Quantum Sensing for Energy Applications

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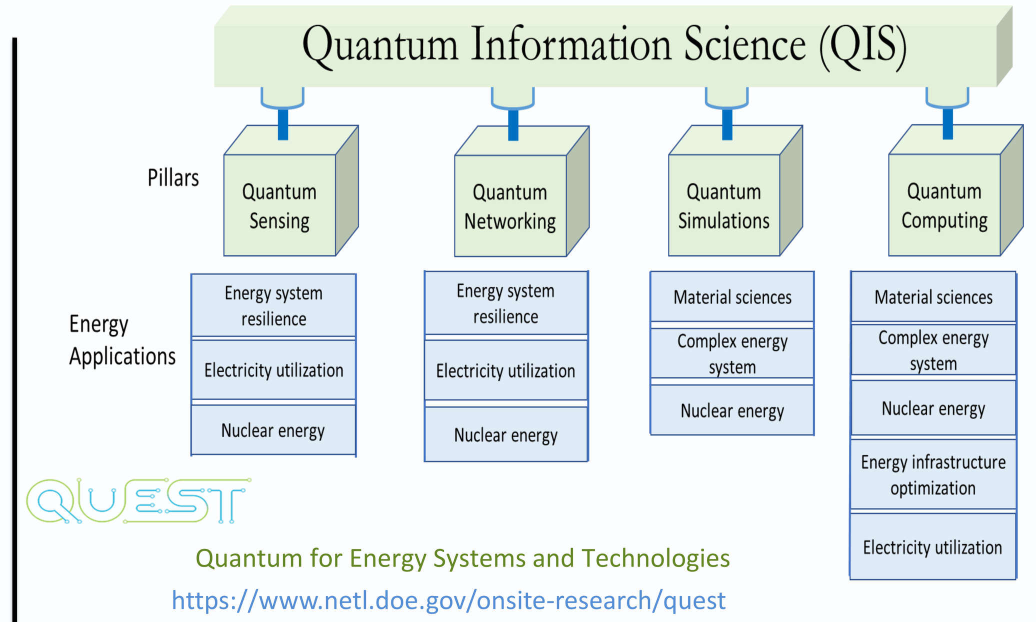
QUEST

Quantum Sensing for Energy Applications

- Quantum sensing is creating potentially transformative opportunities to exploit intricate quantum mechanical phenomena in new ways to make ultrasensitive measurements of multiple parameters.
- A growing interest in quantum sensing has created opportunities for its deployment to improve processes pertaining to energy production, distribution, and consumption.
- NETL is leveraging experimental and computational quantum tools to enhance sensitivity of hybrid quantum-classical ultrasensitive sensor for the detection of hydrocarbons and rare earth elements (REEs).

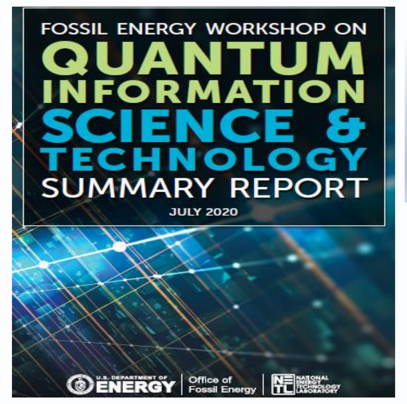


Quantum for Energy Systems and Technologies
https://www.netl.doe.gov/onsite-research/quest

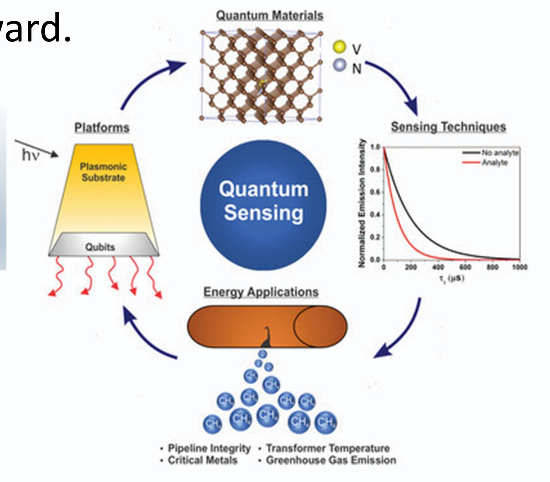
- Crawford, *et al*, *Adv. Quantum Technol.* 4(2021)210049.
- Paudel, *et al*, *Adv. Quantum Technol.* 6(2021)2300096.

Hybrid Quantum-Classical Sensing: Advantages and Scopes

The application of rapidly evolving quantum technologies to real-world systems is challenging. Taking stock of the current state-of-the-art technology in sensing and identifying potential energy sector problems that could benefit from quantum sensing represents a key step forward.



NETL Strategy on Quantum Information Science (04/15/2019)
NETL key initiative on QIS



Paudel, *et al*, *ACS Eng. Au*, 2(2022)151-196

Crawford, *et al*, *Adv. Quantum Technol.* 4(2021)210049.

Traditional Sensors

- Provide wide bandwidth and range
- High update rate and high dynamic range in the data collection
- Sensitivity:
  - ~ 1 nm/°C to 3 nm/°C
  - ~ 100 nm/mT
  - $\sim\Delta n \approx 10^{-10} RIU/\sqrt{Hz}$
- Simple and low cost
- Slow responses (~ms)

Quantum Sensors

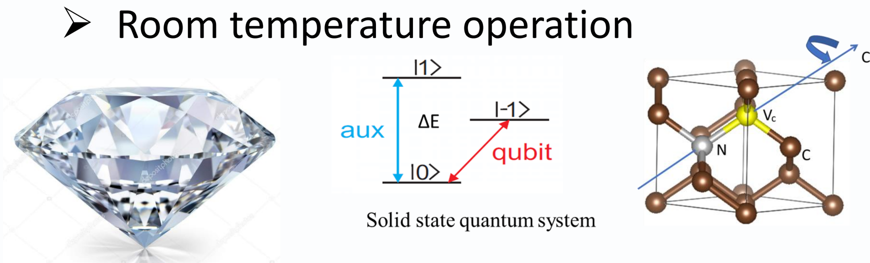
- Provide extreme accuracy without error or noise

(Typically bandwidth is a Hz (one per second))

- ~ 8 nT/sqrt(Hz) @ T = 300 K
- ~ µK/sqrt(Hz) @ 170-700 K
- Low update rate but highly accurate for the measurement at a given point
- Ultrahigh sensitivity
- May not be simple but low cost
- Extremely fast (ns)

Color Centers in Nanodiamond

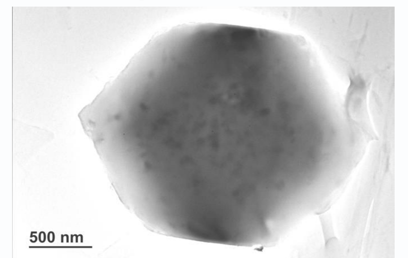
- **Atomic impurity (N, Si, Sn, etc.) and carbon vacancy in a diamond lattice: spin qubits**
- **Information stored in spin states are optically readable:**
  - Optically detected magnetic resonance (magnetometry, thermometry, electrometry)
  - Spin relaxometry (ion and pH sensing)
  - Zero phonon line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



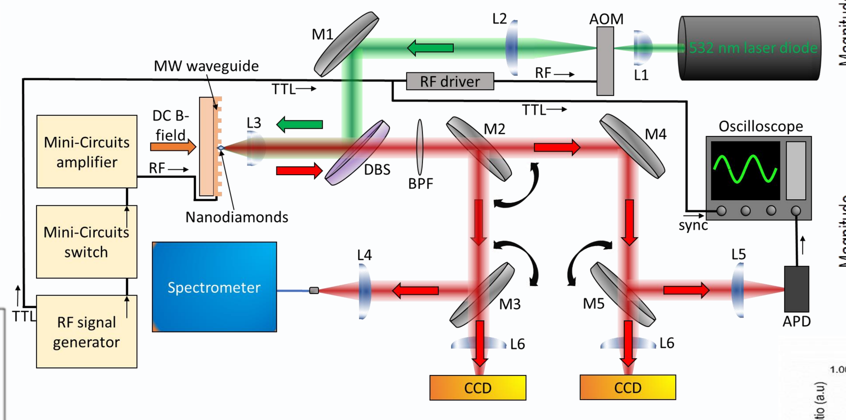
Nanodiamond (ND)/Metal-Organic Framework (MOF) Composites

Functionalization of nanodiamonds (NDs) with a porous coating provides a flexible scaffold for selective analyte uptake for quantum sensing. Quantum sensing properties are preserved in metal organic framework (MOF) embedded ND and enhanced optically-detected magnetic resonance (ODMR) and spin relaxometry performances are observed using a custom-built optical setup.

TEM Image of MOF ZIF-8 NDs

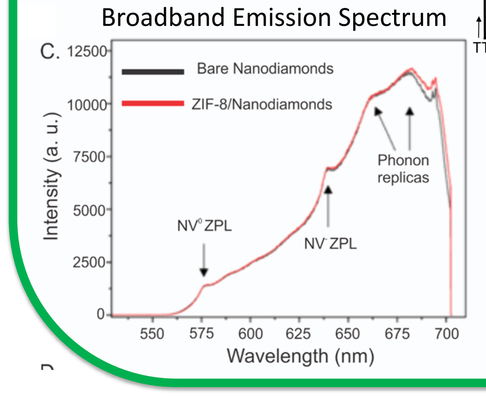


Experimental Configuration

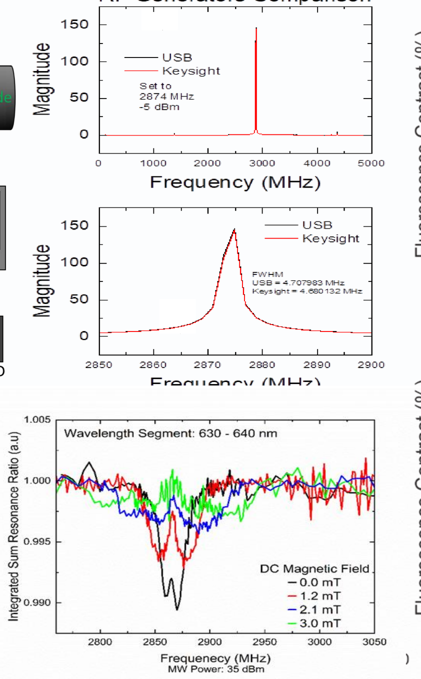


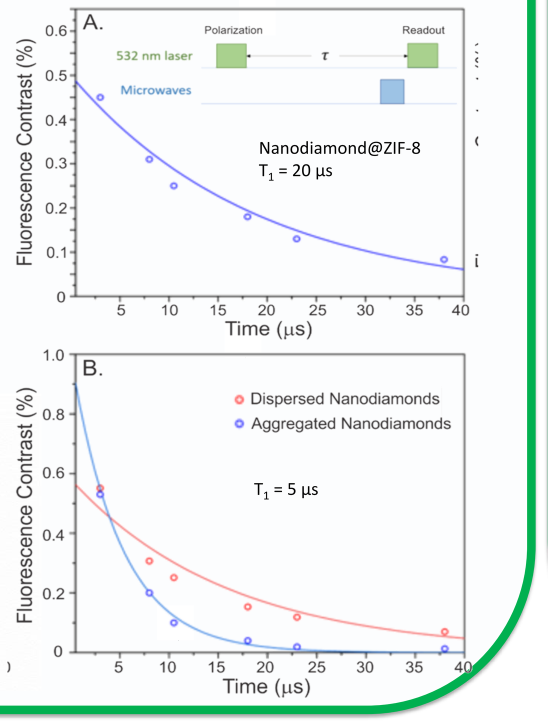
AOM: acousto-optic modulator; M: mirror; L: lens;
DBS: dichroic beam splitter; BS: beam splitter;
APD: avalanche photodiode; BPF: bandpass filter

Broadband Emission Spectrum



RF Generators Comparison



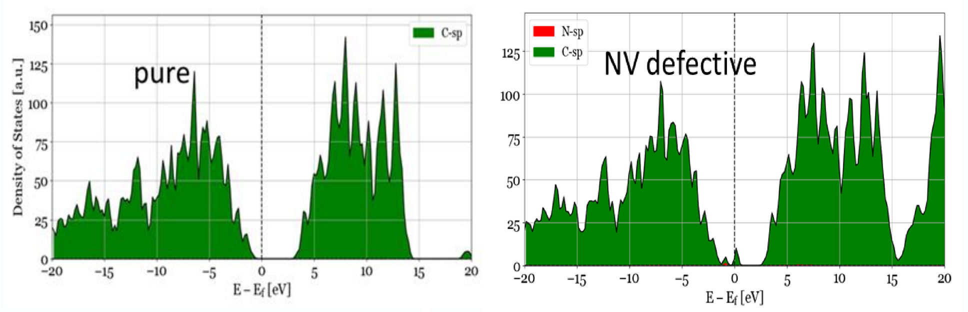


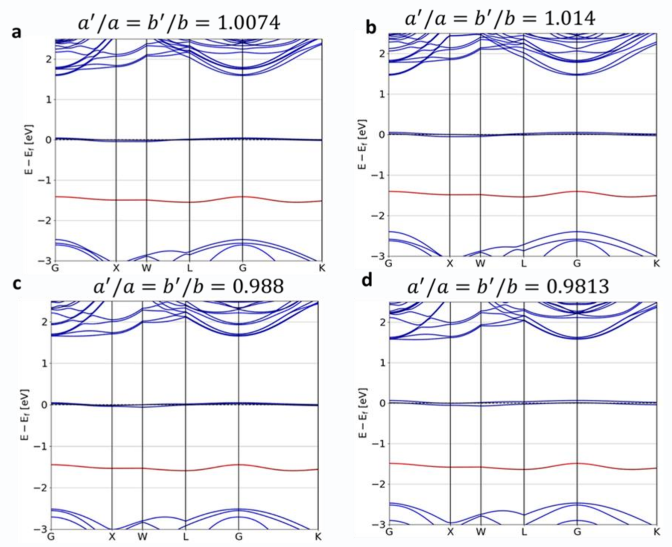
- Shugayev, Crawford, *et al*, *Chem. Mater.* 33(2021)6365–6373.

Modelling of Diamond with NV center for field and pressure sensing

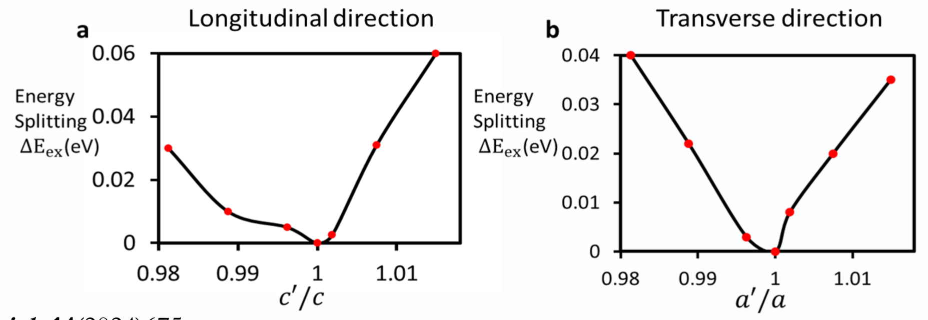
$$H = D_0S_z^2 + M_zS_z^2 + N_x\{S_x,S_z\} + N_y\{S_y,S_z\} + M_x(S_y^2 - S_x^2) + M_y\{S_x,S_y\} + \gamma_e B\cdot S$$

- Changes in the electronic and optical properties of bulk diamond with N impurities and/or N with a carbon (C) vacancy defect on sensing-related applications.
- Sensitivity at the nanoscale can be achieved using NV centers in diamond. NV center-based sensor shows almost few order of magnitude improvement over the traditional sensors.



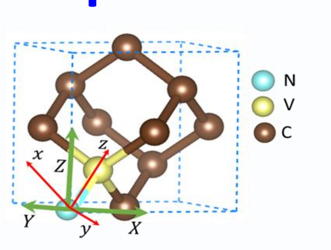


- Shifting of band gap and splitting of band edge under (up to ±2%) changes in the lattice parameters
- The split is up to 40 meV due to a tensile strain under up to 2 %



Both a and b were changed simultaneously.

- Paudel, Lander, Crawford, Duan, *Nanomaterials* 14(2024)675

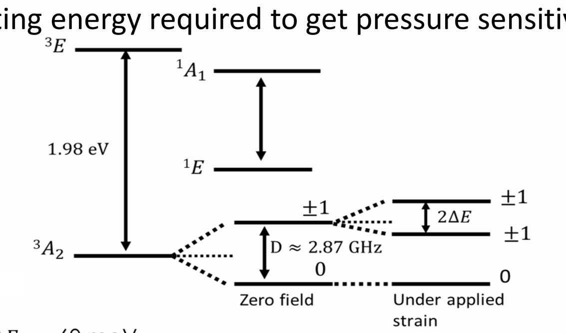


NV dipole orientation along [111]

Pressure sensitivity $\eta_{gs} = \frac{1}{2\pi\frac{dD(p)}{dp}K\sqrt{T_2^*}}$

$$\omega_{|\pm1\rangle} = D_o + M_z \pm \sqrt{(\gamma_e B)^2 + M_x^2 + M_y^2}$$

Spin splitting energy required to get pressure sensitivity



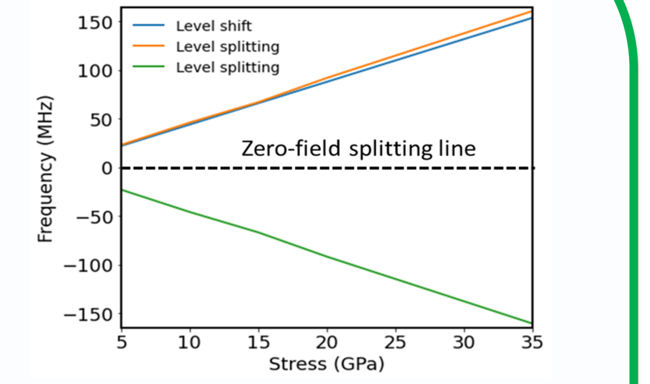
For $\sigma_{xx} = \sigma_{yy}$~25 GPa, the conduction band edge shift, ΔE_{ex}~ 60 meV

Band shift per unit GPa, $\frac{\Delta E_{ex}}{DP}$ ~ 2.4 meV
Wavelength shift per unit GPa, $\Delta\lambda$~ 2 nm

$\eta_{gs} \approx 0.32$ MP a/$\sqrt{Hz}$

(0,0,B_z)= 10 mT, the Zeeman splitting ($\gamma_e B_z$) ~140 MHz from the center energy line

This is equivalent to applying more than 30 GPa pressure!



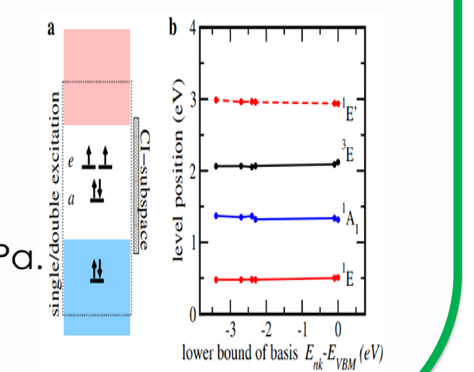
NV center oriented along [111] direction with applied stress along [100]

ND dipole $e_z \in 111$

Applied stress $p \parallel [111]$,

Level shift dD/dP = 3 MHz/GPa.

Spin dephasing $T_2^* \approx 10\ \mu s$



- Shugayev, Crawford, et al, *Chem. Mater.* 33(2021)6365–6373.
- Bockstedte, *et al*, *npj Quantum Mater.* 3(2018)31

A Quantum Manometer

- Hydraulic fracturing of clay, sand, and rocks requires fluid injection under tens of MPa pressure through high-pressure well bores.
- Monitoring deep geological CO_2 storage and the potential induced seismic vibration triggering earthquakes (stress could reach up to 10-15 MPa).

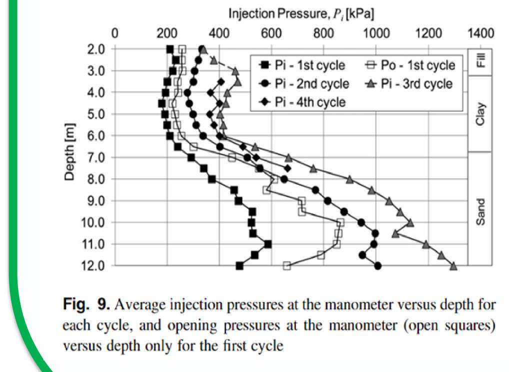
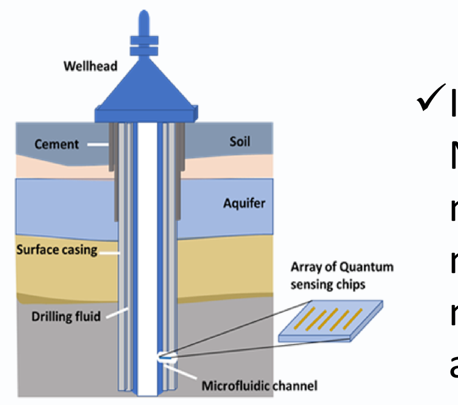
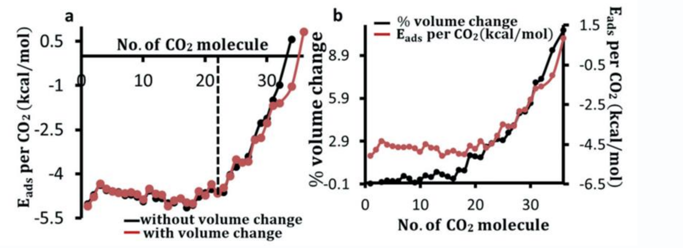


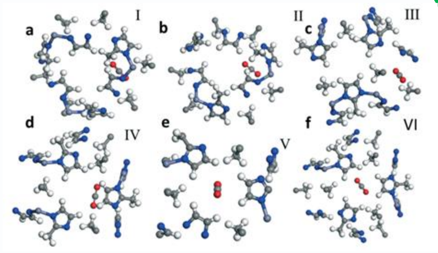
Fig. 9. Average injection pressures at the manometer versus depth for each cycle, and opening pressures at the manometer (open squares) versus depth only for the first cycle



- M. Marchi, *et al*, *J. Geotech. Geoenviron. Eng.* 140(2014) 04013008

Sensing of Gas Molecules in Porous Materials



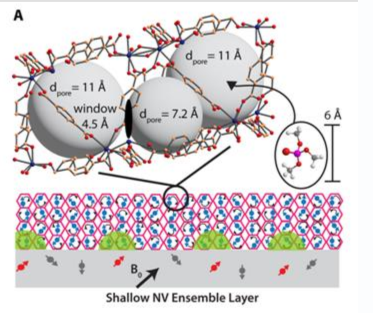


It is possible to detect presence or absence of $CO_2/CH_4/N_2$ and their concentration level in porous material such as ZIF-8 using nuclear spins.

- Paudel, Shi, Hopkinson, Steckel, Duan, *React. Chem. Eng.* 6(2021)990–1001

Probing Liquid Samples Using NV Center NMR

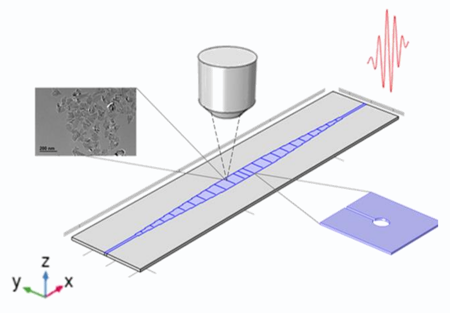
✓It has been shown that UiO-66 grown on a NV diamond can realize the confinement of nanoscale volumes of liquid-state sample nuclei near the NV-quantum sensors for nuclear magnetic resonance spectroscopy applications.

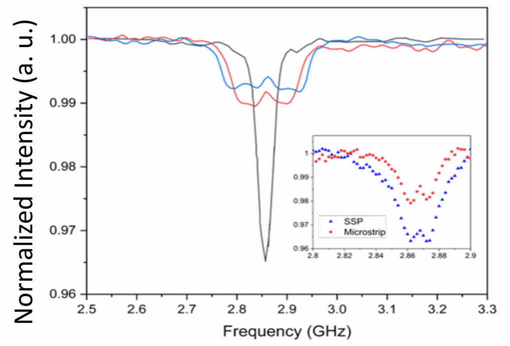


- Liu *et al*, *Nano Lett.* 22(2022)9876–9882

Spoof Plasmons for Enhanced ND Emission

Microwave interactions are crucial for many quantum experiments, but the weak spontaneous emission of quantum emitters makes implementation challenging. Here, significant emission enhancement (up to 10^{11}) using microwave spoof plasmon (SPP) waveguides is demonstrated.

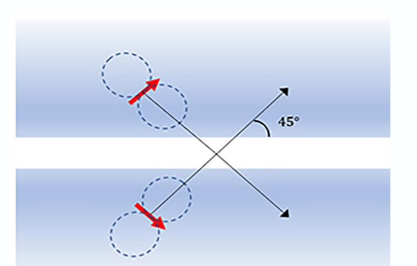


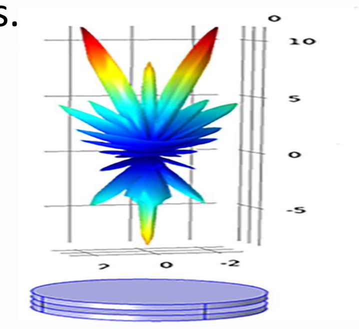


- Shugayev, Devkota, Crawford, Lu, Buric, *Adv. Quantum Technol.* 4(6)(2021) 2000151

Hong-Ou-Mandel Effect Quantum Sensor

Theoretical research indicates that by using superradiant near field coupled emitters positioned across the beamsplitter gap, the coincident emission source required for Hong-Ou-Mandel interference can be created locally. Such a set-up can be integrated into a practical sensor set-up for quantum sensing applications.





- Shugayev, Lu, Duan, Buric, *AVS Quantum Science*, 4 (2022)034402.

Comparison with traditional optical sensors

Compare resolve frequency per unit pressure

Band shift per unit GPa, $\frac{\Delta E}{DP}$ ~ 2.4 meV from the bandstructure calculations ↔ 3 × 10⁵ MHz/Gpa	Typical spin level shift/split per unit Gpa ≈2-4 MHz/GPa

- Quantitatively this is about 4th order of magnitude improvement over traditional optical sensor!
- This shows a superiority of stress sensitivity behavior that could be achieved by manipulating the ground state spin levels in NV center nanodiamond over the traditional optical sensor based on the band edge or band gap shifting.

- Paudel, Lander, Crawford, Duan, *Nanomaterials* 14(2024)675

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