UPISC UNIVERSITY OF PITTSBURGH INFRASTRUCTURE SENSING COLLABORATION WORKSHOP

NATIONAL ENERGY TECHNOLOGY LABORATORY

# Quantum for Energy Systems and Technologies

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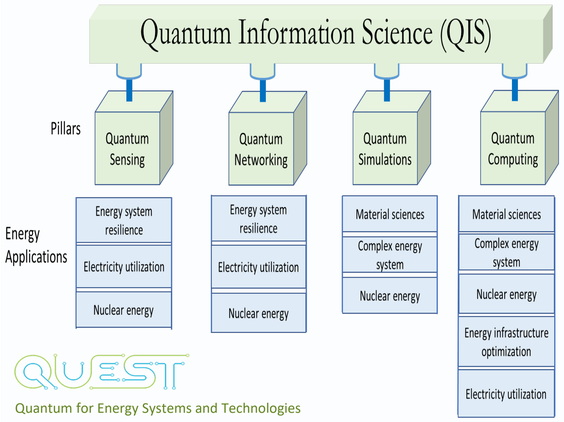
## Quantum Information Science for Energy Applications

On its revolutionary threshold, quantum information science (QIS) is creating potentially transformative opportunities to exploit intricate quantum mechanical phenomena in new ways to make ultrasensitive measurements of multiple parameters. Concurrently, growing interest in quantum sensing, quantum computing, and quantum networks has created opportunities for its deployment to improve processes pertaining to energy production, distribution, and consumption. In that spirit, NETL is leveraging experimental and computational quantum tools to enhance U.S. energy competitiveness.



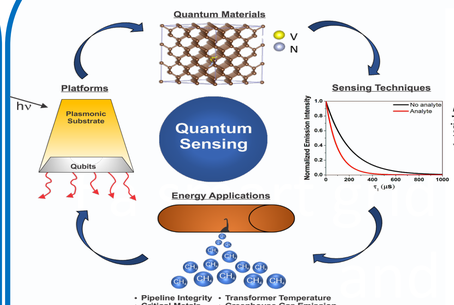

QUEST

Quantum for Energy Systems and Technologies

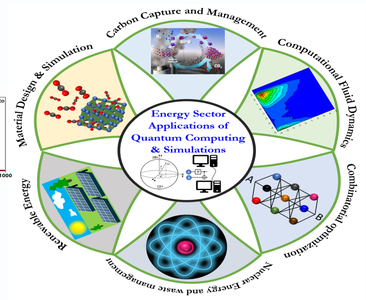
https://www.netl.doe.gov/onsite-research/quest

- Crawford, Shugayev, Paudel, Lu, Syamlal, Ohodnicki, Chorpening, Gentry, Duan, *Adv. Quantum Technol.* **4**(8)(2021) 210049.

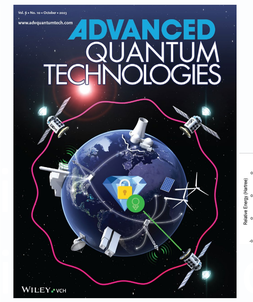
## Identifying Critical Areas for QIS Deployment



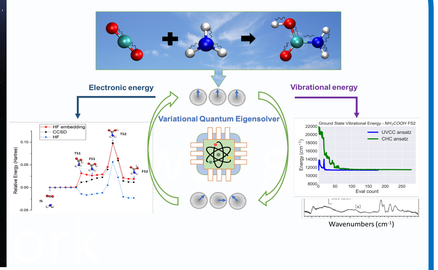

Crawford, *et al*, *Adv. Quantum Technol.* 2021, **4**(8), 210049.




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




Paudel, *et al., Adv. Quantum Technol. 2023,* **6**, 2300096

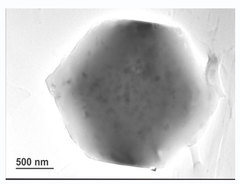


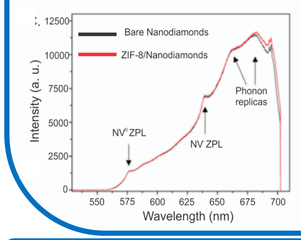

Nguyen, *AVS Quant. Sci.* 2023, **5**, 013801.

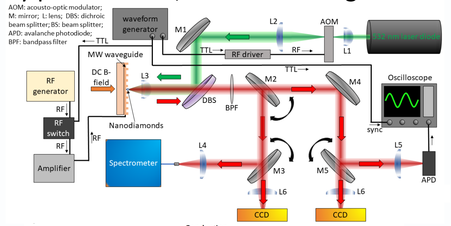
The application of rapidly evolving quantum technologies to real-world systems is challenging. Taking stock of the current state-of-the-art in QIS and identifying potential energy sector problems that could benefit from QIS represents a key first step. In 2019, NETL established a strategy on QIS and held a workshop. Since then, NETL has published three open-access comprehensive review articles on quantum computing, quantum networking, and quantum sensing for energy sector applications, with a fourth in preparation, along with a computational study applying quantum simulation to carbon capture.

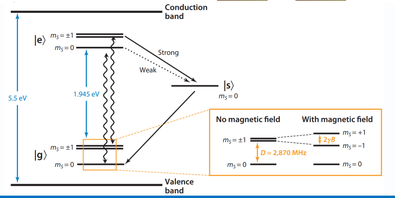
## Nanodiamond (ND)/Metal-Organic Framework (MOF) Composites

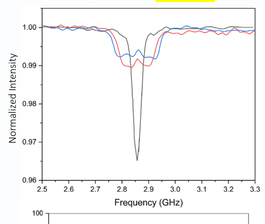
Functionalization of NDs with a porous coating provides a flexible scaffold for selective analyte uptake for quantum sensing. Here, we present a facile synthetic strategy for the controlled encapsulation of NDs with the MOF ZIF-8. Quantum sensing properties are preserved, including an enhanced spin relaxometry performance, measured using a custom-made optical setup.

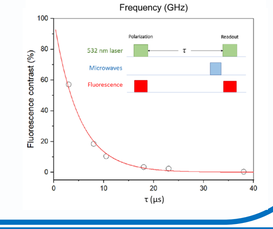


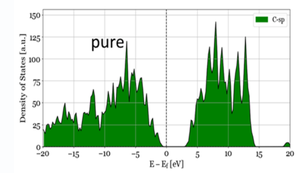



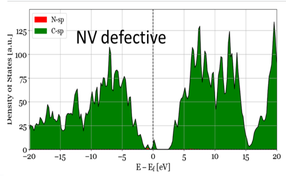




## Modeling of Bulk & Surface of Diamond with NV Center

The role of 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 is still not well understood. Diamond surfaces with a shallow NV center that are doped with different elements provide information on the electronic and optical signatures of spin-related properties.



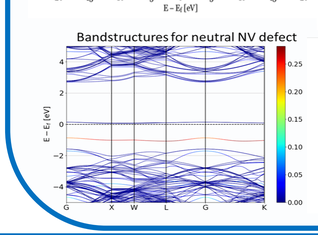



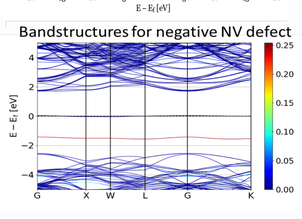

$$\hat{H}_{gs} = D_{gs}\left[\hat{S}_z^2 - S(S+1)/3\right] + A_{gs}^{\parallel}\hat{S}_z\hat{I}_z + A_{gs}^{\perp}\left[\hat{S}_x\hat{I}_x + \hat{S}_y\hat{I}_y\right] + P_{gs}\left[\hat{I}_z^2 - I(I+1)/3\right]$$

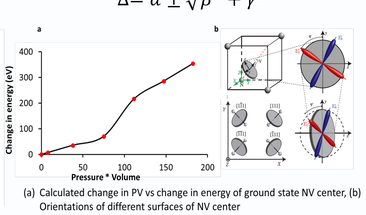
$$\textit{Pressure sensitivity}\ \ \eta_{gs} = \frac{1}{2\pi\frac{dD(p)}{dp}K\sqrt{T_2^*}}$$

Spin splitting energy required to get pressure sensitivity

$$\Delta = \alpha \pm \sqrt{\beta^2 + \gamma^2}$$

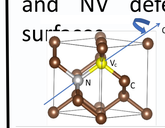


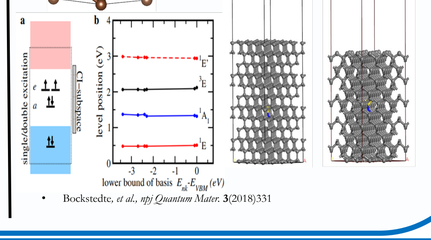




(a) Calculated change in PV vs change in energy of ground state NV center, (b) Orientations of different surfaces of NV center

In order to understand the defect properties and energy levels within the defect bands for different sensing related applications, *ab initio* density functional theory (DFT) calculations were performed on the bulk and surface properties of the N and NV defective bulk and diamond surfaces.




Surfaces of NV defective diamond crystal




- Bockstedte, *et al., npj Quantum Mater.* **3**(2018)331