Quantum Information Science for Energy Sector Applications

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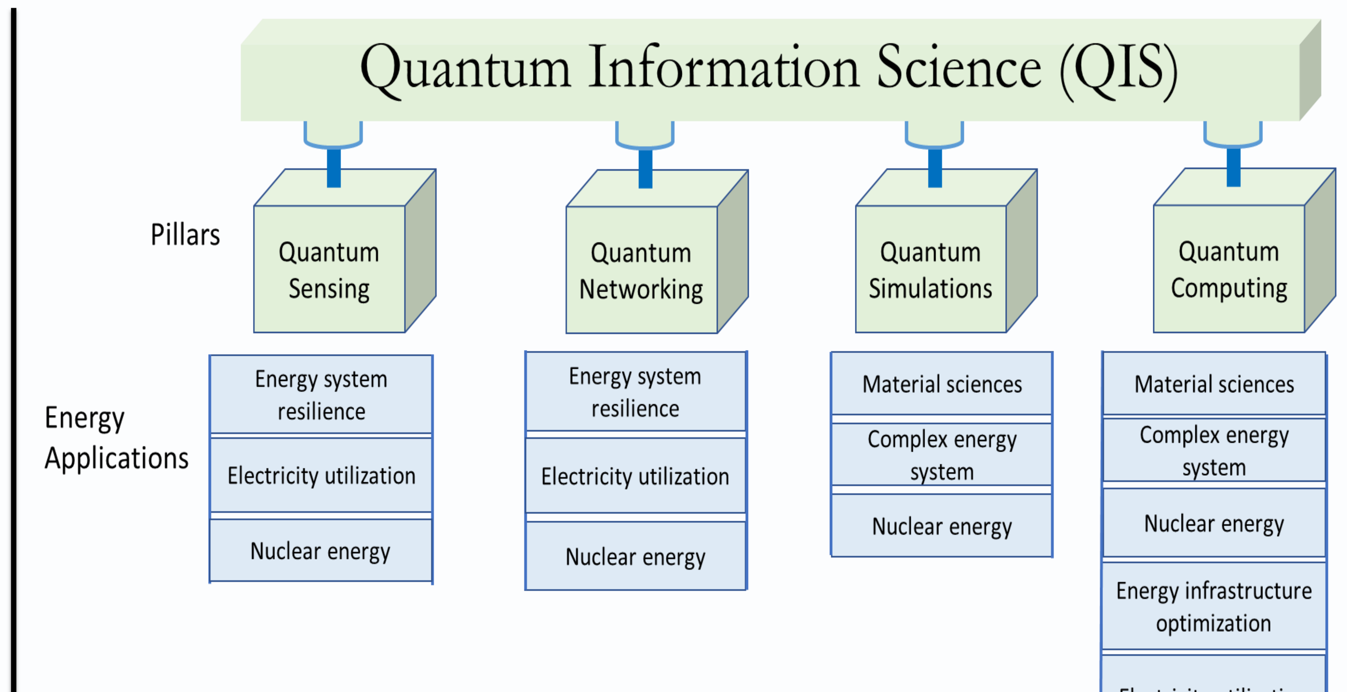
Research & Innovation Center

NATIONAL ENERGY TECHNOLOGY LABORATORY

Quantum Information Science for Energy Applications

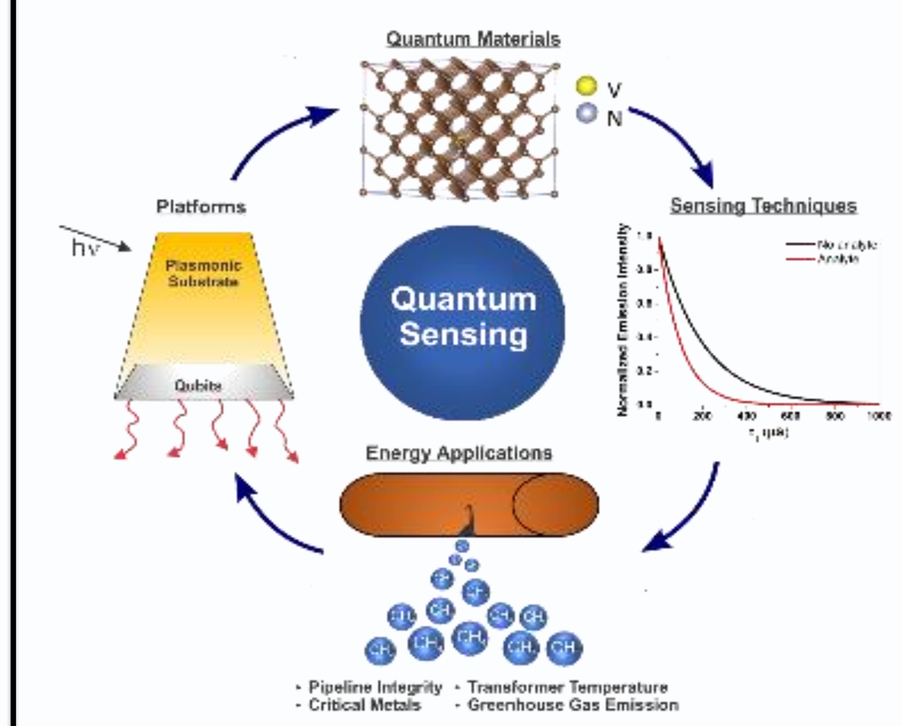
On its revolutionary threshold, quantum sensing is creating potentially transformative opportunities to exploit intricate quantum mechanical phenomena in new ways to make ultrasensitive measurements of multiple parameters. Concurrently, growing interest in quantum sensing has created opportunities for 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.



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

Identifying Critical Areas for QIS Deployment

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. NETL has published two open-access comprehensive review articles on quantum computing and quantum sensing for energy, with a third article in progress.



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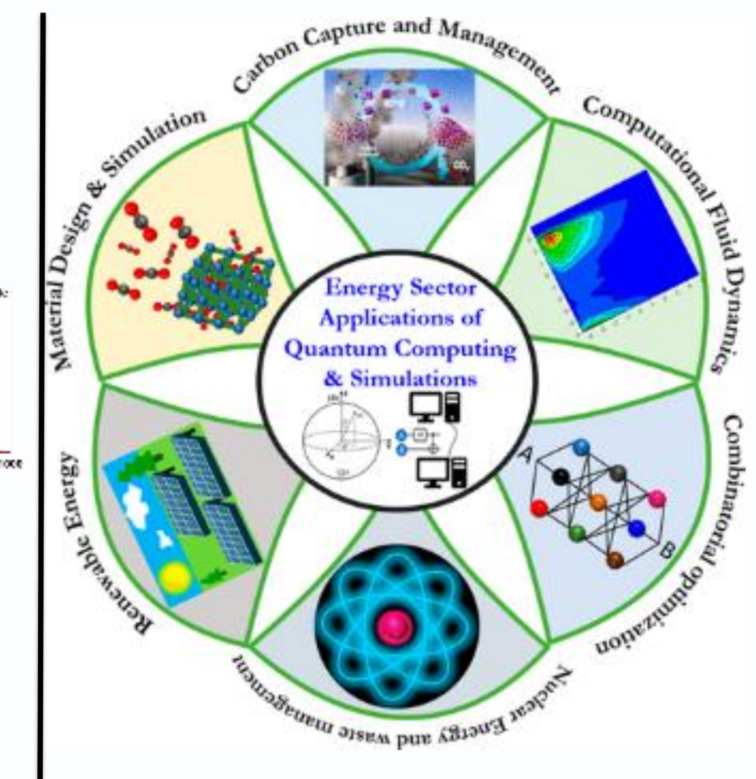
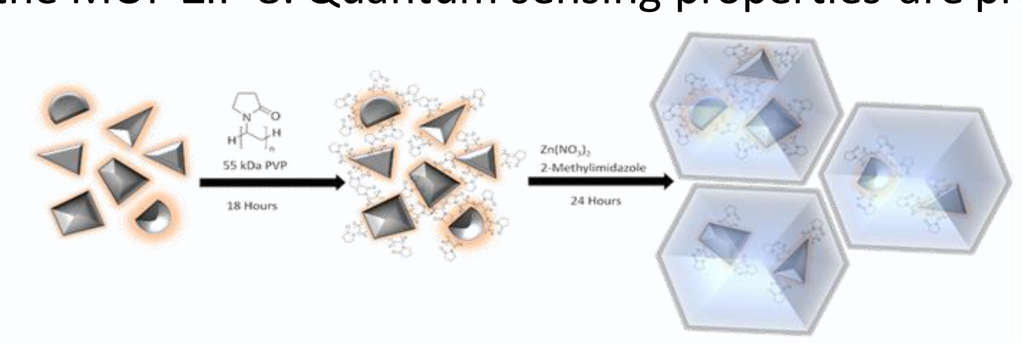
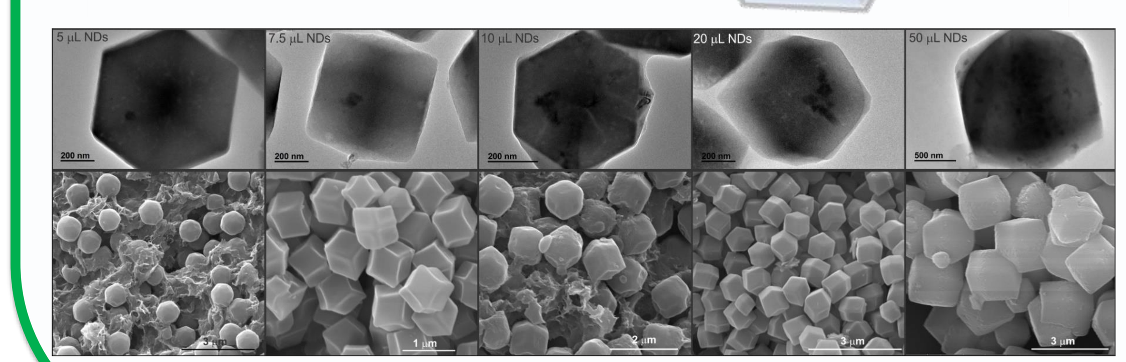


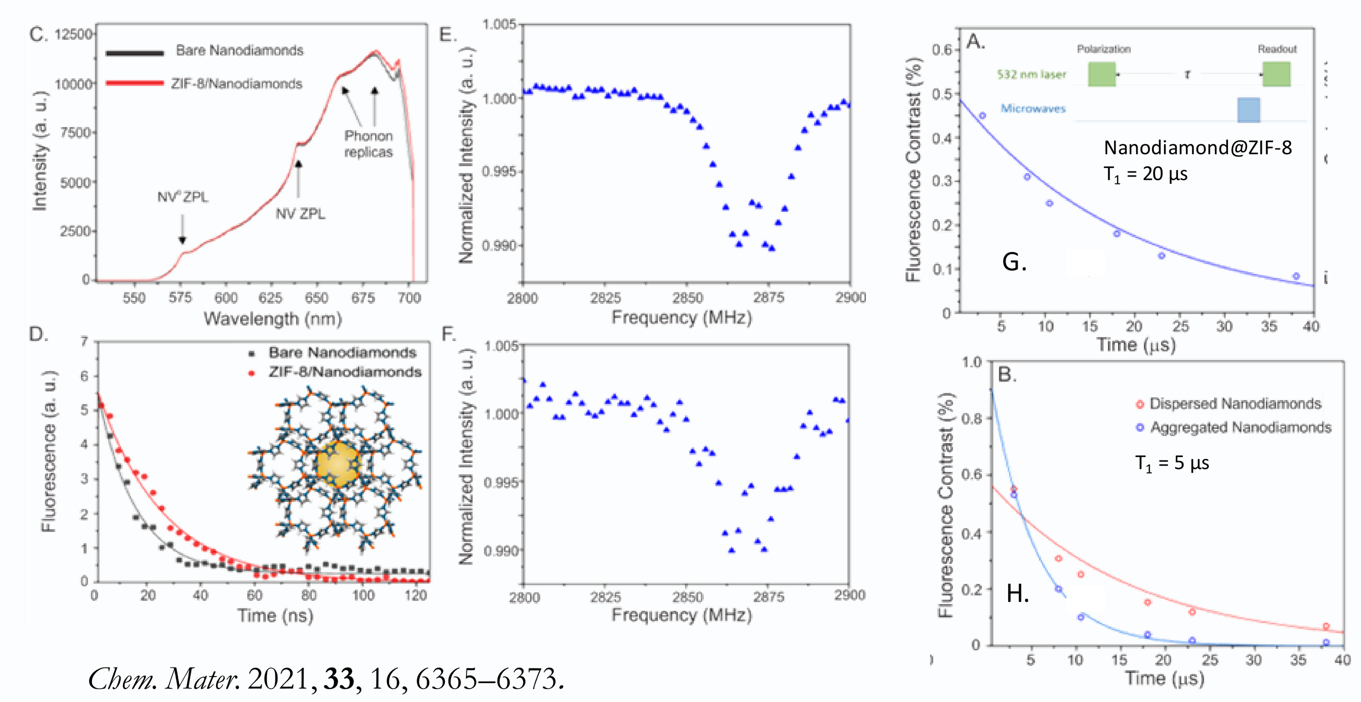
ACS Eng. Au, 2022, *ASAP*

Nanodiamond/Metal-Organic Framework (MOF) Composites

Functionalization of nanodiamonds 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 nanodiamonds with the MOF ZIF-8. Quantum sensing properties are preserved, including an enhanced spin relaxometry performance.



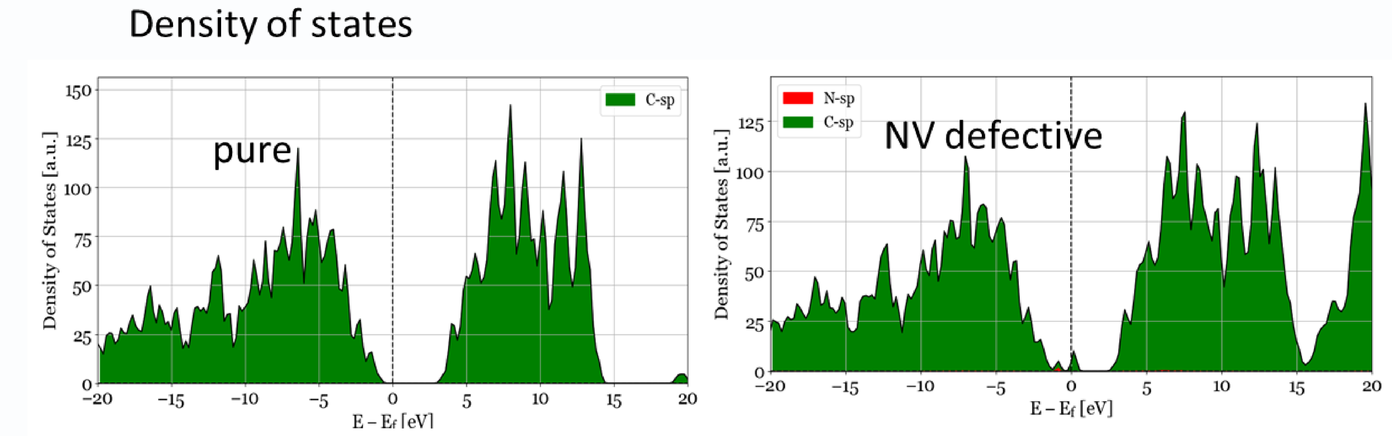


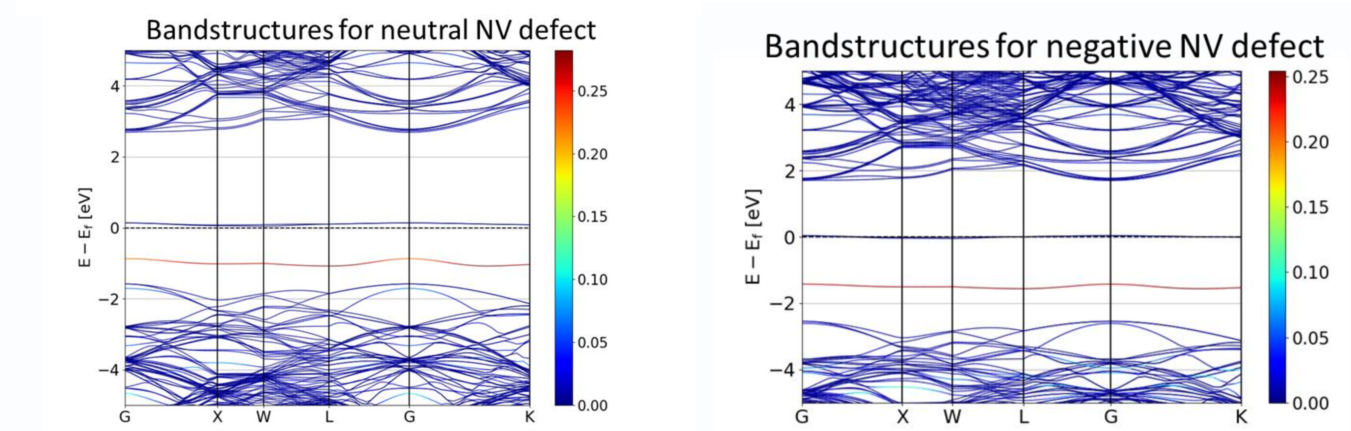


Chem. Mater. 2021, **33**, 16, 6365–6373.

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. The density of states and bandstructures of diamond crystal provides insight on the light-mater interaction needed for optical sensing.

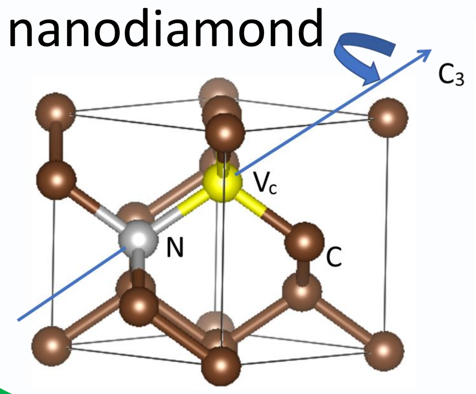




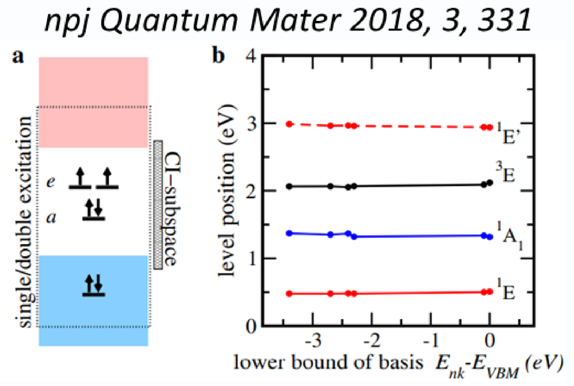
Modeling Diamond with an NV Center

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

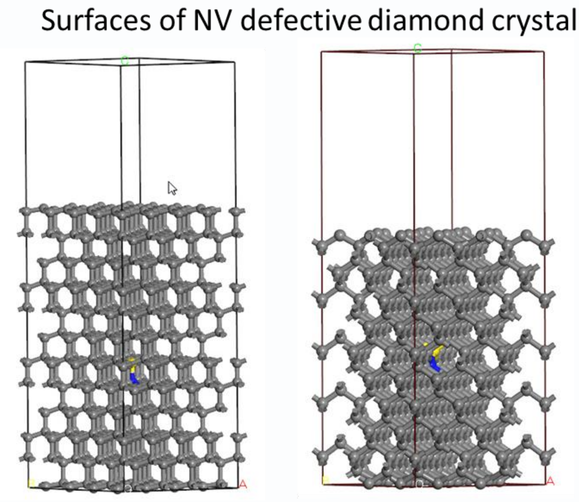
Vacancy in nanodiamond



Bockstedte, et al., npj Quantum Mater 2018, 3, 331

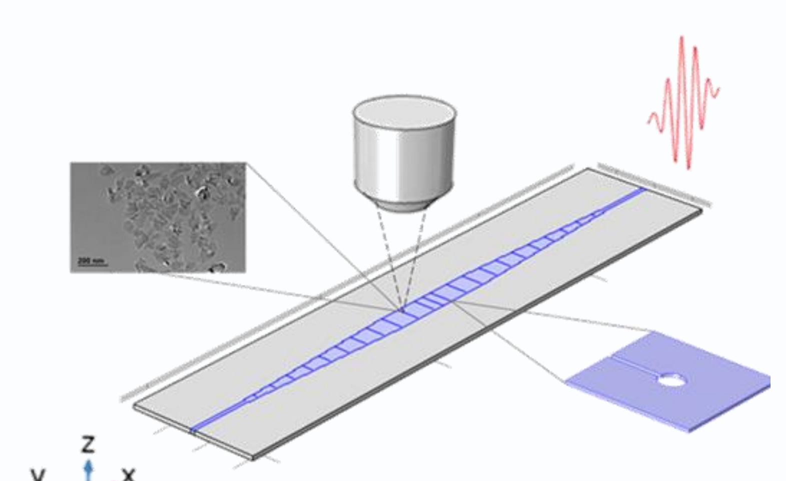


Surfaces of NV defective diamond crystal

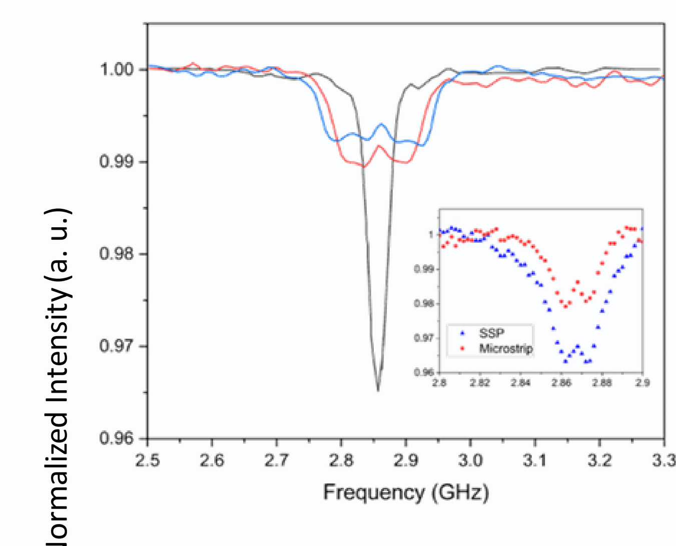


Spoof Plasmons for Enhanced ND Emission

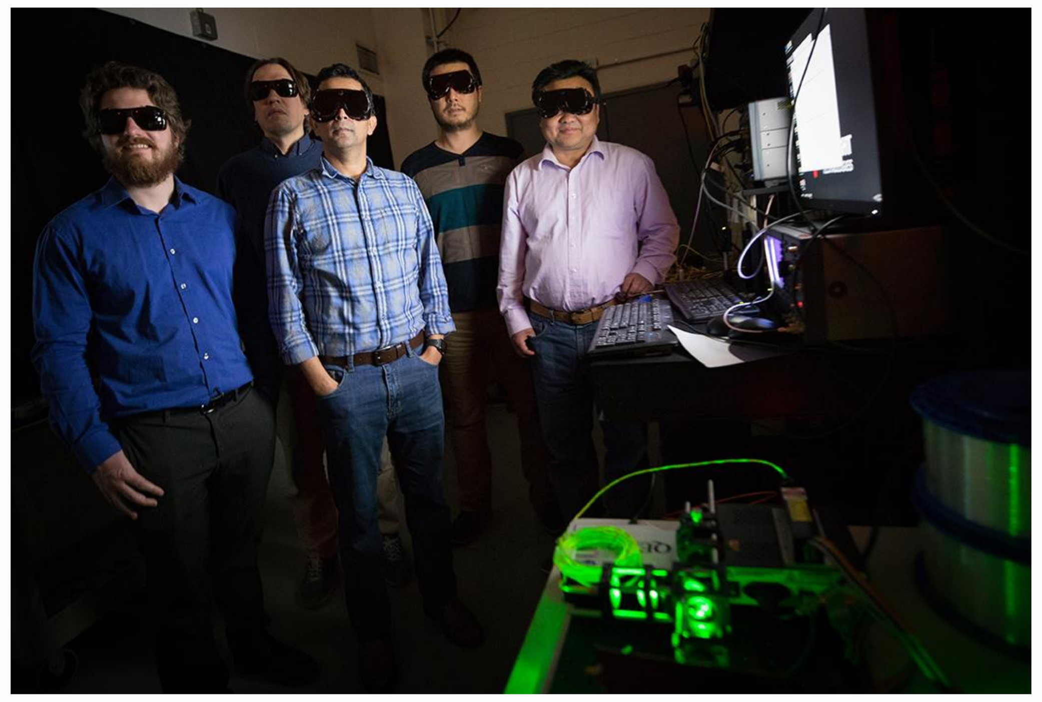
Microwave interactions are crucial for many quantum experiments, but the weak spontaneous emission of quantum emitters makes implementation challenging. Here, significant emission enhancement (up to 10^{11}) using microwave spoof plasmon (SPP) waveguides is demonstrated.



Adv. Quantum Technol. 2021, **4**, 6, 2000151



The Team



L to R: Dr. Scott Crawford, Dr. Roman Shugayev, Dr. Hari Paudel, Dr. Ping Lu, and Dr. Yuhua Duan