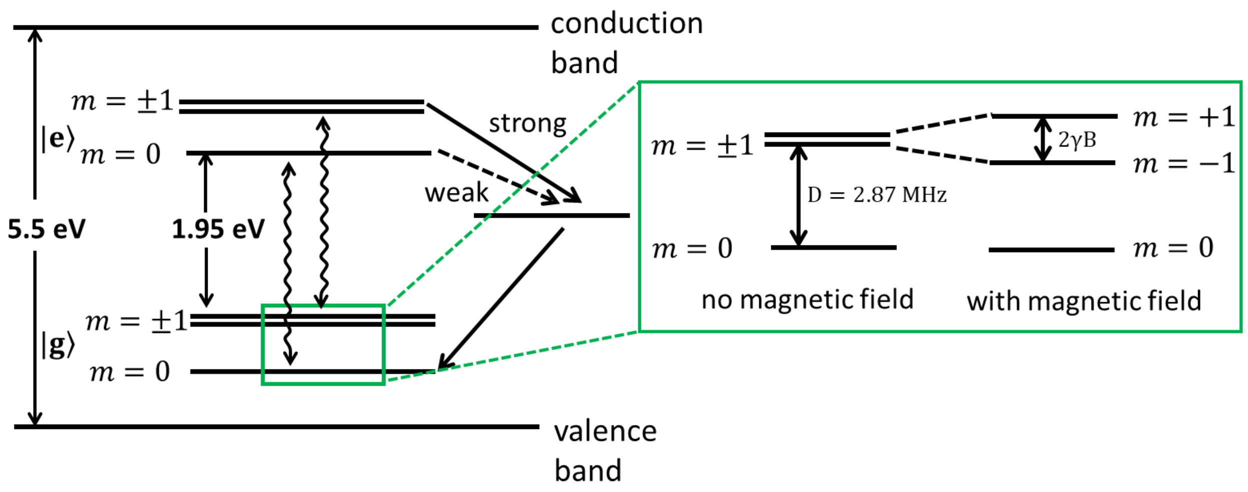
- Atomic impurity (N, Si, Sn, etc.) and carbon vacancy in a diamond lattice: spin qubits
- Information stored in spin states are optically readable
  - Optically-detected magnetic resonance (magnetometry, thermometry, electrometry)
  - Spin relaxometry (ion and pH sensing)
  - Zero-phonon lime emission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



Vacancy in nano-diamond

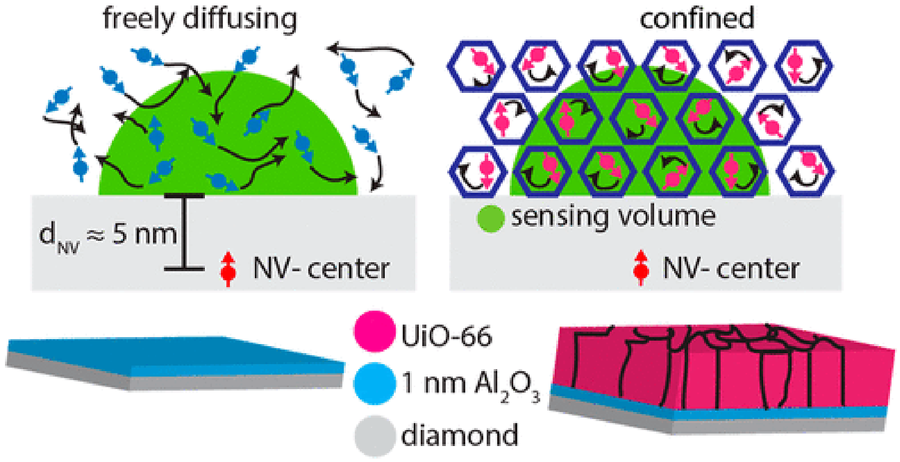


Solid state quantum system

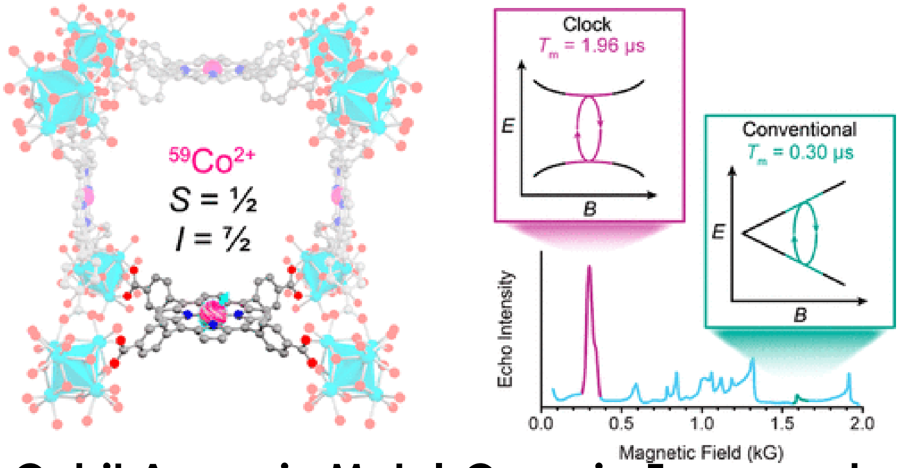


Electronic bands of nitrogen vacancy (NV) center in nano-diamond

Porous Materials Enhance Qubit Performance

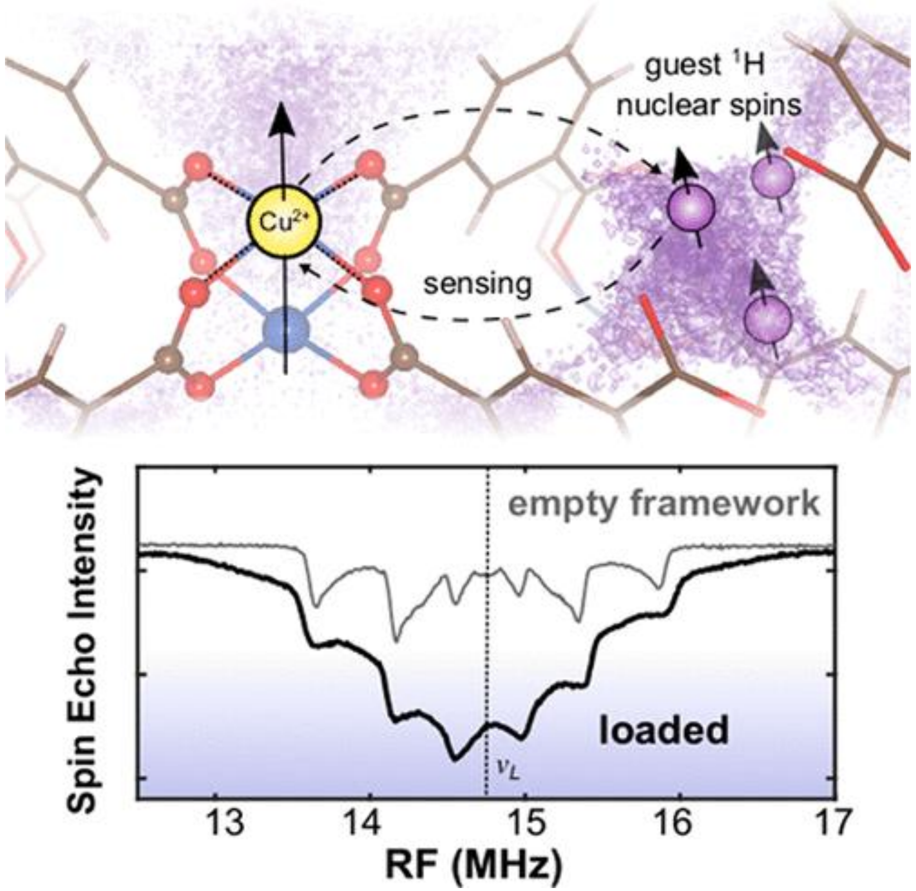


Nano Lett. 2022, 22, 24, 9876–9882



Qubit Arrays in Metal-Organic Frameworks

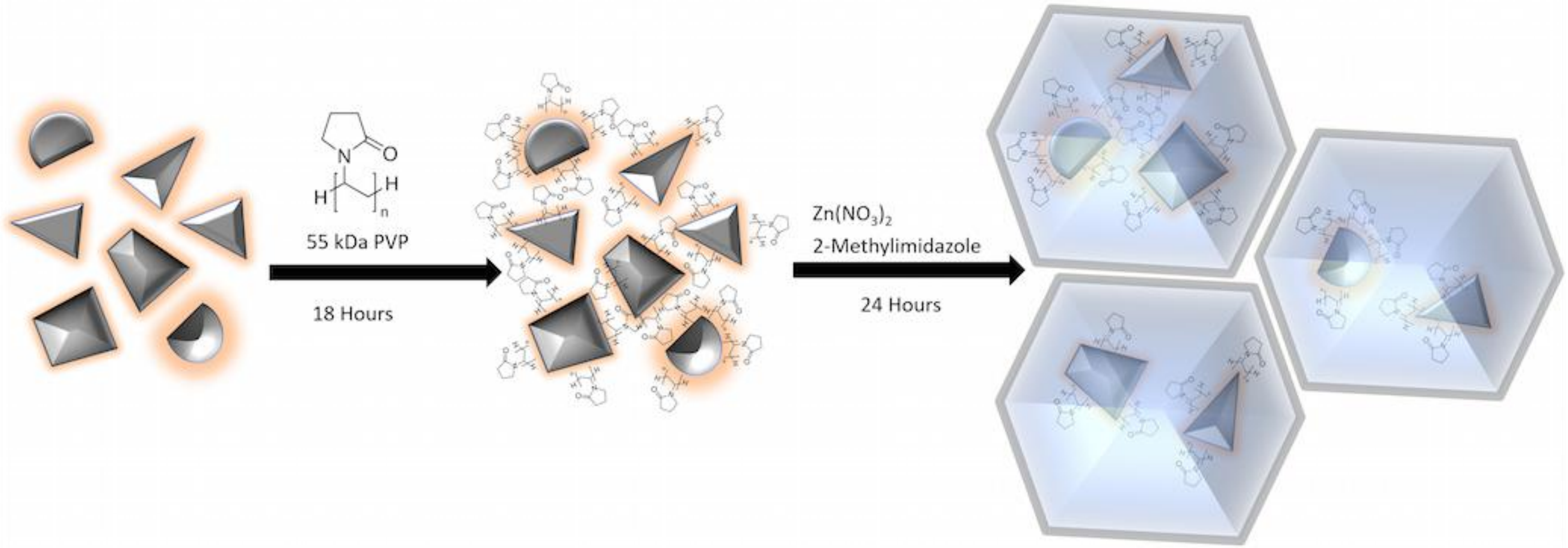
J. Am. Chem. Soc. 2017, 139, 20, 7089–7094

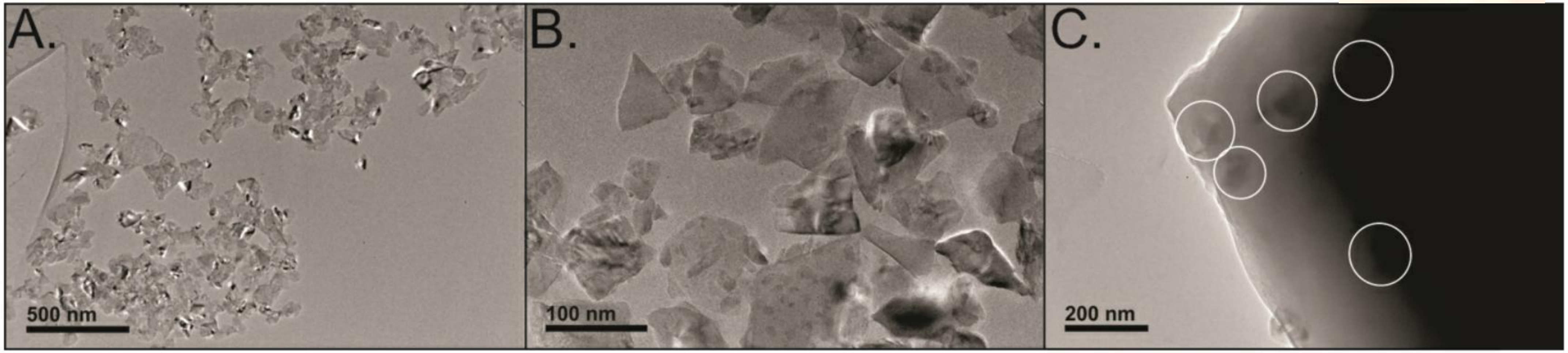


Quantum Sensing of Non-Interacting Gasses

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

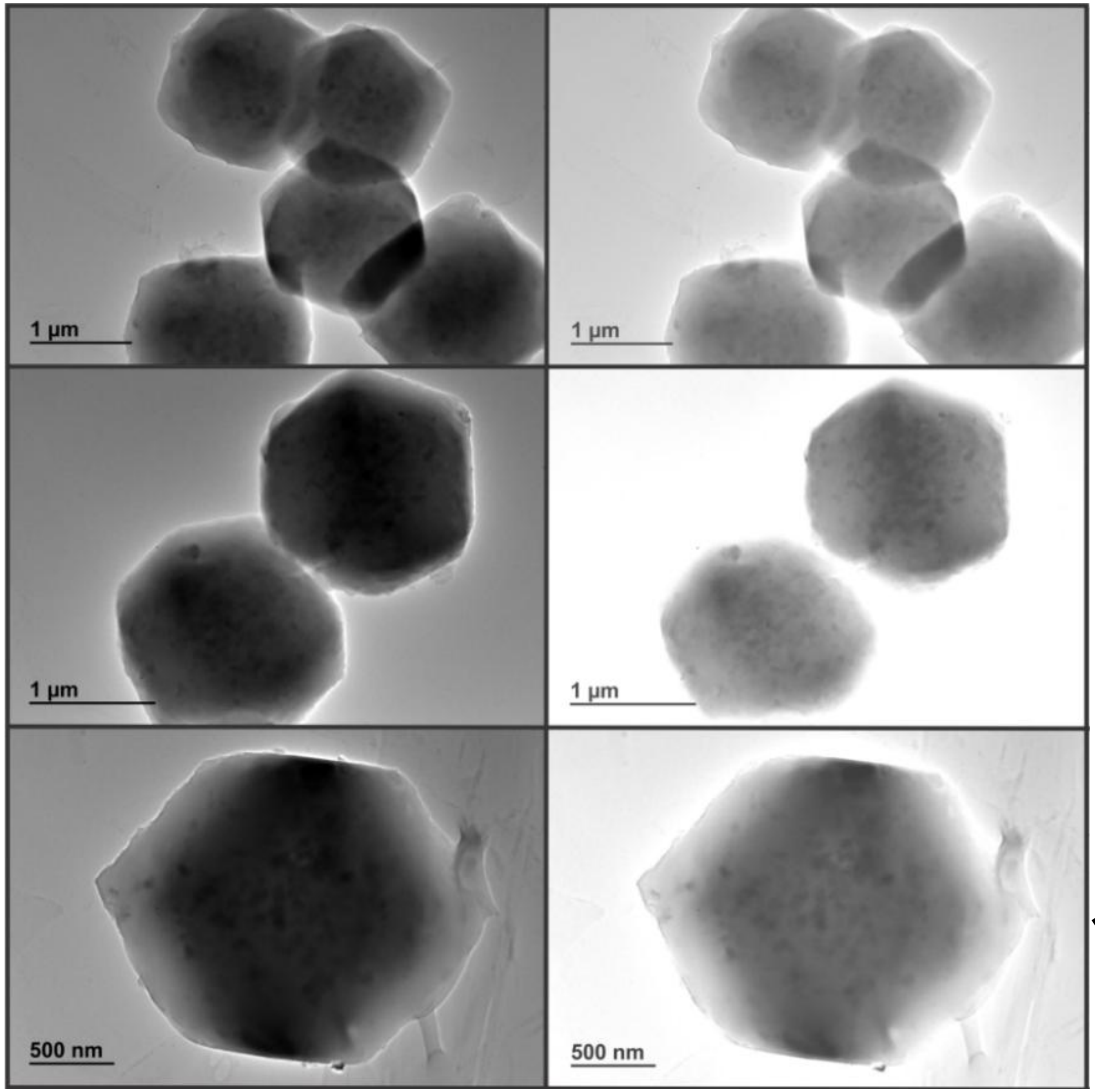
Nanodiamond@ZIF-8* Composite

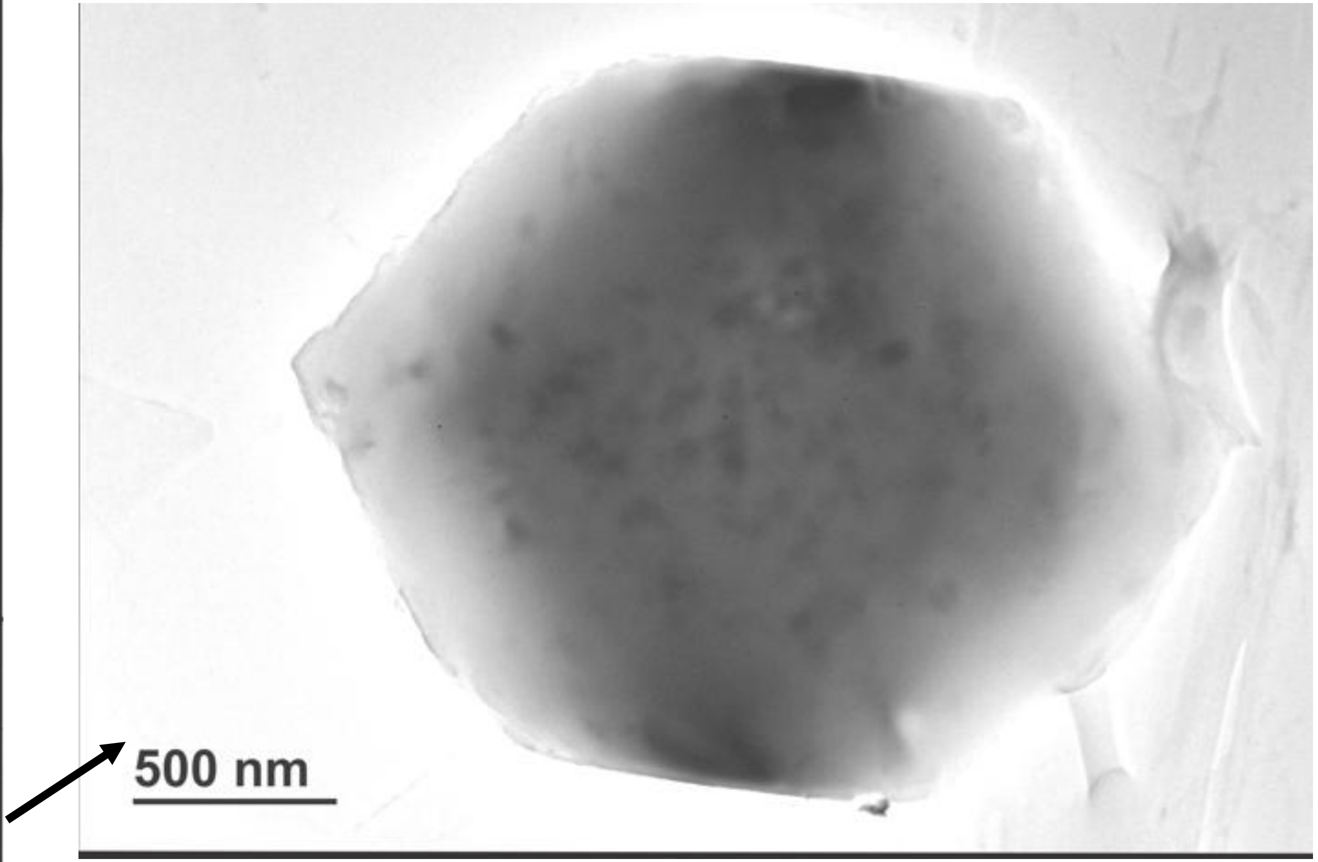




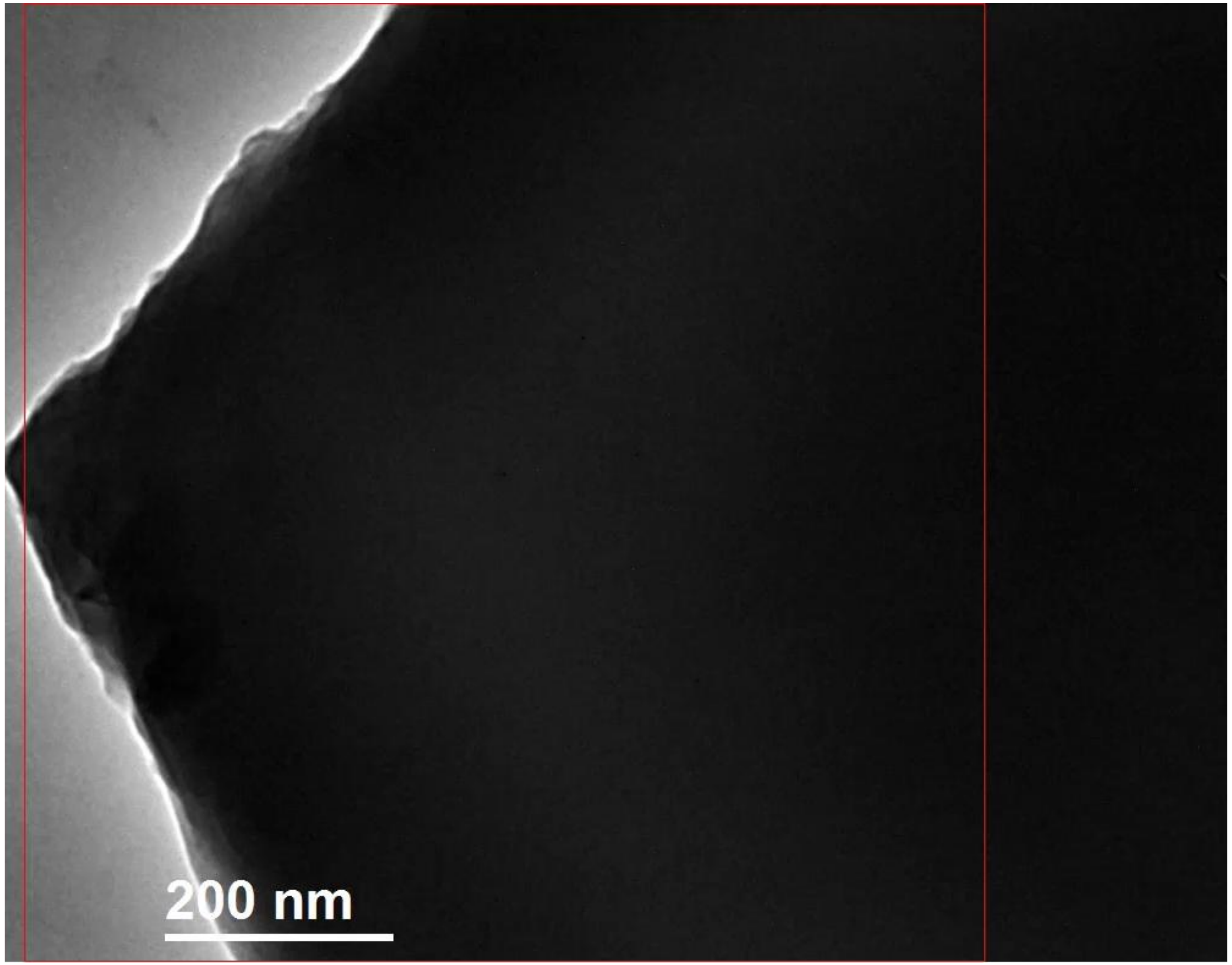
*ZIF-8: zeolitic imidazole framework 8

Transmission Electron Microscope Characterization





Dispersion on Nanodiamonds in ZIF-8



Dispersion on Nanodiamonds in ZIF-8

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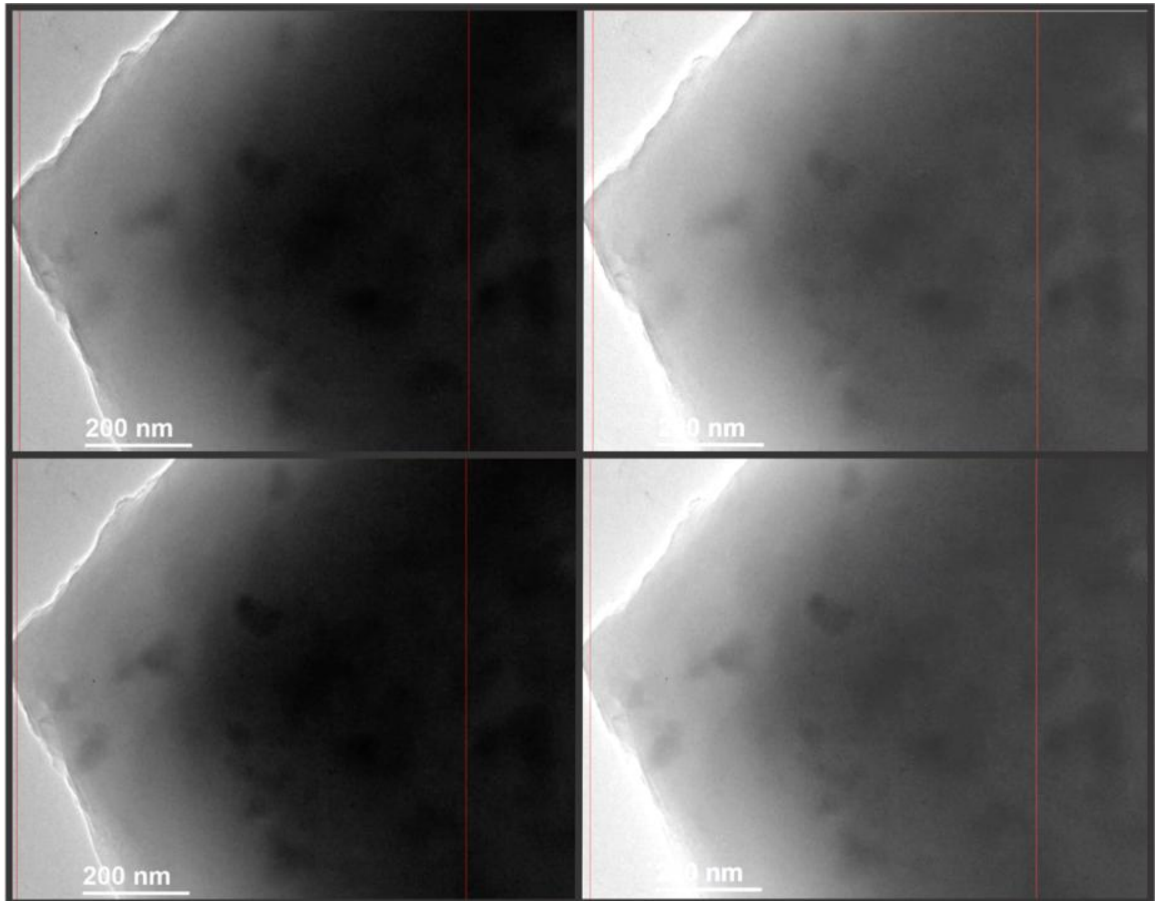
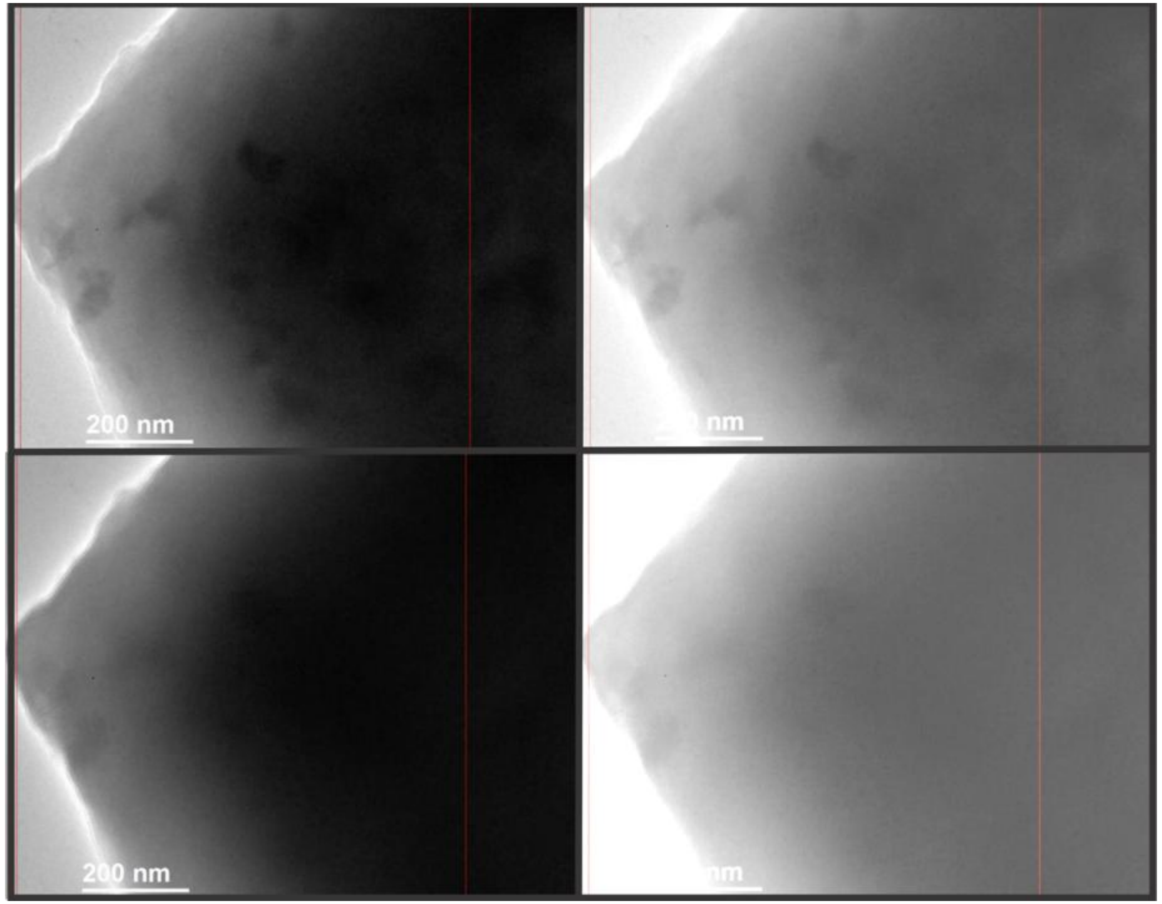
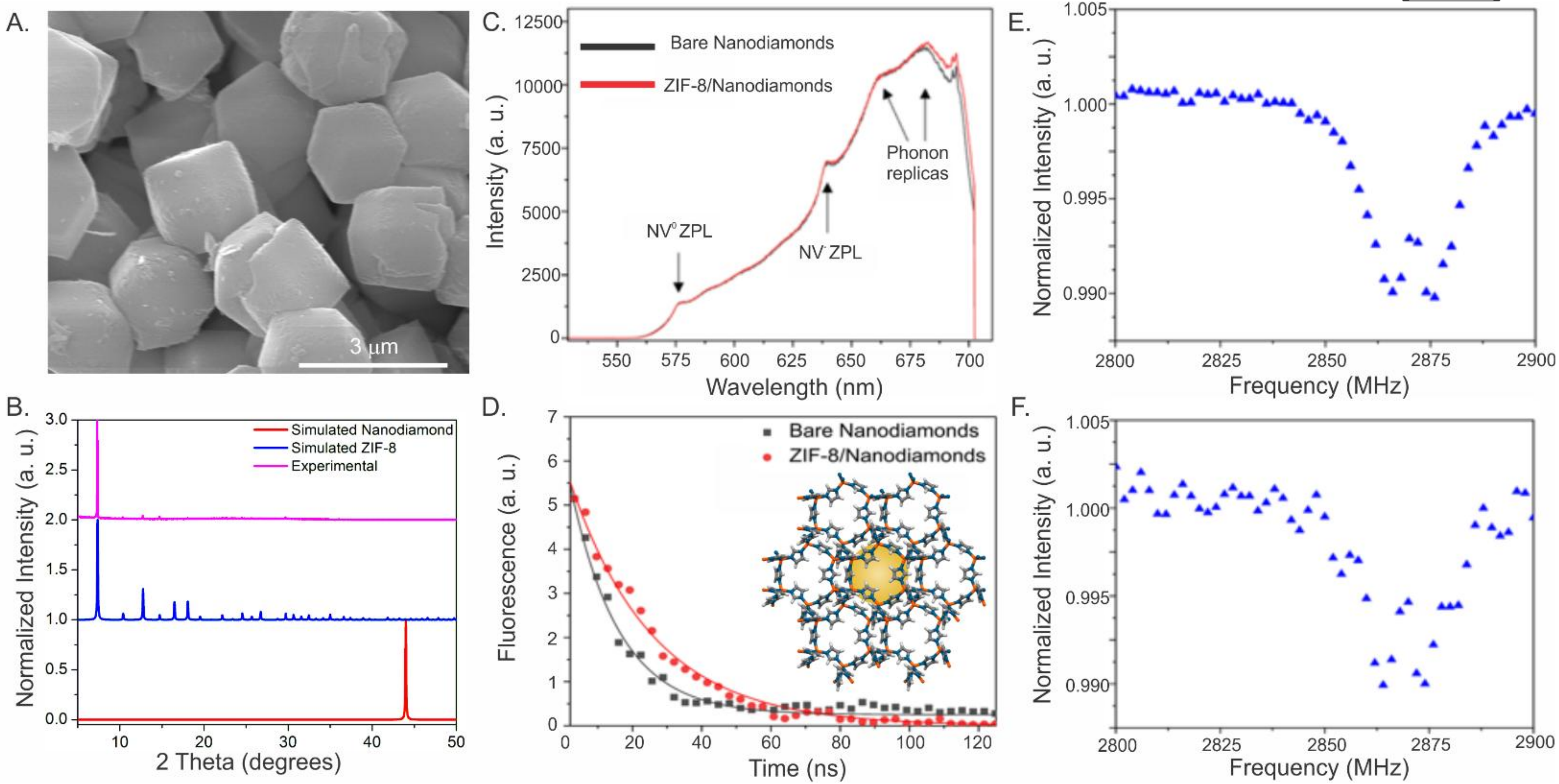
Raw Image **Enhanced Contrast**



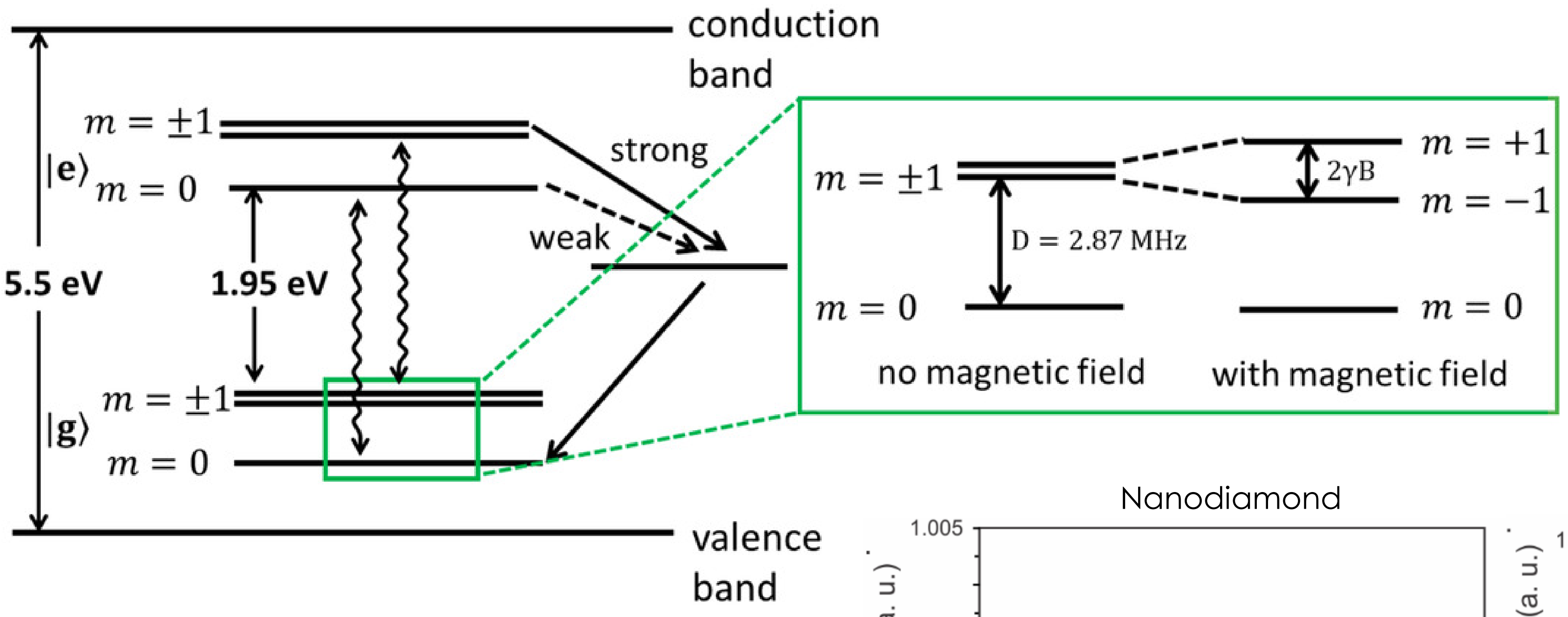
Raw Image

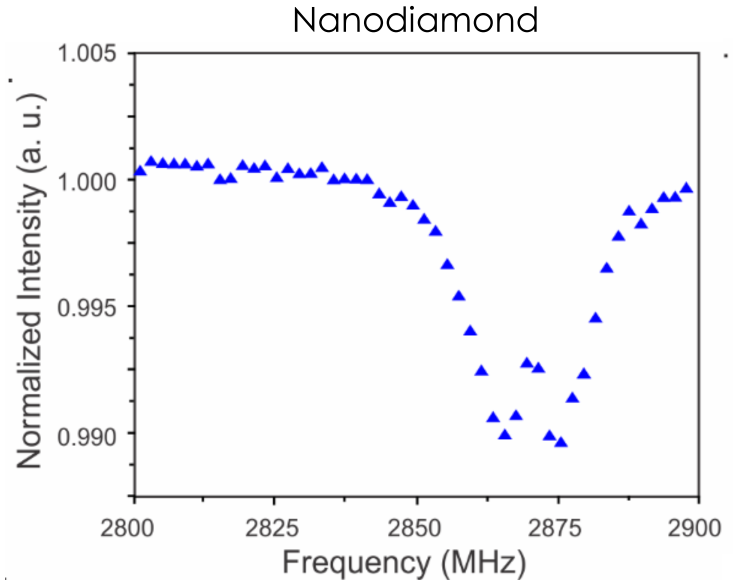


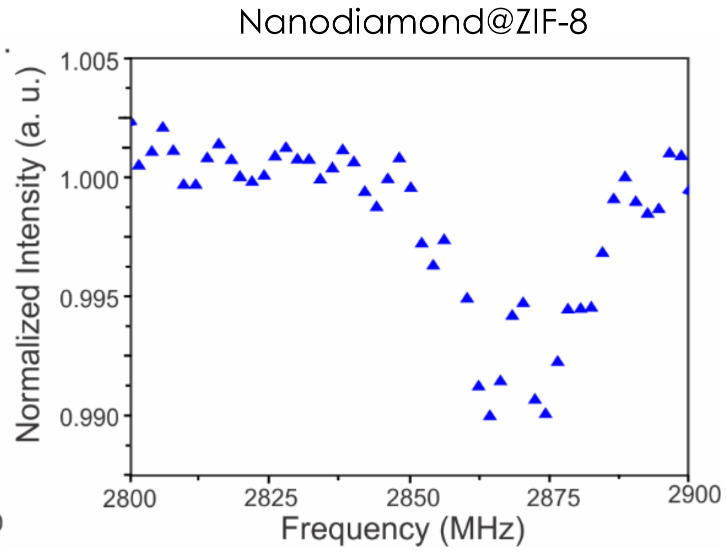
Optical Properties are Unchanged in ZIF-8



Quantum Sensing Experiments: ODMR*

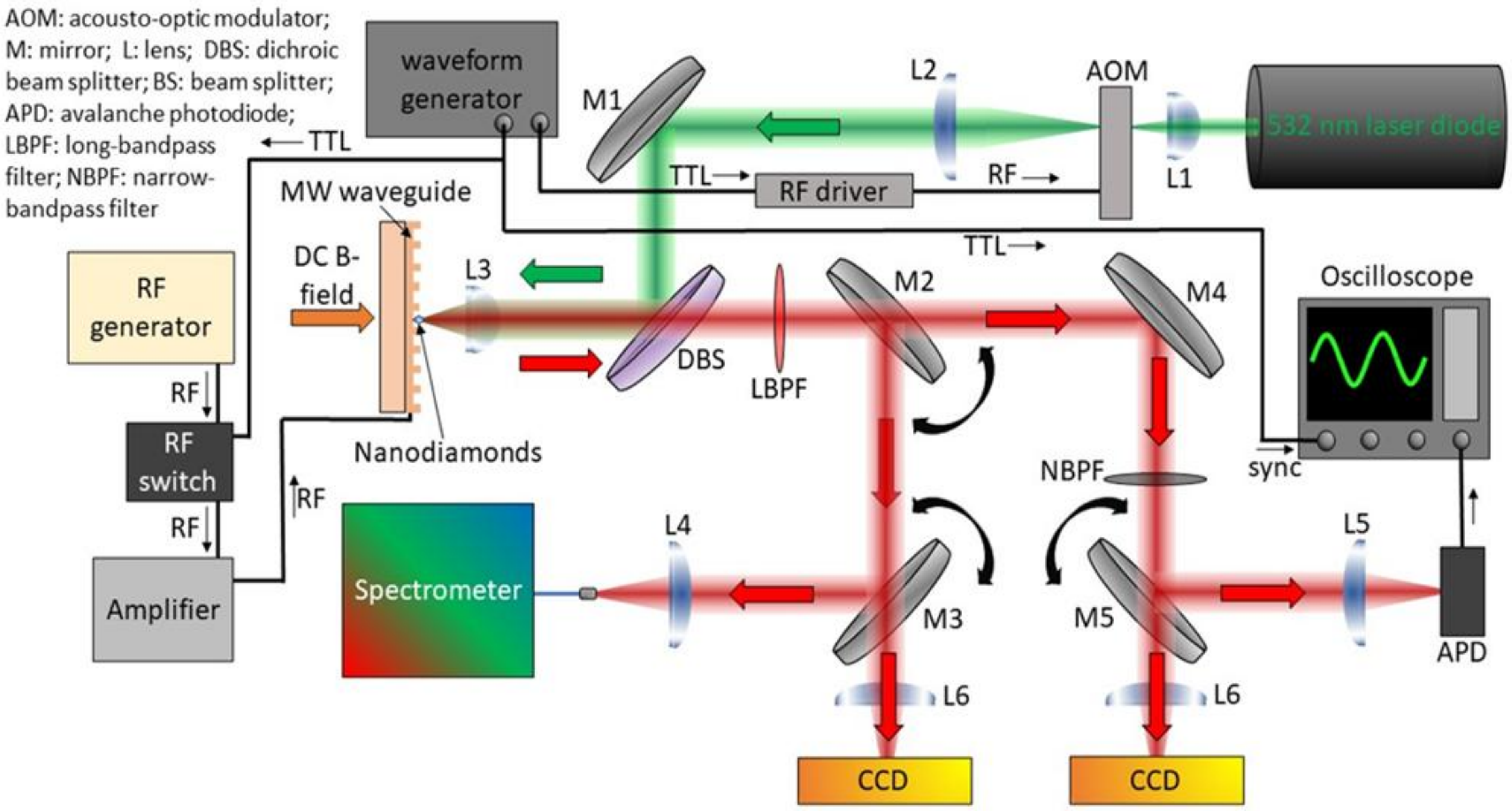






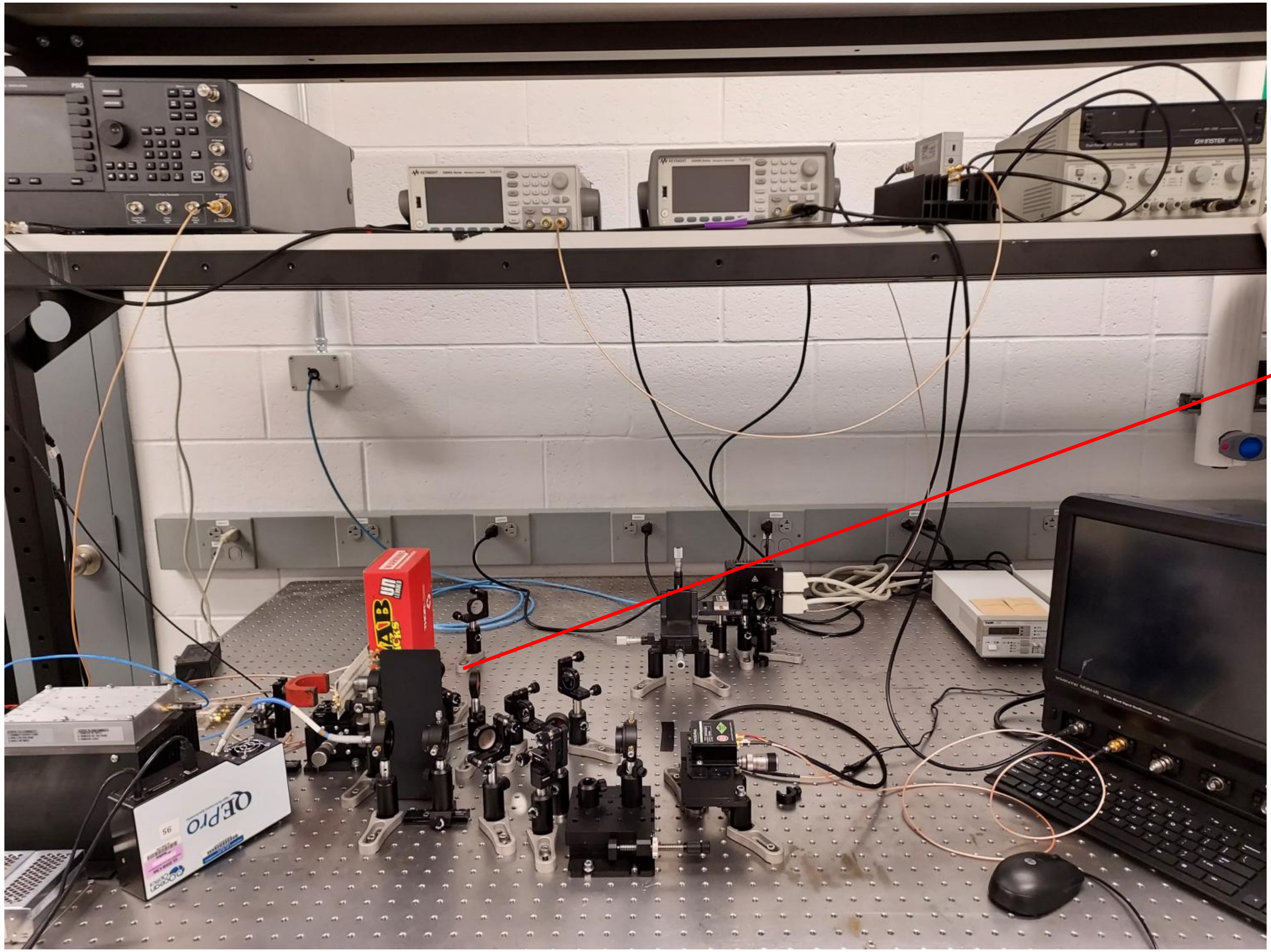
*ODMR: Optically Detected Magnetic Resonance

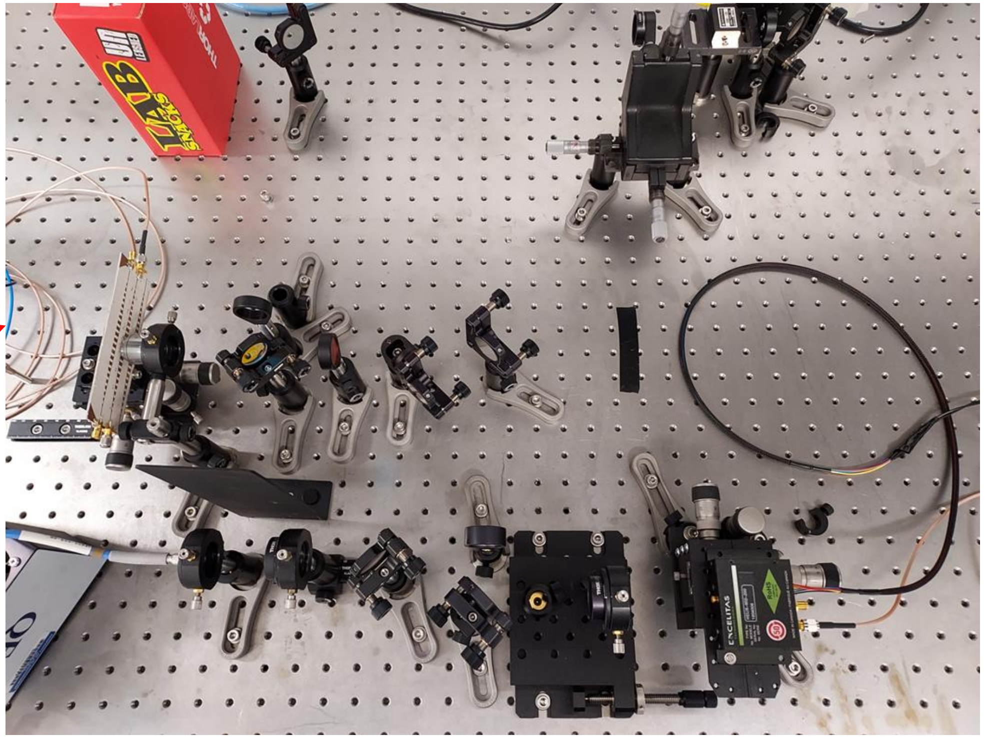
Setup for ODMR/Spin Relaxometery



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

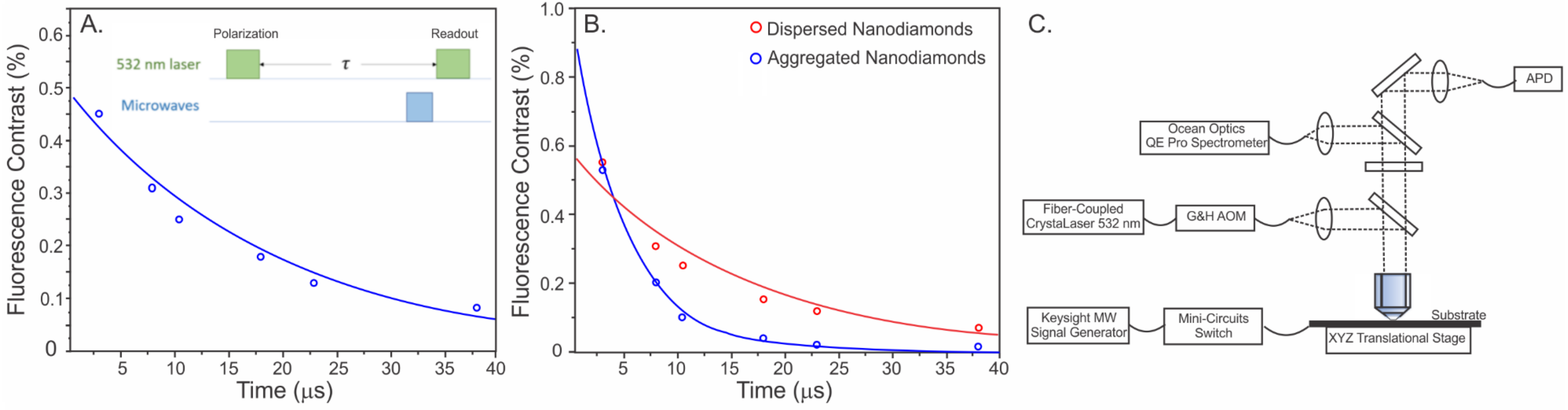
Setup for ODMR/Spin Relaxometery





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

ZIF-8 Enhances Spin Relaxometry Performance



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

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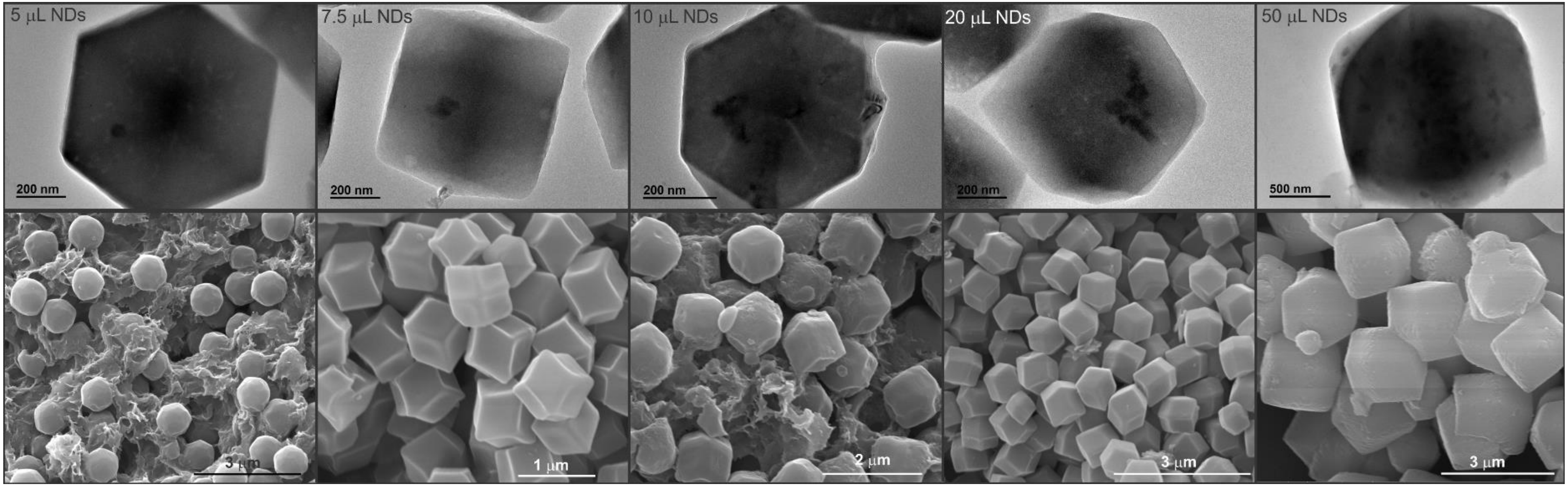
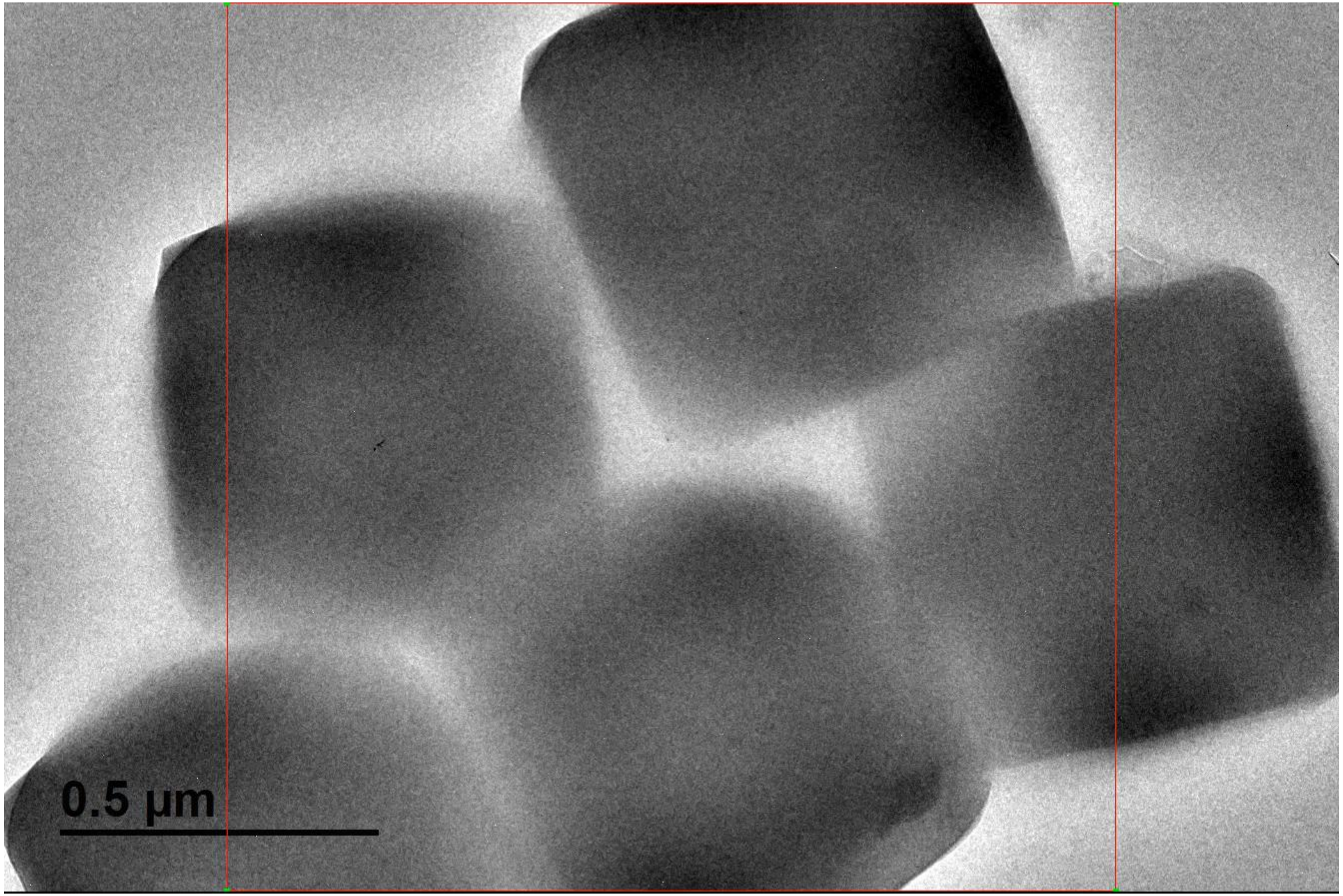


Increasing the concentration of nanodiamonds used in the synthesis correlates with the number of nanodiamonds per MOF

Imaging Single Nanodiamonds in ZIF-8



Conclusions and Next Steps

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- 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

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