

Optical ^{13}C hyperpolarization in nanodiamond particles: Avenues for DNP and imaging

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In recent years, electronic spins associated with Nitrogen Vacancy (NV) centers in diamond have been proposed as room temperature optical hyperpolarizing agents, providing a compelling means for dynamic nuclear polarization (DNP) without the need for cryogenic temperatures or strong magnetic fields [1]. This stems from the fact that the NV defects can be optically polarized close to 100% with modest optical pumping, and this polarization transferred to ^{13}C nuclei in the diamond lattice. Especially attractive therefore are diamond particles in “nanodiamond” form, because their intrinsically large surface area allows one to potentially relay this optical ^{13}C hyperpolarization to external nuclei.

However, due to various problems originating from the strong orientation dependence of the NV centers, realization of an “*optical nanodiamond hyperpolarizer*”, has been technically challenging to develop at room temperature. In this work, we overcome these challenges by uncovering surprising new physics in a recently introduced low-field DNP mechanism [2,3]. This allows hyperpolarization in nanodiamonds to be achieved with very modest resources -- the magnetic field of a refrigerator magnet, very low-power optical irradiation and microwave excitation conveniently set in the WiFi regime. We harness this remarkable new physics to develop a miniature room temperature optical diamond hyperpolarizer. The ultracompact device can retrofit any existing NMR or MRI magnet and produce ^{13}C hyperpolarized diamond particles with high throughput. In several ways, the ability to build such a device is itself surprising, and a fortunate confluence of several interesting attributes of the physics of optically pumped spin-1 electrons at low-fields.

Using the device, we obtain the best reported ^{13}C hyperpolarization in diamond particles, corresponding to a bulk nuclear polarization close to 1%, enhanced over 720 times the Boltzmann value at 7T (acceleration in MRI by over ten-million). Besides this, the ^{13}C hyperpolarization can be rendered completely background-free. It can also be retained (stored) for long periods, typically in excess of ten-minutes. Since the diamond particles optically fluoresce brightly, hyperpolarization opens the possibility to obtain “*dual-mode*” co-registered optical and MRI imaging on a single platform, both imaging modalities being amenable to lock-in techniques, enabling high image SNR retrieval. We demonstrate such dual mode imaging on phantoms using the diamond hyperpolarizer retrofitting a 9.4T vertical bore imaging system.

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References:

1. R. Fisher, et al., *Phys. Rev. Lett.* 111, 057601 (2013).
2. A. Ajoy, et al. *Science Advances*, 4, eaar5492 (2018).
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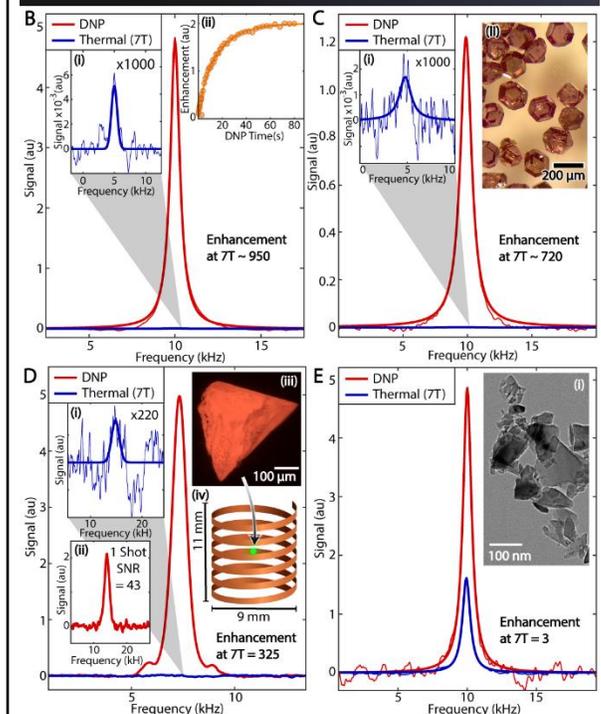
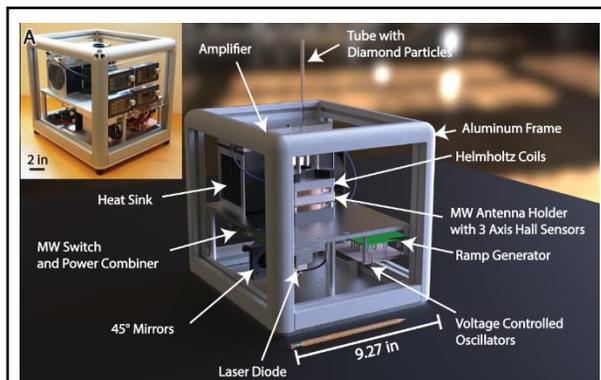


Figure 1: **Optical nanodiamond hyperpolarizer.** (A) Model of compact tabletop device, retrofitting NMR magnets. Inset: photograph of device. DNP results on (B) Single crystal diamond, with 7T enhancement ~ 950 (C) Diamond microparticles (shown in inset), with 7T enhancement >700 , (D) Single 300um diamond particle, with sample fill factor $<10^{-6}$ (E) Commercial 100nm nanodiamonds in solution.