TQT Transformative Quantum Technologies

QUANTUM OPPORTUNITIES + SHOWCASE

Quantum Sensor Based on Spin Defects in Nanodiamonds

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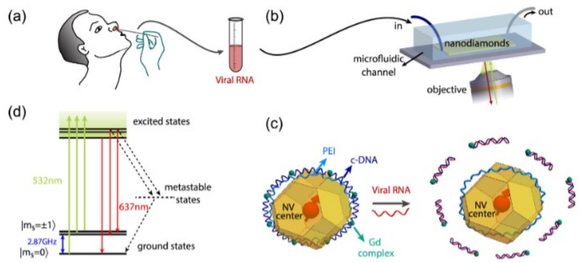
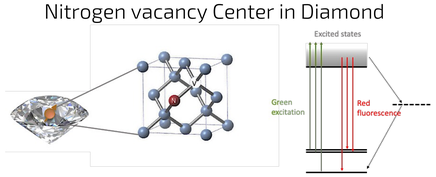
Motivation

- The rapid spread of the COVID-19 has shown the importance for rapid and cost-effective testing of emerging new viruses. Diagnostics that can detect active infections are typically molecular based, gauging the presence of the pathogen. For example, the SARS-CoV-2 can be detected by various virology methods, most pre-eminently by the reverse transcriptase quantitative polymerase chain reaction (RT-PCR) which requires trained personnel, special equipment, and careful design of the primer and probe.



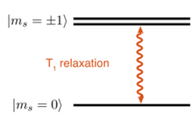
- To solve these problems, we proposed a quantum sensor based on Nitrogen-vacancy (NV) centers in nanodiamonds (NDs) that is capable to detect virus RNA, or any other RNA based stimulus. NV centers in diamond act as stable fluorescence markers and magnetic field sensors and have been investigated as quantum sensors for applications ranging from material science to chemistry and biology. A promising avenue to detect biological signals is to transduce them into magnetic noise - using, e.g., magnetic molecules, such as gadolinium (Gd) complexes. Then, like FRET-based biosensors, the presence of a stimulus (in this case the virus) is detected as it induces a change in the NV fluorescence, following its separation from the magnetic nanoparticle.

Nitrogen vacancy Center in Diamond



Ground State: Triple System

Relaxation of NV center can be quenched by external magnetic noise



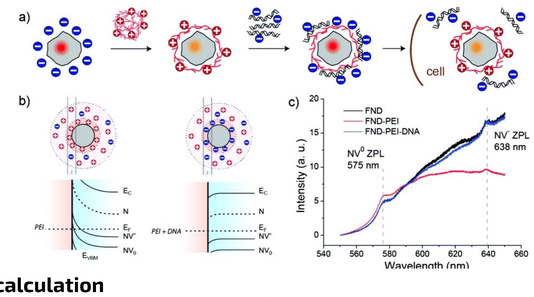
- Spin state can be optically polarized & readout at room temperature;
- NV centers in host nanodiamond (ND) with size down to ~20 nm;
- NDs are biocompatible and have high photo-stability;

Reference:

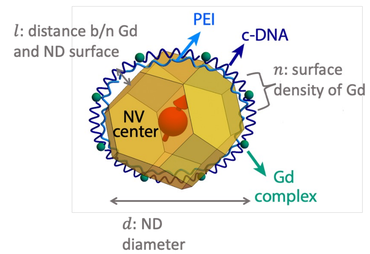
- Changhao Li, Rouhollah Soleyman, Mohammad Kohandel, and Paola Cappellaro, "SARS-CoV-2 Quantum Sensor Based on Nitrogen-Vacancy Centers in Diamond", Nano Lett. 2022, 22, 1, 43–49 and references in this article

Design/Simulation

(a) Development of an FND device for intracellular nucleic acids delivery and monitoring using nanodiamond particles that are coated with PEI. (b) Schematics of electrical charge density for FND–PEI and FND–PEI–DNA complexes and the corresponding band bending of energetic levels in the diamond. (c) The results for the intensity of oxidized FNDs and FND–PEI and FND–PEI–DNA complexes as a function of wavelength.



Model of T_1 calculation



$$\frac{1}{T_1} \sim \frac{1}{T_{1,bulk}} + \gamma_e^2 B_s^2 S_s(\omega) + \gamma_e^2 B_{Gd}^2 S_{Gd}(\omega)$$

$$\omega = \omega_0$$

1. B_{Gd}: Noise strength.
Dipole-dipole interaction between Gd and NV

$$B_{\perp,Gd}^2 = (\frac{\mu_0 \gamma_e \hbar}{\pi})^2 C_{s,Gd} \pi \frac{n}{(d_0/2+l)^4}$$

2. S_{Gd}: Noise spectrum

$$S_{Gd} = R_{Gd}/(R_{Gd}^2 + \omega_0^2)$$

$$\hbar R_{Gd,dip} = \sqrt{\sum_{i \neq j} \langle H_{ij}^2 \rangle} = \frac{\mu_0 \gamma_e^2 \hbar^2 \sqrt{6} C_{s,Gd}}{4\pi} (\frac{\pi}{2})^{1/2} \frac{n^{1/2}}{r_{min}^2} \Rightarrow R_{dip,Gd} \approx 21.1 \mathrm{ns}^{-1}\mathrm{nm} \times n^{1/2}.$$

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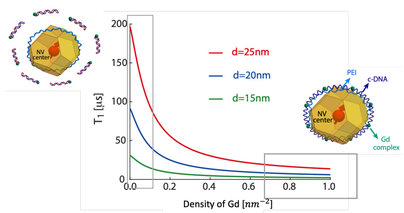
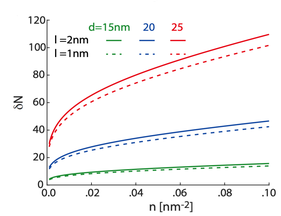
Simulation results

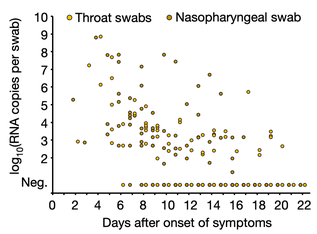


Quantum sensitivity



Meaning: the minimal detectable copies of virus RNA in one second

Quantum sensitivity



Meaning: the minimal detectable copies of virus RNA in one second
Results: sensitivity down to several hundreds of RNA copies in one second (single NV)

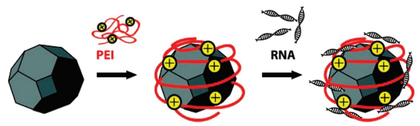
Performance Evaluation

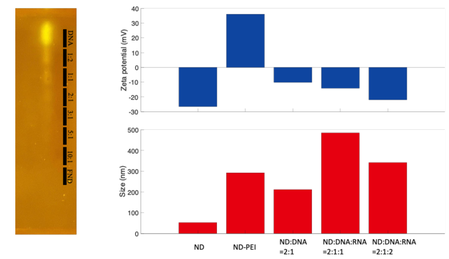
Desired Property	meaning	Our sensor
Sensitivity	low false negative	sensitivity >> RT-PCR
Specificity	low false positive	comparable with RT-PCR
Speed	return result as soon	< RT-PCR*
Quantitative	amount of virus	High sensitivity

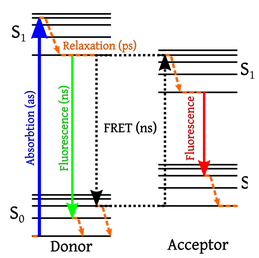
Fabrication/Results

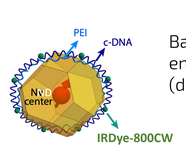
Sensor synthesis:

We coated PEI on ND particles and immobilized different ratio of DNA to our ND particles and found the best DNA/ND ratio. Measuring Zeta potential shows the attachment and detachment of PEI and DNA to the ND surface.





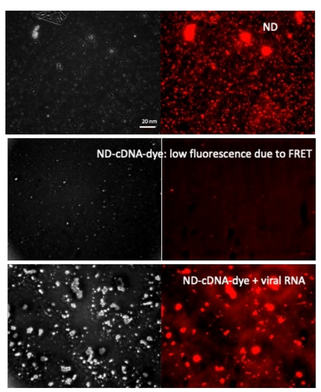


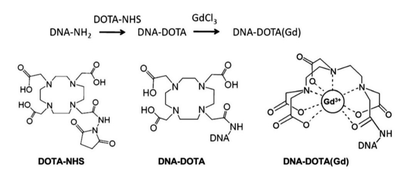


Based of the Fluorescence resonance energy transfer (FRET) between NV center (donor) and dye molecule (acceptor)

Based of the Fluorescence resonance energy transfer (FRET) of NDs, we attached a Fl-dye to NDs to confirm RNA coupling and DNA detachment:

Next step: replace dye with Gd complex, and measure T_1





Using NHS chemistry to couple aptamers to gadolinium-tetraazacyclododecanetetraacetic acid (DOTA-Gd). DOTA-Gd is a common T1-weighted MRI contrast agent, and its structure is shown here.

Acknowledgment: This work was supported in part by the U.S. Army Research Office through Grant W911NF-15-1-0548, Canada First Research Excellence Fund Canada and TQT First Research Excellence Fund.