Project title: **Low-field NMR and MRI with *in situ* parahydrogen hyperpolarisation**
Supervisor name(s): Dr Meghan Halse
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**Project Description:**

Magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR) spectroscopy are powerful tools for applications that range from synthetic chemistry to medical diagnosis. However, these methods suffer from low sensitivity because only tens out of every million atomic nuclei in the sample being studied are actually detected. Hyperpolarisation methods amplify signals by several orders of magnitude by dramatically increasing the fraction of nuclei detected. By overcoming the sensitivity barrier in NMR and MRI, hyperpolarisation holds great transformative potential. This is particularly true for applications of low-cost and portable NMR and MRI, where devices have low magnetic fields, ranging from μT (Earth’s field) up to 2T (permanent magnet arrays,) and so suffer from significantly lower sensitivity than traditional NMR spectrometers based on superconducting magnets with fields of 7 T and above. This project concerns the application of hyperpolarisation to NMR in the very low-field range (μT – mT) and will focus on the implementation and optimisation of the hyperpolarisation as well as the development of new applications for hyperpolarised low-field NMR and MRI more generally.

In the project we will focus primarily on the SABRE (signal amplification by reversible exchange) approach to hyperpolarisation that was developed in York by Prof Simon Duckett, the director of the Centre for Hyperpolarisation in Magnetic resonance (CHyM). SABRE is a catalytic process for transferring polarisation from *parahydrogen* (the singlet nuclear spin isomer of H₂) to a molecule of interest in solution. SABRE is an attractive hyperpolarisation approach, particularly for low-field NMR, because it benefits from fast polarisation times (seconds), high potential polarisation levels (approaching 100%) that are detection-field independent and a relatively simple experimental implementation. A key feature of SABRE is that the exchange reaction step, where the polarisation transfer takes place, must be carried out in a very low field of a few mT in order for the transfer to be efficient. In the standard approach, SABRE polarisation transfer is achieved over a period of seconds in a mT field (called the polarisation transfer field or PTF) and then the sample is transported (either manually or under flow) to the NMR spectrometer for signal detection at a much stronger field (> 1T). In this project, the SABRE polarisation transfer and the subsequent NMR detection will be carried out *in situ*, without the need to shuttle the sample between two detection fields. This will be implemented in two ways: first with NMR and MRI detection in the Earth’s magnetic field and second with NMR detection in the polarisation transfer field itself. The project will involve adapting currently available low-field NMR and MRI hardware to suit the purpose, the design and implementation of novel experiment protocols and the application of these new experiments to study and optimise the hyperpolarisation process for a range of chemical systems of potential interest to industrial process monitoring and/or clinical diagnosis.

**Training:**

All research students follow our innovative Doctoral Training in Chemistry (iDTC): cohort-based training to support the development of scientific, transferable and employability skills. All research students take the core training package which provides both a grounding in the skills required for their research, and transferable skills to enhance employability opportunities following graduation. Core training is progressive and takes place at appropriate points throughout a student’s higher degree programme, with the majority of training taking place in Year 1. In conjunction with the Core training, students, in consultation with their supervisor(s), select training related to the area of their research. The iDTC themes are broad, interdisciplinary, and fit within the Department’s research expertise. Themes are flexible and adapt in line with the evolving research landscape. Each theme has a leader who oversees the training offered. Students may select courses from other themes where appropriate.

The project will be carried out under the supervision of Dr Meghan Halse and will be based in the Centre for Hyperpolarisation in Magnetic Resonance (CHyM), a cutting edge research facility in the Department of Chemistry that specializes in the development of *p-H₂* based methodologies in liquid-state NMR, with a particular focus on the
development of hyperpolarised agents for use in clinical MRI. Throughout the project the student will gain advanced training in MR based analytical chemistry with additional skills in the theoretical basis of NMR and MRI, advanced data analysis and NMR and MRI experiment design and implementation on a range of instruments. This project will be carried out within the context of the large multidisciplinary research program within CHyM and therefore, through participation in group meetings, the student will be exposed to the wide range of expertise within the centre including NMR spectroscopy, hyperpolarisation, MR theory, photochemistry, catalysis and kinetics.

Equality and Diversity:

The Department of Chemistry holds an Athena SWAN Gold Award and is committed to supporting equality and diversity for all staff and students. The Department strives to provide a working environment which allows all staff and students to contribute fully, to flourish, and to excel. Chemistry at York was the first academic department in the UK to receive the Athena SWAN Gold award, first attained in 2007 and then renewed in October 2010 and in April 2015. This PhD project is available to study full-time or part-time (50%).

Funding:

Value: Studentships are fully funded either by (1) the EPSRC for 3 years (2) a Department of Chemistry Teaching Studentship for 3 years or (3) a Department of Chemistry NMR Studentship for 4 years, and cover: (i) a tax-free annual stipend at the standard Research Council rate (£14,553 for 2017-18), (ii) tuition fees at the UK/EU rate.

Eligibility: EPSRC studentships are available to UK and EU students who meet the UK residency requirements. Students from EU countries who do not meet the residency requirements may still be eligible for a fees-only award. Chemistry Teaching Studentships are available to any student who is eligible to pay tuition fees at the home rate. Further information about eligibility for Research Council UK funding can be found at the following website: http://www.bbsrc.ac.uk/documents/studentship-eligibility-pdf/

Candidate selection process:

- Applicants should submit an application for a PhD in Chemistry by **17:00 on Wednesday 28 February 2018**
- Supervisors will interview their preferred candidates either by email, telephone, web-chat or in person
- Supervisors may nominate up to two candidates to the assessment panel
- Nominated candidates will be invited to a panel interview at the University of York on **Wednesday 21 March 2018**
- The Chemistry Graduate Awards Panel will award studentships following the panel interviews
- Candidates will be notified of the outcome of the panel’s decision by email

For more information contact chemgrad@york.ac.uk or see our web page: http://www.york.ac.uk/chemistry/postgraduate/