Hyperpolarized nano-diamonds as molecular imaging and sensing probes for MRI | 7GS	**Start Date:** February 1st 2015
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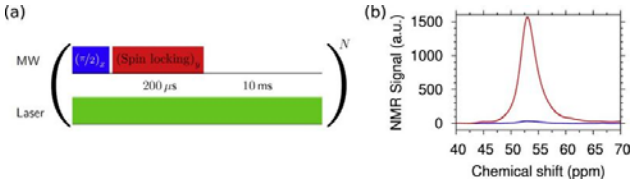
Abstract: The ability to recognize molecular processes using novel imaging techniques is crucial for medicine, biology and biochemistry in the 21st century. Non-invasively detecting small numbers of molecular probes, to help image particular targets or pathways in vivo, is currently undergoing a technological revolution. Recent breakthroughs in molecular hyperpolarization proved a more than 10,000-fold increase in sensitivity on conventional magnetic resonance imaging (MRI) systems, thus providing insight into previously unseen metabolic processes. They variety of molecules which can be used in hyperpolarized MRI is unfortunately very limited, as the signal increase decays with the T1 relaxation time of the molecule. Our project goal is the development and realization of a novel hyperpolarization scheme for nano-diamonds (NDs), using the unique properties of Nitrogen-Vacancy (NV) centres. In this project we will develop polarization schemes which can overcome the challenges of DNP in nanodiamonds and achieve a high room-temperature hyperpolarization of nanodiamond ensembles



Recent results: We have introduced a new dynamic nuclear polarization scheme, termed PulsePol, for transferring polarisation from electron to nuclear spins by Hamiltonian engineering. Contrary to current pulsed DNP sequences for which the polarisation transfer occurs during a long pulse (e.g. spin-locking), the polarisation transfer in PulsePol occurs through the accumulated dynamics between very fast pulses. We show that in PulsePol robustness to detuning or spectral width and pulse errors can be greatly enhanced with no efficiency cost and demonstrate the efficiency and remarkable robustness of PulsePol in transferring polarisation from an optically polarized NV-centre in diamond to the surrounding 13C nuclear spin bath over a range of 60 MHz detuning. This improves performance of ensembles of shallow NV centres to hyperpolarise nuclear spins in external molecules.

We also investigated polarization transfer from optically-pumped NV-centers in diamond to external molecules at room temperature. This polarization transfer is described by both an extensive analytical analysis and numerical simulations based on spin bath bosonization and is supported by experimental data. These results set the route to hyperpolarization of diffusive molecules in different scenarios and consequently, due to increased signal, to high-resolution NMR.

Publications:

Resonance-inclined optical nuclear spin polarization of liquids in diamond structures Q. Chen, I. Schwarz, F. Jelezko, A. Retzker, and M. B. Plenio Phys. Rev. B 93, 060408(R) (2016)

Optically induced dynamic nuclear spin polarisation in diamond J. Scheuer, I. Schwarz, Q. Chen, D. Schulze-Sünninghausen, P. Carl, P. Höfer, A. Retzker, H. Sumiya, J. Isoya, B. Luy, M.B. Plenio, B. Naydenov, and F. Jelezko New Journal of Physics 18, 013040 (2016)

Optical hyperpolarization of 13C nuclear spins in nanodiamond ensembles Chen, I. Schwarz, F. Jelezko, A. Retzker, M.B. Plenio Phys. Rev. B 92, 184420 (2015)

Pulsed polarization for robust DNP I. Schwartz, J. Scheuer, B. Tratzmiller, S. Müller, Q. Chen, I. Dhand, Z.-Y. Wang, Ch. Müller, B. Naydenov, F. Jelezko, and M.B. Plenio
Submitted to Phys. Rev. X

Towards hyperpolarization of oil molecules via nitrogen-vacancy centers in diamond P. Fernandez-Acebal, O. Rosolio, J. Scheuer, C. Müller, S. Müller, S. Schmitt, L.P.
McGuinness, I. Schwarz, Q. Chen, A. Retzker, B. Naydenov, F. Jelezko, M.B. Plenio

Further Collaborators: NVision Imaging Technologies GmbH